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Distributed and Preconditioned Space–Time Boundary Element Methods for the Heat Equation

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Abstract

In this work we describe space–time boundary element methods for the numerical solution of the time-dependent heat equation. Solutions of initial boundary value problems can be expressed in terms of the boundary and initial data. Unknown boundary data can be determined by solving appropriate boundary integral equations. For the numerical approximation we consider a discretization which is done with respect to a space–time decomposition of the boundary of the space–time domain. Besides the widely used tensor product approach we also consider an arbitrary decomposition of the space–time boundary into boundary elements, allowing us to apply adaptive refinement in space and time simultaneously. In addition to the analysis of the boundary integral operators and the formulation of boundary element methods for a variety of different boundary value problems, we state a priori error estimates of the approximations and comment on non-symmetric FEM–BEM coupling methods for parabolic transmission problems.

The space–time discretization technique allows us to parallelize the computation of the global solution of the whole space–time system. We introduce a parallel solver for space–time boundary integral equations. The boundary mesh is decomposed into a given number of submeshes. Pairs of the submeshes represent dense blocks in the system matrices, which are distributed among computational nodes by an algorithm based on a cyclic decomposition of complete graphs, ensuring load balance. Additionally, we employ threading and vectorization in shared memory to ensure intra-node efficiency. All levels of parallelism allow us to tackle large problems and lead to an almost optimal speedup.

In order to obtain an efficient space–time solver for the global linear system, the application of robust preconditioners is required. We present a preconditioning strategy which is based on using boundary integral operators of opposite order, known as operator preconditioning, and extend the introduced parallel solver to the preconditioned system.

We present numerous numerical experiments to confirm the theoretical findings and to evaluate the performance of the proposed parallelization and preconditioning techniques.

Zusammenfassung

In dieser Arbeit wird die Randelementmethode zur Diskretisierung von zeitabhängigen Anfangsrandwertproblemen am Modell der Wärmeleitungsgleichung beschrieben. Die Lösungen der betrachteten Anfangsrandwertprobleme sind durch die Vorgabe der zugehörigen Rand- und Anfangsdaten eindeutig bestimmt. Die noch unbekannten Randdaten können durch Lösen von entsprechenden Randintegralgleichungen berechnet werden. Anders als bei klassischen Zeitschrittverfahren betrachten wir eine globale Zerlegung des Randes des Raum–Zeit-Gebiets für die numerische Approximation des Problems. Neben dem weitverbreiteten Tensorprodukt-Ansatz wird auch eine beliebige Zerlegung (Triangulierung) des Randes im Raum–Zeit-Bereich analysiert. Eine solche Zerlegung erlaubt das Anwenden von adaptiven Verfeinerungsstrategien bezüglich des gesamten Raum–Zeit-Bereichs. Neben der Analysis der Randintegraloperatoren und Randintegralgleichungen, und der Herleitung von Randelementmethoden für verschiedene Randwertprobleme werden auch a priori Fehlerabschätzungen der Näherungslösungen angegeben. Ebenso wird die nichtsymmetrische FEM–BEM Kopplung für parabolische Transmissionsprobleme diskutiert.

Eine Raum–Zeit-Diskretisierung bietet zudem die Möglichkeit, iterative Lösungsverfahren bezüglich des gesamten Raum–Zeit-Systems zu parallelisieren. In der vorliegenden Arbeit wird eine passende parallele Lösungsmethode beschrieben. Das aus der Zerlegung des Randes entstehende Netz wird in eine vorgegebene Anzahl von Teilnetzen zerlegt. Paare dieser Teilnetze stellen dichtbesetzte Blöcke in den aus der Diskretisierung der Randintegralgleichungen entstehenden Matrizen dar. Diese Blöcke werden dann anhand eines Algorithmus basierend auf einer zyklischen Zerlegung von vollständigen Graphen auf Rechenknoten verteilt, was einen Ausgleich der Rechenlast zwischen den Knoten mit sich bringt. An den Rechnern selbst wird zudem Threading und Vektorisierung zur Performancesteigerung eingesetzt. Alle verfügbaren Level an Parallelisierungsmöglichkeiten erlauben es, große Probleme, insbesondere Raum–Zeit-Systeme, zu lösen und haben eine nahezu optimale Skalierbarkeit zur Folge.

Um ein effizientes Lösen des globalen linearen Gleichungssystems zu gewährleisten, ist die Anwendung von passenden Vorkonditionierern notwendig. Ein Teil dieser Arbeit befasst sich deshalb mit der Erweiterung der sogenannten Operator-Vorkonditionierung auf Randelementmethoden im Raum–Zeit-Bereich. Diese Strategie verwendet Randintegraloperatoren entgegengesetzter Ordnung. Der beschriebene parallele Löser wird anschließend auf das vorkonditionierte System ausgeweitet.

Die Richtigkeit der erarbeiteten theoretischen Aussagen als auch die Effizienz der Parallelisierung und Vorkonditionierung werden anhand numerischer Experimente demonstriert.

CONTENTS

1 INTRODUCTION

There exists a variety of numerical methods in order to compute an approximate solution of time-dependent initial boundary value problems. Standard techniques for parabolic evolution problems are based on semi-discretizations, see, e.g., [69]. These methods typically lead to a scheme where the structure of the discrete system is based on some tensor product of space–time elements. The basic idea behind space–time methods is to think of the time variable as an additional spatial dimension and discretize the whole space–time domain at once, see, e.g., [1, 32, 42, 56, 63]. Space–time discretization methods in general are gaining in popularity due to their ability to drive adaptivity in space and time simultaneously [5,44] and to use parallel iterative solution strategies for time-dependent problems [20,43]. Besides space–time finite element methods one can also use boundary element methods to obtain an approximate solution of parabolic intial boundary value problems, assuming that the underlying structure of the partial differential equation allows for an application of this discretization technique. In this work we will focus on space–time boundary element methods for the numerical solution of the time-dependent heat equation [3, 10, 66].

Let $\Omega \subset \mathbb{R}^n$ $(n = 1,2,3)$ be a bounded domain with, for $n = 2,3$, Lipschitz boundary $\Gamma := \partial\Omega$, $T \in \mathbb{R}$ some time horizon with $T > 0$, and $\alpha \in \mathbb{R}$ a fixed heat capacity constant with $\alpha > 0$. We consider the initial boundary value problem for the heat equation

$$\begin{aligned} \alpha\partial_t u(x,t) - \Delta_x u(x,t) &= f(x,t) \qquad \text{for } (x,t) \in Q := \Omega \times (0,T), \\ u(x,0) &= u_0(x) \qquad \text{for } x \in \Omega \end{aligned} \tag{1.1}$$

with given source term f, initial datum u_0 and appropriate boundary conditions on the space–time boundary $\Sigma := \Gamma \times (0,T)$, e.g. Dirichlet or Neumann boundary conditions. Unique solvability of problem (1.1) with Dirichlet or Neumann boundary conditions in the setting of anisotropic Sobolev spaces [35] was shown in, e.g., [10, 19, 65]. An explicit formula describing the solution of problem (1.1) is given by the so-called representation formula for the heat equation, see, e.g., [3], i.e. for $(x,t) \in Q$ we have

$$\begin{aligned} u(x,t) =& \frac{1}{\alpha}\int_\Sigma U^\star(x-y,t-\tau)\gamma_1^{\mathrm{int}}u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau - \frac{1}{\alpha}\int_\Sigma \partial_{n_y}U^\star(x-y,t-\tau)\gamma_0^{\mathrm{int}}u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau \\ &+ \int_\Omega U^\star(x-y,t)u_0(y)\,\mathrm{d}y + \frac{1}{\alpha}\int_Q U^\star(x-y,t-\tau)f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau, \end{aligned} \tag{1.2}$$

where

$$U^\star(x-y,t-\tau) = \begin{cases} \left(\dfrac{\alpha}{4\pi(t-\tau)}\right)^{n/2} \exp\left(\dfrac{-\alpha|x-y|^2}{4(t-\tau)}\right), & x,y \in \mathbb{R}^n, 0 \le \tau < t, \\ 0\,, & \text{else} \end{cases}$$

denotes the fundamental solution of the heat equation [18]. Here, $\gamma_0^{\mathrm{int}} u$ and $\gamma_1^{\mathrm{int}} u$ denote the Dirichlet and Neumann trace of the solution u on the space–time boundary Σ, respectively. Due to this representation of the solution it suffices to determine the unknown Cauchy data on Σ in order to compute the solution u of problem (1.1), e.g. for given Dirichlet boundary conditions $\gamma_0^{\mathrm{int}} u = g$ we have to compute the unknown Neumann datum $\gamma_1^{\mathrm{int}} u$ on Σ, whereas for given Neumann boundary conditions $\gamma_1^{\mathrm{int}} u = w$ the computation of the unknown Dirichlet datum $\gamma_0^{\mathrm{int}} u$ on Σ is required. Hence the problem is reduced to the boundary Σ of the space–time domain Q. We can determine the unknown Cauchy data by applying the Dirichlet and Neumann trace operator to the representation formula (1.2) and solving related space–time boundary integral equations. The approximation of the solution only requires a decomposition of the space–time boundary Σ into boundary elements. Thus, in the case of space–time boundary element methods, the dimension of the problem is reduced to n compared to $n+1$ for space–time finite elements methods discussed in, e.g., [63, 65].

Boundary integral equations and corresponding boundary element methods for the approximation of the solution of initial boundary value problems for the heat equation (1.1) have been studied for a long time [3, 4, 10, 26]. Besides well known time-stepping methods [7], the convolution quadrature method [36] or the Nyström method [67, 68], one can use the Galerkin approach [10, 22, 39–41, 45] for the discretization of the global space–time integral equation. However, in order to get a competitive space–time solver compared to, e.g., time-stepping schemes, an efficient iterative solution technique for the global space–time system is necessary, i.e. the solution requires an application of suitable preconditioners and parallel space–time solvers.

In this work we analyze the heat potentials in (1.2) and the arising boundary integral operators and discuss the solvability of related space–time boundary integral equations. The analysis of the boundary integral operators and equations is mainly based on [3, 4, 10]. We start with a discussion of the domain variational formulation of (1.1) with given Dirichlet boundary conditions, see [65], and derive the mapping properties of the related boundary integral operators as well as the ellipticity of the single layer and hypersingular boundary integral operator. Moreover, we discuss two different space–time discretization methods in order to compute an approximation of the unknown Cauchy data on Σ. The first one is the so-called tensor product approach [40, 45], originating from a separate decomposition of the boundary Γ and the time interval $(0,T)$. In this case we use space–time tensor product spaces for the discretization of the boundary integral equations. The second approach is using boundary element spaces which are defined with respect to a shape-regular triangulation of the whole space–time boundary Σ into boundary elements. This approach additionally allows for an application of adaptive refinement in space and time simultaneously while maintaining the regularity of the boundary element mesh. We also present some numerical experiments to confirm the theoretical results.

For the solution of the discretized boundary integral equations we use a preconditioned

GMRES method. We establish a robust preconditioning strategy which is based on boundary integral operators of opposite order. This preconditioning technique, also referred to as Calderón preconditioning or operator preconditioning, was introduced and analyzed in [64] in the case of the Laplace equation, where the involved integral operators are in general self adjoint, and extended to a more general setting in [23]. Here we extend this method to space–time integral equations, see also [11, 13].

The matrices related to the discretized space–time integral equations are dense and their dimension is much higher than in the case of stationary problems. Even with fast methods, see, e.g. [40,41], the computational times and the memory requirements of the huge space–time system are demanding. Thus, the solution of even moderately sized problems requires the use of computer clusters. Although there is a simple parallelization by OpenMP in the FMM code of [39], parallelization of boundary element methods for the heat equation in HPC environments has not been closely investigated yet. In this work we concentrate on hybrid parallelization in shared and distributed memory. The global space–time nature of the system matrices leads to improved parallel scalability in distributed memory systems in contrast to time-stepping methods, where the parallelization is usually limited to spatial dimensions. For this reason, parallel-in-time algorithms have been considered suitable for tackling the problems of the upcoming exascale era when more than 100 million way concurrency will be required [15, 16, 58]. Methods such as parareal [33] or space–time parallel multigrid [20] are gaining in popularity. While time-stepping may be more tractable on smaller parallel architectures, here we focus on the parallelization for large scale systems and thus, aim to exploit the global space–time matrices, see also [11, 14].

An advantage of boundary element methods is the natural handling of problems in exterior, unbounded domains. Thus, boundary element methods are a popular choice when solving transmission problems. The introduced domain variational formulation in [65] in the setting of anisotropic Sobolev spaces allows us to establish symmetric and non-symmetric FEM–BEM coupling methods in an appropriate functional framework. In this work we will discuss both BEM and FEM discretizations of the interior problem of parabolic transmission problems and present numerical experiments.

The structure of the thesis is as follows. In Chapter 2 we give a short overview of the functional framework for the numerical analysis of problem (1.1), i.e. introducing anisotropic Sobolev spaces on the space–time domain Q as well as anisotropic Sobolev spaces on the space–time boundary Σ [34, 35]. In Chapter 3 we recall existence and uniqueness results [19, 32, 65] for the domain variational formulation of problem (1.1) with Dirichlet boundary conditions. This domain variational formulation is later on used to prove the ellipticity of the single layer and hypersingular boundary integral operators. Chapters 4 and 5 are devoted to the analysis of the arising heat potentials, boundary integral operators and boundary integral equations. In Chapter 6 we introduce the already mentioned space–time decomposition techniques, define suitable boundary element spaces and derive approximation properties of related L^2 projection operators. The space–time trial and test spaces are then used for the discretization of boundary integral equations in Chapter 7, where we also derive a priori error estimates for Galerkin approximations of the unknown Cauchy data for different types of boundary value problems and provide numerical experiments validating the introduced discretization techniques. Chapter 8 is devoted to the extension of the well known operator preconditioning strategy [23, 64] to the space–time setting. Parallelization in distributed and shared memory is discussed in Chapter 9. In Chapter 10 we briefly motivate the non-symmetric space–time FEM–BEM coupling method for parabolic transmission problems with respect to the introduced functional framework, and we conclude with a brief summary and outlook in Chapter 11.

2 FUNCTIONAL FRAMEWORK

The analysis of problem (1.1) is done in the setting of anisotropic Sobolev spaces which are introduced and discussed in this chapter. Under certain conditions we can define trace operators acting on those spaces and therefore provide conditions for the Dirichlet datum $u_{|\Sigma}$ and the Neumann datum $\partial_{n_x} u_{|\Sigma}$ of the solution, resulting in existence and uniqueness theorems for solutions of the model problem (1.1). The definitions and results in this chapter are mainly based on [12, 34, 35, 65, 72]. We start with the definition of fractional order Sobolev spaces on the time interval $(0,T)$ in Section 2.1 and use the results to introduce anisotropic Sobolev spaces on the space–time domain $Q = \Omega \times (0,T)$ in Section 2.2. The extension of the anisotropic setting to the space–time boundary $\Sigma = \Gamma \times (0,T)$ is discussed in Section 2.3.

2.1 Sobolev Spaces on the Time Interval $(0,T)$

Let $H^1(0,T)$ denote the standard Sobolev space on the time interval $(0,T)$. The norm of a function $u \in H^1(0,T)$ is given by

$$\|u\|_{H^1(0,T)}^2 := \|u\|_{L^2(0,T)}^2 + \|\partial_t u\|_{L^2(0,T)}^2 .$$

Moreover, we define the space of functions in $H^1(0,T)$ with homogeneous initial conditions as

$$H_{0,}^1(0,T) := \left\{ v \in H^1(0,T) : v(0) = 0 \right\}$$

with norm

$$\|u\|_{H_{0,}^1(0,T)} := \|\partial_t u\|_{L^2(0,T)} .$$

Analogously we define $H_{,0}^1(0,T)$ to be the space of functions in $H^1(0,T)$ vanishing at the time horizon T. Fractional order Sobolev spaces on $(0,T)$ are introduced as corresponding interpolation spaces [6, 34, 35], i.e. for $s \in (0,1)$ we set

$$\begin{aligned} H^s(0,T) &:= \left[L^2(0,T), H^1(0,T) \right]_s, \\ H_{0,}^s(0,T) &:= \left[L^2(0,T), H_{0,}^1(0,T) \right]_s, \\ H_{,0}^s(0,T) &:= \left[L^2(0,T), H_{,0}^1(0,T) \right]_s. \end{aligned}$$

Note that for $s \in (0,1/2)$ we have $H^s(0,T) = H_{0,}^s(0,T) = H_{,0}^s(0,T)$, i.e. the homogeneous initial and final conditions are not seen by the interpolation spaces [32]. The interpolation norm of a function $u \in H^s(0,T)$ for $s \in (0,1)$ is equivalent to the norm

$$\|u\|_{H^s(0,T)}^2 := \|u\|_{L^2(0,T)}^2 + |u|_{H^s(0,T)}^2,$$

where
$$|u|^2_{H^s(0,T)} := \int\limits_0^T \int\limits_0^T \frac{[u(t)-u(\tau)]^2}{|t-\tau|^{1+2s}} \, \mathrm{d}\tau \, \mathrm{d}t.$$

The space $H^{1/2}_{0,}(0,T)$ in particular will be important in the analysis of the domain variational formulation of problem (1.1). The Sobolev space $H^{1/2}_{0,}(0,T)$ is a dense subspace of $H^{1/2}(0,T)$, see, e.g., [71], and its interpolation norm is equivalent to the norm
$$\|u\|^2_{H^{1/2}_{0,}(0,T)} := \|u\|^2_{L^2(0,T)} + |u|^2_{H^{1/2}(0,T)} + |u|^2_{H^{1/2}_{0,}(0,T)}$$

with
$$|u|^2_{H^{1/2}_{0,}(0,T)} := \int\limits_0^T \frac{[u(t)]^2}{t} \, \mathrm{d}t.$$

Similarly, a norm of a function $u \in H^{1/2}_{,0}(0,T)$ is given by
$$\|u\|^2_{H^{1/2}_{,0}(0,T)} := \|u\|^2_{L^2(0,T)} + |u|^2_{H^{1/2}(0,T)} + |u|^2_{H^{1/2}_{,0}(0,T)}$$

with
$$|u|^2_{H^{1/2}_{,0}(0,T)} := \int\limits_0^T \frac{[u(t)]^2}{T-t} \, \mathrm{d}t.$$

A more detailed discussion of the space $H^{1/2}_{0,}(0,T)$ and its importance for the analysis of problem (1.1) in the anisotropic setting can be found in [32,65]. For $s > 1$ with $s = k + \kappa$, $k \in \mathbb{N}$ and $\kappa \in (0,1)$, we define
$$H^s(0,T) := \left\{ u \in H^k(0,T) : |\partial_t^k u|_{H^\kappa(0,T)} < \infty \right\}$$

where $H^k(0,T)$ denotes the standard Sobolev space of order k with norm
$$\|u\|^2_{H^k(0,T)} := \sum_{\ell=0}^k \left\| \partial_t^\ell u \right\|^2_{L^2(0,T)}.$$

The corresponding Sobolev spaces of functions with homogeneous initial or final conditions are then defined as
$$H^s_{0,}(0,T) := H^s(0,T) \cap H^1_{0,}(0,T), \quad H^s_{,0}(0,T) := H^s(0,T) \cap H^1_{,0}(0,T).$$

Moreover, Sobolev spaces on $(0,T)$ with negative order $s < 0$ are given by
$$H^s_{,0}(0,T) := [H^{-s}_{0,}(0,T)]', \quad H^s_{0,}(0,T) := [H^{-s}_{,0}(0,T)]', \quad \widetilde{H}^s(0,T) := \left[H^{-s}(0,T)\right]'.$$

2.2 Anisotropic Sobolev Spaces on the Space–Time Domain Q

Let $H^r(\Omega)$ and $H^r_0(\Omega)$ for $0 \le r \in \mathbb{R}$ denote the standard Sobolev spaces on Ω, see, e.g., [38, 62]. The anisotropic Sobolev space $H^{r,s}(Q)$ for $r \ge 0$ and $s \ge 0$ is defined as

$$H^{r,s}(Q) := L^2(0,T;H^r(\Omega)) \cap H^s(0,T;L^2(\Omega)),$$

where [34, 35]

$$H^s(0,T;L^2(\Omega)) := \left\{ u \in L^2(Q) : |u|_{H^s(0,T;L^2(\Omega))} < \infty \right\}$$

with

$$|u|^2_{H^s(0,T;L^2(\Omega))} := \int_\Omega \|u(x,\cdot)\|^2_{H^s(0,T)} \,\mathrm{d}x.$$

The space $L^2(0,T;H^r(\Omega))$ denotes the Bochner space as introduced in, e.g., [72, Section 23.2]. The analysis of the model problem (1.1) is done in the space $H^{1,1/2}(Q)$ and therefore we are interested in the properties of this specific anisotropic setting. The norm of a function $u \in H^{1,1/2}(Q)$ is given by

$$\|u\|^2_{H^{1,1/2}(Q)} := \|u\|^2_{L^2(Q)} + \|\nabla_x u\|^2_{L^2(Q)} + |u|^2_{H^{1/2}(0,T;L^2(\Omega))}.$$

Moreover, we define the space of functions in $H^{1,1/2}(Q)$ with homogeneous initial conditions

$$H^{1,1/2}_{;0,}(Q) := \left\{ u \in H^{1,1/2}(Q) : |u|_{H^{1/2}_{0,}(0,T;L^2(\Omega))} < \infty \right\},$$

where

$$|u|^2_{H^{1/2}_{0,}(0,T;L^2(\Omega))} := \int_\Omega |u(x,\cdot)|^2_{H^{1/2}_{0,}(0,T)} \,\mathrm{d}x \tag{2.1}$$

and

$$\|u\|^2_{H^{1,1/2}_{;0,}(Q)} := \|u\|^2_{H^{1,1/2}(Q)} + |u|^2_{H^{1/2}_{0,}(0,T;L^2(\Omega))}.$$

We write $H^{1,1/2}_{;0,}(Q) = L^2(0,T;H^1(\Omega)) \cap H^{1/2}_{0,}(0,T;L^2(\Omega))$ with

$$H^{1/2}_{0,}(0,T;L^2(\Omega)) := \left\{ u \in H^{1/2}(0,T;L^2(\Omega)) : |u|_{H^{1/2}_{0,}(0,T;L^2(\Omega))} < \infty \right\}.$$

The space of functions in $H^{1,1/2}_{;0,}(Q)$ with homogeneous boundary conditions is defined as

$$H^{1,1/2}_{0;0,}(Q) := L^2(0,T;H^1_0(\Omega)) \cap H^{1/2}_{0,}(0,T;L^2(\Omega))$$

and is equipped with the norm

$$\|u\|^2_{H^{1,1/2}_{0;0,}(Q)} := \|\nabla_x u\|^2_{L^2(Q)} + |u|^2_{H^{1/2}(0,T,L^2(\Omega))} + |u|^2_{H^{1/2}_{0,}(0,T;L^2(\Omega))}.$$

In the same way we introduce the space of functions in $H^{1,1/2}(Q)$ vanishing at the time horizon T, i.e.

$$H^{1,1/2}_{;,0}(Q) := L^2(0,T;H^1(\Omega)) \cap H^{1/2}_{,0}(0,T;L^2(\Omega))$$

and

$$H^{1,1/2}_{0;,0}(Q) := L^2(0,T;H^1_0(\Omega)) \cap H^{1/2}_{,0}(0,T;L^2(\Omega)).$$

In this case, the semi-norm (2.1) is replaced by

$$|u|^2_{H^{1/2}_{,0}(0,T;L^2(\Omega))} := \int_\Omega |u(x,\cdot)|^2_{H^{1/2}_{,0}(0,T)} \, \mathrm{d}x.$$

Moreover, we define the space

$$H^{1,1/2}_{;0,}(Q,\mathcal{L}) := \left\{ u \in H^{1,1/2}_{;0,}(Q) : \mathcal{L}u \in L^2(Q) \right\},$$

where $\mathcal{L} := \alpha\partial_t - \Delta_x$ denotes the differential operator of the heat equation. The norm of a function $u \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ is then given by

$$\|u\|^2_{H^{1,1/2}_{;0,}(Q,\mathcal{L})} := \|u\|^2_{H^{1,1/2}_{;0,}(Q)} + \|\mathcal{L}u\|^2_{L^2(Q)}.$$

The definition of the space $H^{1,1/2}_{;,0}(Q,\mathcal{L}')$, where $\mathcal{L}' := -\alpha\partial_t - \Delta_x$ denotes the operator of the adjoint heat equation, follows the same path. Analogously we define the spaces

$$H^{1,1/2}(Q,\mathcal{L}) := \left\{ u \in H^{1,1/2}(Q) : \mathcal{L}u \in L^2(Q) \right\}$$

and

$$H^{1,1/2}(Q,\mathcal{L}') := \left\{ u \in H^{1,1/2}(Q) : \mathcal{L}'u \in L^2(Q) \right\}.$$

2.3 Anisotropic Sobolev Spaces on the Space–Time Boundary Σ

Let $H^r(\Gamma)$ for $0 \le r \in \mathbb{R}$ denote the standard Sobolev spaces on Γ, see, e.g., [38, 62]. For a smooth lateral boundary Γ the space $H^r(\Gamma)$ is defined for arbitrary $r \ge 0$. However, for a general Lipschitz boundary Γ the definition is only valid for $0 \le r \le 1$. The anisotropic Sobolev spaces $H^{r,s}(\Sigma)$ for $r,s \ge 0$ are defined in a similar way as $H^{r,s}(Q)$ described in Section 2.2, see [35]. We set

$$H^{r,s}(\Sigma) := L^2(0,T;H^r(\Gamma)) \cap H^s(0,T;L^2(\Gamma)),$$

where

$$H^s(0,T;L^2(\Gamma)) := \left\{ u \in L^2(\Sigma) : |u|_{H^s(0,T;L^2(\Gamma))} < \infty \right\}$$

with

$$|u|^2_{H^s(0,T;L^2(\Gamma))} := \int\limits_{\Gamma} \|u(x,\cdot)\|^2_{H^s(0,T)} \, \mathrm{d}s_x.$$

Again, the space $L^2(0,T;H^r(\Gamma))$ denotes the Bochner space as introduced in, e.g., [72, Section 23.2]. For $r,s \in (0,1)$ a norm is given by

$$\|u\|^2_{H^{r,s}(\Sigma)} := \|u\|^2_{L^2(\Sigma)} + |u|^2_{L^2(0,T;H^r(\Gamma))} + |u|^2_{H^s(0,T;L^2(\Gamma))}$$

with

$$|u|^2_{L^2(0,T;H^r(\Gamma))} := \int\limits_{\Gamma}\int\limits_{\Gamma} \frac{\|u(x,\cdot)-u(y,\cdot)\|^2_{L^2(0,T)}}{|x-y|^{n-1+2r}} \, \mathrm{d}s_y \, \mathrm{d}s_x$$

and

$$|u|^2_{H^s(0,T;L^2(\Gamma))} := \int\limits_0^T\int\limits_0^T \frac{\|u(\cdot,t)-u(\cdot,\tau)\|^2_{L^2(\Gamma)}}{|t-\tau|^{1+2s}} \, \mathrm{d}\tau \, \mathrm{d}t.$$

The following lemma is essential for the numerical analysis of the approximation properties of L^2 projections on boundary element spaces which are defined with respect to an arbitrary triangulation of the space–time boundary Σ. Since we will work with shape regular elements, the lemma basically implies that we can use the approximation properties in standard Sobolev spaces $H^s(\Sigma)$ for $s \geq 0$, see, e.g., [38, 62], to obtain the convergence results with respect to the anisotropic setting.

Lemma 2.1. *For $r,s \in [0,1]$ the continuous embeddings*

$$H^{\max(r,s)}(\Sigma) \hookrightarrow H^{r,s}(\Sigma) \hookrightarrow H^{\min(r,s)}(\Sigma)$$

hold.

Proof. Let $u \in H^{r,s}(\Sigma)$ for $r,s \in [0,1]$ and define $m := \min(r,s)$, $M := \max(r,s)$. Since $H^r(\Gamma) \hookrightarrow H^m(\Gamma)$ [27, Theorem 4.2.2] and $H^s(0,T) \hookrightarrow H^m(0,T)$, we have

$$\begin{aligned} \|u\|^2_{H^{m,m}(\Sigma)} &\cong \|u\|^2_{H^{m,0}(\Sigma)} + \|u\|^2_{H^{0,m}(\Sigma)} \quad \leq c\left(\|u\|^2_{H^{r,0}(\Sigma)} + \|u\|^2_{H^{0,s}(\Sigma)}\right) \\ &\leq c\,\|u\|^2_{H^{r,s}(\Sigma)}, \end{aligned} \tag{2.2}$$

and therefore $H^{r,s}(\Sigma) \hookrightarrow H^{m,m}(\Sigma)$. According to [38, Theorem B.11 ff.] and [34, 35], and since $H^1(\Sigma) \cong H^{1,1}(\Sigma)$, we have

$$H^{m,m}(\Sigma) = \left[L^2(\Sigma), H^{1,1}(\Sigma)\right]_m \cong \left[L^2(\Sigma), H^1(\Sigma)\right]_m = H^m(\Sigma). \tag{2.3}$$

Hence $\|u\|_{H^{m,m}(\Sigma)} \cong \|u\|_{H^m(\Sigma)}$ and therefore $H^{r,s}(\Sigma) \hookrightarrow H^m(\Sigma)$. The proof of the first equality in (2.3) follows the same path as described in [35, Proposition 2.1] in the case of anisotropic Sobolev spaces on Q.

To prove the continuous embedding $H^M(\Sigma) \hookrightarrow H^{r,s}(\Sigma)$, we use $H^M(\Gamma) \hookrightarrow H^r(\Gamma)$ and $H^M(0,T) \hookrightarrow H^s(0,T)$. Analogously to estimate (2.2) and relation (2.3) we obtain $H^M(\Sigma) \cong H^{M,M}(\Sigma)$ and $\|u\|^2_{H^{r,s}(\Sigma)} \le c\,\|u\|^2_{H^{M,M}(\Sigma)}$, and therefore conclude the continuous embedding $H^M(\Sigma) \hookrightarrow H^{r,s}(\Sigma)$. □

Let us now introduce the spaces

$$H^{r,s}_{;0,}(\Sigma) := L^2(0,T;H^r(\Gamma)) \cap H^s_{0,}(0,T;L^2(\Gamma)),$$
$$H^{r,s}_{;,0}(\Sigma) := L^2(0,T;H^r(\Gamma)) \cap H^s_{,0}(0,T;L^2(\Gamma)),$$

which are the closures in $H^{r,s}(\Sigma)$ of the subspaces of functions vanishing in a neighborhood of $t=0$ and $t=T$, respectively. Anisotropic Sobolev spaces on Σ with negative order $r,s<0$ are defined as

$$H^{r,s}_{;,0}(\Sigma) := \left[H^{-r,-s}_{;0,}(\Sigma)\right]', \quad H^{r,s}_{;0,}(\Sigma) := \left[H^{-r,-s}_{;,0}(\Sigma)\right]', \quad \widetilde{H}^{r,s}(\Sigma) := \left[H^{-r,-s}(\Sigma)\right]'.$$

For convenience we additionally set $H^{-r,-s}(\Sigma) := H^{-r,-s}_{;,0}(\Sigma)$ and $\widetilde{H}^{r,s}(\Sigma) := H^{r,s}_{;0,}(\Sigma)$ for $r,s \ge 0$.

Remark 2.1. *For $r \ge 0$ and $0 \le s < \frac{1}{2}$ we have $H^{r,s}(\Sigma) = H^{r,s}_{;0,}(\Sigma) = H^{r,s}_{;,0}(\Sigma)$ and therefore $H^{-r,-s}_{;0,}(\Sigma) = H^{-r,-s}_{;,0}(\Sigma) = \widetilde{H}^{-r,-s}(\Sigma)$.*

For a function $u \in C(\overline{Q})$ we define the interior Dirichlet trace as

$$\gamma_0^{\text{int}} u(x,t) := \lim_{\Omega \ni \widetilde{x} \to x \in \Gamma} u(\widetilde{x},t) \quad \text{for } (x,t) \in \Sigma.$$

Hence $\gamma_0^{\text{int}} u$ coincides with the restriction of u to the space–time boundary Σ, i.e. we have $\gamma_0^{\text{int}} u = u_{|\Sigma}$. This operator can be extended to the anisotropic Sobolev space $H^{1,1/2}(Q)$.

Theorem 2.2 (Trace Theorem, [35, Theorem 2.1] and [10])**.** *The interior Dirichlet trace operator*

$$\gamma_0^{int} : H^{1,1/2}(Q) \to H^{1/2,1/4}(\Sigma)$$

is linear and bounded, satisfying

$$\left\|\gamma_0^{int} u\right\|_{H^{1/2,1/4}(\Sigma)} \le c_T\,\|u\|_{H^{1,1/2}(Q)} \quad \textit{for all } u \in H^{1,1/2}(Q).$$

Lemma 2.3 ([10, Lemma 2.4])**.** *The interior Dirichlet trace operator γ_0^{int} is bounded and surjective from $H^{1,1/2}_{;0,}(Q)$ to $H^{1/2,1/4}(\Sigma)$.*

Theorem 2.4 (Inverse Trace Theorem). *The interior Dirichlet trace operator*

$$\gamma_0^{int} : H^{1,1/2}_{;0,}(Q) \to H^{1/2,1/4}(\Sigma)$$

has a continuous right inverse operator

$$\mathcal{E}_0 : H^{1/2,1/4}(\Sigma) \to H^{1,1/2}_{;0,}(Q)$$

satisfying $\gamma_0^{int}\mathcal{E}_0 v = v$ for all $v \in H^{1/2,1/4}(\Sigma)$, i.e. there exists a constant $c_{IT} > 0$ such that

$$\|\mathcal{E}_0 v\|_{H^{1,1/2}_{;0,}(Q)} \le c_{IT}\, \|v\|_{H^{1/2,1/4}(\Sigma)} \quad \textit{for all } v \in H^{1/2,1/4}(\Sigma).$$

Proof. The proof is similar to [19, Theorem 4.9]. See also [10]. □

Piecewise Smooth Functions on Σ

For a closed, piecewise smooth boundary $\Gamma = \bigcup_{j=1}^{J} \overline{\Gamma}_j$ with $\Gamma_i \cap \Gamma_j = \emptyset$ for $i \neq j$, where Γ_j are open parts of the boundary Γ, we set $\Sigma_j := \Gamma_j \times (0,T)$ for $j = 1,\dots,J$. We then have $\overline{\Sigma} = \bigcup_{j=1}^{J} \overline{\Sigma}_j$. For $r \ge 0$ and $s \ge 0$ we define the anisotropic Sobolev space on the open part Σ_j of the space–time boundary Σ

$$H^{r,s}(\Sigma_j) := \left\{ v = \widetilde{v}_{|\Sigma_j} : \widetilde{v} \in H^{r,s}(\Sigma) \right\}$$

and the space of piecewise smooth functions on Σ

$$H^{r,s}_{\mathrm{pw}}(\Sigma) := \left\{ v \in L^2(\Sigma) : v_{|\Sigma_j} \in H^{r,s}(\Sigma_j) \text{ for } j = 1,\dots,J \right\}$$

with norm

$$\|v\|_{H^{r,s}_{\mathrm{pw}}(\Sigma)} := \left(\sum_{j=1}^{J} \left\| v_{|\Sigma_j} \right\|^2_{H^{r,s}(\Sigma_j)} \right)^{1/2}.$$

For $r,s < 0$ the anisotropic Sobolev space on Σ_j is defined as the corresponding dual space

$$\widetilde{H}^{r,s}(\Sigma_j) := \left[H^{-r,-s}(\Sigma_j) \right]'.$$

The space of piecewise smooth functions on Σ with negative order is then given by

$$H^{r,s}_{\mathrm{pw}}(\Sigma) := \prod_{j=1}^{J} \widetilde{H}^{r,s}(\Sigma_j)$$

with norm

$$\|w\|_{H^{r,s}_{\mathrm{pw}}(\Sigma)} := \sum_{j=1}^{J} \left\| w_{|\Sigma_j} \right\|_{\widetilde{H}^{r,s}(\Sigma_j)}.$$

Lemma 2.5. *For $r,s<0$ and $w\in H^{r,s}_{pw}(\Sigma)$ there holds*

$$\|w\|_{\widetilde{H}^{r,s}(\Sigma)} \le \|w\|_{H^{r,s}_{pw}(\Sigma)}\,.$$

Proof. Let $w\in H^{r,s}_{\mathrm{pw}}(\Sigma)$. By duality we conclude

$$\begin{aligned}
\|w\|_{\widetilde{H}^{r,s}(\Sigma)} &= \sup_{0\neq v\in H^{-r,-s}(\Sigma)} \frac{|\langle w,v\rangle_\Sigma|}{\|v\|_{H^{-r,-s}(\Sigma)}} \le \sup_{0\neq v\in H^{-r,-s}(\Sigma)} \sum_{j=1}^{J} \frac{|\langle w,v\rangle_{\Sigma_j}|}{\|v\|_{H^{-r,-s}(\Sigma)}}\\
&\le \sup_{0\neq v\in H^{-r,-s}(\Sigma)} \sum_{j=1}^{J} \frac{|\langle w_{|\Sigma_j}, v_{|\Sigma_j}\rangle_{\Sigma_j}|}{\left\|v_{|\Sigma_j}\right\|_{H^{-r,-s}(\Sigma_j)}}\\
&\le \sum_{j=1}^{J} \sup_{0\neq v_j\in H^{-r,-s}(\Sigma_j)} \frac{|\langle w_{|\Sigma_j}, v_j\rangle_{\Sigma_j}|}{\left\|v_j\right\|_{H^{-r,-s}(\Sigma_j)}} = \|w\|_{H^{r,s}_{\mathrm{pw}}(\Sigma)}\,.
\end{aligned}$$

□

Note that for a general Lipschitz boundary Γ we have to assume $|r|\le 1$ to keep the validity of the statements above.

3 DOMAIN VARIATIONAL FORMULATION

In this chapter we introduce and analyze the domain variational formulation of problem (1.1) with given Dirichlet boundary conditions in the setting of anisotropic Sobolev spaces. In Sections 3.1 - 3.2 we recall existence and uniqueness results for the solution of the variational formulation of the model problem with Dirichlet boundary conditions and homogeneous initial conditions and introduce a transformation operator $\mathcal{H}_T$ in order to obtain an equivalent Galerkin–Bubnov variational formulation, which is important for the stability of the discretized space–time system [65]. In Section 3.3 we define and analyze the Neumann trace of solutions of initial Dirichlet boundary value problems, and we derive Green's identities for the heat equation in Section 3.4. The unique solvability of problem (1.1) with given initial datum and homogeneous Dirichlet boundary conditions is discussed in Section 3.5. The presented results are based on [12, 65, 71, 72].

3.1 Homogeneous Initial Datum

In the following section we discuss the unique solvability of problem (1.1) with given Dirichlet datum and homogeneous initial conditions based on [65,71]. Let $f \in [H^{1,1/2}_{0;,0}(Q)]'$ and $g \in H^{1/2,1/4}(\Sigma)$ be given. We consider the initial Dirichlet boundary value problem

$$\begin{aligned} \alpha\partial_t u(x,t) - \Delta_x u(x,t) &= f(x,t) \quad && \text{for } (x,t) \in Q, \\ u(x,t) &= g(x,t) && \text{for } (x,t) \in \Sigma, \\ u(x,0) &= 0 && \text{for } x \in \Omega. \end{aligned} \tag{3.1}$$

The variational formulation of problem (3.1) is to find $u \in H^{1,1/2}_{;0,}(Q)$ with $u_{|\Sigma} = g$ such that

$$a(u,v) = \langle f, v\rangle_Q \quad \text{for all } v \in H^{1,1/2}_{0;,0}(Q) \tag{3.2}$$

with the bilinear form

$$a(u,v) := \alpha\langle \partial_t u, v\rangle_Q + \langle \nabla_x u, \nabla_x v\rangle_{L^2(Q)} \tag{3.3}$$

for $u \in H^{1,1/2}_{;0,}(Q)$ and $v \in H^{1,1/2}_{;,0}(Q)$. Here we have to ensure that the term $\langle \partial_t u, v\rangle_Q$ is well defined. In [65] it was shown that the bilinear form $\langle \partial_t u, v\rangle_Q$ can be extended to functions $u \in H^{1,1/2}_{;0,}(Q)$ and $v \in H^{1,1/2}_{;,0}(Q)$, and that there exists a constant $c > 0$ such that

$$\langle \partial_t u, v\rangle_Q \le c\, \|u\|_{H^{1,1/2}_{;0,}(Q)} \|v\|_{H^{1,1/2}_{;,0}(Q)} \quad \text{for all } u \in H^{1,1/2}_{;0,}(Q), v \in H^{1,1/2}_{;,0}(Q).$$

The bilinear form $\langle \cdot, \cdot\rangle_Q$ in (3.2) denotes the duality pairing on $[H^{1,1/2}_{0;,0}(Q)]' \times H^{1,1/2}_{0;,0}(Q)$ as extension of the inner product in $L^2(Q)$.

Hence
$$a(\cdot,\cdot) : H^{1,1/2}_{;0,}(Q) \times H^{1,1/2}_{;,0}(Q) \to \mathbb{R}$$
is bounded, i.e. there exists a constant $c_2^A > 0$ such that
$$|a(u,v)| \le c_2^A \, \|u\|_{H^{1,1/2}_{;0,}(Q)} \, \|v\|_{H^{1,1/2}_{;,0}(Q)} \quad \text{for all } u \in H^{1,1/2}_{;0,}(Q), v \in H^{1,1/2}_{;,0}(Q).$$

For the given Dirichlet datum $g \in H^{1/2,1/4}(\Sigma)$ we consider the decomposition $u := \bar{u} + \tilde{u}_g$, where $\tilde{u}_g := \mathcal{E}_0 g$ is an extension of the boundary datum g to the space–time domain Q satisfying $\gamma_0^{\text{int}} \tilde{u}_g = g$. The boundedness of $\mathcal{E}_0 : H^{1/2,1/4}(\Sigma) \to H^{1,1/2}_{;0,}(Q)$ then implies
$$\left\|\tilde{u}_g\right\|_{H^{1,1/2}_{;0,}(Q)} \le c_{IT} \, \|g\|_{H^{1/2,1/4}(\Sigma)} \,. \tag{3.4}$$

Hence the variational formulation (3.2) changes to: Find $\bar{u} \in H^{1,1/2}_{0;0,}(Q)$ such that
$$a(\bar{u},v) = \langle f,v\rangle_Q - a(\tilde{u}_g,v) \quad \text{for all } v \in H^{1,1/2}_{0;,0}(Q). \tag{3.5}$$

Theorem 3.1 (Existence and uniqueness [65, Theorem 3.2])**.** *The variational formulation* (3.5) *implies an isomorphism*
$$\mathcal{L} : H^{1,1/2}_{0;0,}(Q) \to [H^{1,1/2}_{0;,0}(Q)]'$$
satisfying
$$\|\bar{u}\|_{H^{1,1/2}_{0;0,}(Q)} \le 2 \, \|\mathcal{L}\bar{u}\|_{[H^{1,1/2}_{0;,0}(Q)]'} \quad \textit{for all } \bar{u} \in H^{1,1/2}_{0;0,}(Q).$$

Hence we conclude that the variational problem (3.5) is uniquely solvable and therefore $u = \bar{u} + \tilde{u}_g$ is the unique solution of the variational problem (3.2). A direct consequence of Theorem 3.1 is the stability estimate
$$\frac{1}{2} \, \|\bar{u}\|_{H^{1,1/2}_{0;0,}(Q)} \le \sup_{0 \ne v \in H^{1,1/2}_{0;,0}(Q)} \frac{a(\bar{u},v)}{\|v\|_{H^{1,1/2}_{0;,0}(Q)}} \quad \text{for all } \bar{u} \in H^{1,1/2}_{0;0,}(Q). \tag{3.6}$$

Theorem 3.2. *For $f \in [H^{1,1/2}_{0;,0}(Q)]'$ and $g \in H^{1/2,1/4}(\Sigma)$ there exists a unique solution $u \in H^{1,1/2}_{;0,}(Q)$ of the variational problem* (3.2) *satisfying*
$$\|u\|_{H^{1,1/2}_{;0,}(Q)} \le c_R \, \|f\|_{[H^{1,1/2}_{0;,0}(Q)]'} + c_B \, \|g\|_{H^{1/2,1/4}(\Sigma)} \,.$$

Proof. Unique solvability is a result of Theorem 3.1. The stability condition (3.6) and the boundedness of the bilinear form $a(\cdot,\cdot)$ imply

$$\begin{aligned}\frac{1}{2}\|\bar{u}\|_{H^{1,1/2}_{0;0,}(Q)} &\leq \sup_{0\neq v\in H^{1,1/2}_{0;,0}(Q)} \frac{a(\bar{u},v)}{\|v\|_{H^{1,1/2}_{0;,0}(Q)}} = \sup_{0\neq v\in H^{1,1/2}_{0;,0}(Q)} \frac{\langle f,v\rangle_Q - a(\tilde{u}_g,v)}{\|v\|_{H^{1,1/2}_{0;,0}(Q)}} \\ &\leq \|f\|_{[H^{1,1/2}_{0;,0}(Q)]'} + c\,\|\tilde{u}_g\|_{H^{1,1/2}_{;0,}(Q)}.\end{aligned}$$

The assertion follows by using the triangle inequality for $u=\bar{u}+\tilde{u}_g$, the Poincaré inequality, and the stability (3.4) of the inverse trace operator. □

Note that (3.5) is a Galerkin–Petrov variational formulation with different trial and test spaces. In order to obtain an equivalent Galerkin–Bubnov variational formulation, which is important for the stability of the discretized space–time system when using conforming finite element spaces, we have to establish some suitable bijective transformation operator $\mathcal{H}_T : H^{1,1/2}_{;0,}(Q) \to H^{1,1/2}_{;,0}(Q)$.

3.2 The Transformation Operator $\mathcal{H}_T$

The definition and analysis of the transformation operator in the following section is based on [65]. Here we only recall the main results. Let us consider the eigenvalue problem

$$-\partial_{tt}u(t) = \lambda u(t) \quad \text{for } t\in(0,T), \quad u(0)=0, \quad \partial_t u(T)=0. \tag{3.7}$$

The eigenfunctions $\{v_k\}_{k\in\mathbb{N}_0}$ with eigenvalues $\{\lambda_k\}_{k\in\mathbb{N}_0}$ of (3.7) are given as

$$v_k(t) = \sin\left(\left(\frac{\pi}{2}+k\pi\right)\frac{t}{T}\right), \quad \lambda_k = \frac{1}{T^2}\left(\frac{\pi}{2}+k\pi\right)^2, \quad k\in\mathbb{N}_0 \tag{3.8}$$

and form an orthogonal basis in $L^2(0,T)$ satisfying

$$\int_0^T v_k(t)v_l(t)\,\mathrm{d}t = \frac{T}{2}\delta_{kl}.$$

Hence, for $u\in L^2(0,T)$ we may consider the representation

$$u(t) = \sum_{k=0}^{\infty} u_k \sin\left(\left(\frac{\pi}{2}+k\pi\right)\frac{t}{T}\right)$$

with

$$u_k = \frac{2}{T}\int_0^T u(t)\sin\left(\left(\frac{\pi}{2}+k\pi\right)\frac{t}{T}\right)\mathrm{d}t, \quad k\in\mathbb{N}_0.$$

By Parseval's identity we have

$$\|u\|^2_{L^2(0,T)} = \frac{T}{2}\sum_{k=0}^{\infty} u_k^2$$

and for $u \in H^1_{0,}(0,T)$ we further obtain

$$\|\partial_t u\|^2_{L^2(0,T)} = \frac{1}{2T}\sum_{k=0}^{\infty}\left(\frac{\pi}{2}+k\pi\right)^2 u_k^2.$$

Hence, using interpolation, we can define an equivalent norm in $H^{1/2}_{0,}(0,T)$ by

$$\|u\|^2_{H^{1/2}_{0,}(0,T)} = \frac{1}{2}\sum_{k=0}^{\infty}\left(\frac{\pi}{2}+k\pi\right) u_k^2,$$

as well as an inner product

$$\langle u,v\rangle_{H^{1/2}_{0,}(0,T)} = \frac{1}{2}\sum_{k=0}^{\infty}\left(\frac{\pi}{2}+k\pi\right) u_k v_k.$$

The operator $\mathcal{H}_T : L^2(0,T) \to L^2(0,T)$ is then defined by

$$(\mathcal{H}_T u)(t) := \sum_{k=0}^{\infty} u_k \cos\left(\left(\frac{\pi}{2}+k\pi\right)\frac{t}{T}\right) \quad \text{for } u \in L^2(0,T).$$

The transformation operator $\mathcal{H}_T : L^2(0,T) \to L^2(0,T)$ as well as the restriction

$$\mathcal{H}_T : H^{1/2}_{0,}(0,T) \to H^{1/2}_{,0}(0,T)$$

define isometric isomorphisms, i.e. we have

$$\|\mathcal{H}_T u\|_{L^2(0,T)} = \|u\|_{L^2(0,T)} \quad \text{for all } u \in L^2(0,T)$$

and

$$\|\mathcal{H}_T u\|_{H^{1/2}_{,0}(0,T)} = \|u\|_{H^{1/2}_{0,}(0,T)} \quad \text{for all } u \in H^{1/2}_{0,}(0,T).$$

For $u \in L^2(Q)$ we consider the representation

$$u(x,t) = \sum_{i=1}^{\infty} U_i(t)\phi_i(x), \quad U_i(t) = \sum_{k=0}^{\infty} u_{i,k} v_k(t) \tag{3.9}$$

where $\phi_i \in H^1_0(\Omega)$ are the orthonormal eigenfunctions of the spatial Dirichlet eigenvalue problem

$$-\Delta\phi = \mu\phi \quad \text{in } \Omega, \quad \phi = 0 \quad \text{on } \Gamma, \quad \|\phi\|_{L^2(\Omega)} = 1 \tag{3.10}$$

and $v_k \in H^1_{0,}(0,T)$ are given by (3.8). The coefficients in (3.9) are given by

$$u_{i,k} = \frac{2}{T}\int_0^T \int_\Omega u(x,t) v_k(t) \phi_i(x) \mathrm{d}x \, \mathrm{d}t \,.$$

Then $\mathcal{H}_T u$ for $u \in L^2(Q)$ is defined as

$$(\mathcal{H}_T u)(x,t) = \sum_{i=1}^\infty (\mathcal{H}_T U_i)(t) \phi_i(x) \quad \text{for } (x,t) \in Q.$$

Again, the transformation operator $\mathcal{H}_T : L^2(Q) \to L^2(Q)$ and its restriction

$$\mathcal{H}_T : H^{1,1/2}_{;0,}(Q) \to H^{1,1/2}_{;,0}(Q)$$

define isometric isomorphisms, i.e. we have

$$\|\mathcal{H}_T u\|_{L^2(Q)} = \|u\|_{L^2(Q)} \quad \text{for all } u \in L^2(Q)$$

and

$$\|\mathcal{H}_T u\|_{H^{1,1/2}_{;,0}(Q)} = \|u\|_{H^{1,1/2}_{;0,}(Q)} \quad \text{for all } u \in H^{1,1/2}_{;0,}(Q).$$

As mentioned before, a detailed analysis of the operator $\mathcal{H}_T$ is given in [65].

By using the transformation operator $\mathcal{H}_T$ we obtain an equivalent Galerkin–Bubnov variational formulation: Find $\bar{u} \in H^{1,1/2}_{0;0,}(Q)$ such that

$$a(\bar{u}, \mathcal{H}_T v) = \langle f, \mathcal{H}_T v \rangle_Q - a(\tilde{u}_g, \mathcal{H}_T v) \quad \text{for all } v \in H^{1,1/2}_{0;0,}(Q). \tag{3.11}$$

This Galerkin–Bubnov variational formulation is uniquely solvable as well.

For a given conforming space–time finite element space $\mathcal{V}_h \subset H^{1,1/2}_{0;0,}(Q)$ the Galerkin variational formulation of (3.11) is to find $u_h \in \mathcal{V}_h$ such that

$$a(u_h, \mathcal{H}_T v_h) = \langle f, \mathcal{H}_T v_h \rangle_Q - a(\tilde{u}_g, \mathcal{H}_T v_h) \quad \text{for all } v_h \in \mathcal{V}_h. \tag{3.12}$$

The related finite element stiffness matrix is positive definite and therefore unique solvability of (3.12) follows for any conforming choice of $\mathcal{V}_h$. Related numerical experiments for the discretization of the variational problem (3.11) in the spatially one-dimensional case can be found in [65, 71].

3.3 Neumann Trace Operator

For a function $u \in C^1(\overline{Q})$ we define the interior Neumann trace

$$\gamma_1^{\mathrm{int}} u(x,t) := \lim_{\Omega \ni \widetilde{x} \to x \in \Gamma} n_x \cdot \nabla_{\widetilde{x}} u(\widetilde{x},t) \quad \text{for } (x,t) \in \Sigma,$$

which coincides with the normal derivative of u on Σ, i.e. we have $\gamma_1^{\mathrm{int}} u = \partial_{n_x} u_{|\Sigma}$. The definition of the interior Neumann trace operator can be extended to the anisotropic Sobolev space $H^{1,1/2}(Q,\mathcal{L})$ and to functions $u \in H^{1,1/2}_{;0,}(Q)$ with $\mathcal{L}u \in [H^{1,1/2}_{;,0}(Q)]'$.

Lemma 3.3 ([10, Proposition 2.18])**.** *The interior Neumann trace operator*

$$\gamma_1^{int} : H^{1,1/2}(Q,\mathcal{L}) \to H^{-1/2,-1/4}(\Sigma)$$

is linear and bounded satisfying

$$\left\| \gamma_1^{int} u \right\|_{H^{-1/2,-1/4}(\Sigma)} \le c_{NT} \left\| u \right\|_{H^{1,1/2}(Q,\mathcal{L})} \quad \textit{for all } u \in H^{1,1/2}(Q,\mathcal{L}).$$

For $u \in C^2(\overline{Q})$ we have $\gamma_1^{int} u = \partial_{n_x} u_{|\Sigma}$ in the distributional sense.

Note that the continuity of the mapping $\gamma_1^{\mathrm{int}} : H^{1,1/2}(Q,\mathcal{L}') \to H^{-1/2,-1/4}(\Sigma)$ can be shown in the same way, only with respect to the differential operator of the adjoint heat equation.

Recall that the mapping $\mathcal{L} : H^{1,1/2}_{0;0,}(Q) \to [H^{1,1/2}_{0;,0}(Q)]'$ defines an isomorphism, see Theorem 3.1. The corresponding proof in [65] utilizes a Fourier series expansion of functions $u \in H^{1,1/2}_{0;0,}(Q)$ as in 3.9 with eigenfunctions $\phi_i \in H^1_0(\Omega)$ of the spatial Dirichlet eigenvalue problem for the Laplacian (3.10). In the same way, by considering a series expansion of $u \in H^{1,1/2}_{;0,}(Q)$ with eigenfunctions $\phi_i \in H^1(\Omega)$ of the spatial Neumann eigenvalue problem

$$-\Delta \phi = \lambda \phi \quad \text{in } \Omega, \quad \partial_n \phi = 0 \quad \text{on } \Gamma,$$

one can show that

$$\mathcal{L} : H^{1,1/2}_{;0,}(Q) \to [H^{1,1/2}_{;,0}(Q)]'$$

and consequently

$$\mathcal{L}' : H^{1,1/2}_{;,0}(Q) \to [H^{1,1/2}_{;0,}(Q)]'$$

define isomorphisms as well.

For functions $u \in H^{1,1/2}_{;0,}(Q)$ with $\mathcal{L}u \in [H^{1,1/2}_{;,0}(Q)]'$ we can determine the associated conormal derivative $\gamma_1^{\mathrm{int}} u \in H^{-1/2,-1/4}(\Sigma)$ as the solution of the variational problem

$$\langle \gamma_1^{\mathrm{int}} u, z \rangle_\Sigma = a(u, \mathcal{E}_T z) - \langle \mathcal{L}u, \mathcal{E}_T z \rangle_Q \quad \text{for all } z \in H^{1/2,1/4}(\Sigma) \tag{3.13}$$

where $\mathcal{E}_T := \mathcal{H}_T\mathcal{E}_0 : H^{1/2,1/4}(\Sigma) \to H^{1,1/2}_{;,0}(Q)$ and $a(\cdot,\cdot)$ is given by (3.3). Here and in the following chapters $\langle\cdot,\cdot\rangle_Q$ denotes the duality pairing on $[H^{1,1/2}_{;,0}(Q)]' \times H^{1,1/2}_{;,0}(Q)$ or $H^{1,1/2}_{;0,}(Q) \times [H^{1,1/2}_{;0,}(Q)]'$ as extension of the inner product in $L^2(Q)$, whereas $\langle\cdot,\cdot\rangle_\Sigma$ denotes the duality pairing on $H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$ as extension of the inner product in $L^2(\Sigma)$. The stability condition

$$\|w\|_{H^{-1/2,-1/4}(\Sigma)} = \sup_{0\neq z\in H^{1/2,1/4}(\Sigma)} \frac{\langle w,z\rangle_\Sigma}{\|z\|_{H^{1/2,1/4}(\Sigma)}} \quad \text{for all } w \in H^{-1/2,-1/4}(\Sigma)$$

ensures unique solvability of (3.13) and thus, we obtain the following stability estimate for the Neumann trace.

Theorem 3.4. *Let $u \in H^{1,1/2}_{;0,}(Q)$ with $\mathcal{L}u \in [H^{1,1/2}_{;,0}(Q)]'$. Then the interior Neumann trace $\gamma_1^{int}u \in H^{-1/2,-1/4}(\Sigma)$ satisfies the stability estimate*

$$\left\|\gamma_1^{int}u\right\|_{H^{-1/2,-1/4}(\Sigma)} \le c_{IT}\left(c_2^A\,\|u\|_{H^{1,1/2}_{;0,}(Q)} + \|\mathcal{L}u\|_{[H^{1,1/2}_{;,0}(Q)]'}\right).$$

Proof. Let $u \in H^{1,1/2}_{;0,}(Q)$. Using the definition of the Neumann trace (3.13), the boundedness of the bilinear form $a(\cdot,\cdot)$ and the boundedness of the operator $\mathcal{E}_T$ yields

$$\begin{aligned}
\left\|\gamma_1^{\mathrm{int}}u\right\|_{H^{-1/2,-1/4}(\Sigma)} &= \sup_{0\neq z\in H^{1/2,1/4}(\Sigma)} \frac{\langle\gamma_1^{\mathrm{int}}u,z\rangle_\Sigma}{\|z\|_{H^{1/2,1/4}(\Sigma)}} \\
&= \sup_{0\neq z\in H^{1/2,1/4}(\Sigma)} \frac{a(u,\mathcal{E}_T z) - \langle\mathcal{L}u,\mathcal{E}_T z\rangle_Q}{\|z\|_{H^{1/2,1/4}(\Sigma)}} \\
&\le c_{IT}\left(c_2^A\,\|u\|_{H^{1,1/2}_{;0,}(Q)} + \|\mathcal{L}u\|_{[H^{1,1/2}_{;,0}(Q)]'}\right).
\end{aligned}$$

□

In particular, for the solution $u \in H^{1,1/2}_{;0,}(Q)$ of the initial Dirichlet boundary value problem (3.1) with homogeneous source term, i.e. $f \equiv 0$, we get

$$\left\|\gamma_1^{\mathrm{int}}u\right\|_{H^{-1/2,-1/4}(\Sigma)} \le c_{IT}\,c_2^A\,\|u\|_{H^{1,1/2}_{;0,}(Q)}.$$

The definition of the Neumann trace for functions $v \in H^{1,1/2}_{;,0}(Q)$ with $\mathcal{L}'u \in [H^{1,1/2}_{;0,}(Q)]'$ follows the same path, only with respect to the differential operator of the adjoint heat equation and the corresponding bilinear form.

3.4 Green's Identities for the Heat Equation

This section is devoted to the derivation of Green's first and second identity for the heat equation with respect to the previously introduced anisotropic setting. These formulas are later on used to derive the representation formula for the heat equation and for the analysis of related boundary integral operators, see Chapter 4. Recall that $\Omega \subset \mathbb{R}^n$ is assumed to be a bounded domain with, for $n = 2,3$, Lipschitz boundary $\Gamma = \partial\Omega$.

Theorem 3.5 ([2, Corollary 7.8]). *Let $u \in C^2(\Omega) \cap C^1(\overline{\Omega})$. Then there holds the classical Green's formula, i.e.*

$$\int_\Omega \Big[\Delta u(x) v(x) + \nabla u(x) \cdot \nabla v(x)\Big]\, \mathrm{d}x = \int_\Gamma \partial_n u(x) v(x)\, \mathrm{d}s_x$$

for all $v \in C^1(\Omega) \cap C(\overline{\Omega})$.

Now consider $u \in C^2(\overline{Q})$. By applying Theorem 3.5 we get

$$\begin{aligned} \int_0^T \int_\Omega \Big[\alpha \partial_t u(x,t) - \Delta_x u(x,t)\Big] v(x,t)\, \mathrm{d}x\, \mathrm{d}t &= -\int_0^T \int_\Gamma \partial_{n_x} u(x,t) v(x,t)\, \mathrm{d}s_x\, \mathrm{d}t \\ &+ \int_0^T \int_\Omega \Big[\alpha\, \partial_t u(x,t) v(x,t) + \nabla_x u(x,t) \cdot \nabla_x v(x,t)\Big]\, \mathrm{d}x\, \mathrm{d}t\,. \end{aligned} \tag{3.14}$$

This equation is the so-called Green's first identity for the heat equation. Using integration by parts on the first term on the right hand side and rearranging the terms yields

$$\begin{aligned} \alpha \int_\Omega u(x,T) v(x,T)\, \mathrm{d}x &= \alpha \int_\Omega u(x,0) v(x,0)\, \mathrm{d}x \\ &+ \int_0^T \int_\Omega \Big[\alpha \partial_t u(x,t) - \Delta_x u(x,t)\Big] v(x,t)\, \mathrm{d}x\, \mathrm{d}t + \int_0^T \int_\Gamma \partial_{n_x} u(x,t) v(x,t)\, \mathrm{d}s_x\, \mathrm{d}t \\ &+ \int_0^T \int_\Omega \Big[\alpha\, u(x,t) \partial_t v(x,t) - \nabla_x u(x,t) \cdot \nabla_x v(x,t)\Big]\, \mathrm{d}x\, \mathrm{d}t\,. \end{aligned}$$

Again, by applying Theorem 3.5 we get

$$\begin{aligned}
\alpha \int_\Omega u(x,T)v(x,T)\,\mathrm{d}x &= \alpha \int_\Omega u(x,0)v(x,0)\,\mathrm{d}y \\
&+ \int_0^T \int_\Omega \Big[\alpha\partial_t u(x,t) - \Delta_x u(x,t)\Big] v(x,t)\,\mathrm{d}x\,\mathrm{d}t + \int_0^T \int_\Gamma \partial_{n_x} u(x,t)v(x,t)\,\mathrm{d}s_x\,\mathrm{d}t \\
&- \int_0^T \int_\Omega \Big[-\alpha\partial_t v(x,t) - \Delta_x v(x,t)\Big] u(x,t)\,\mathrm{d}x\,\mathrm{d}t - \int_0^T \int_\Gamma \partial_{n_x} v(x,t)u(x,t)\,\mathrm{d}s_x\,\mathrm{d}t\,.
\end{aligned} \tag{3.15}$$

This equation is the so-called Green's second identity for the heat equation. Our aim is to extend these identities to the more general case of functions in $H^{1,1/2}(Q)$. To do so, we use the following density results.

Lemma 3.6 ([10, Lemma 2.22]). *Let $C_0^\infty(\overline{\Omega} \times (0,T])$ denote the space of functions in $C_0^\infty(\mathbb{R}^n \times (0,\infty))$ restricted to $\overline{Q}$. Then $C_0^\infty(\overline{\Omega} \times (0,T])$ is dense in the anisotropic Sobolev spaces $H^{1,1/2}_{;0,}(Q)$ and $H^{1,1/2}_{;0,}(Q,\mathcal{L})$.*

Analogously we obtain the following result, where $C_0^\infty(\overline{\Omega} \times [0,T))$ is the space of functions in $C_0^\infty(\mathbb{R}^n \times (-\infty,T))$ restricted to $\overline{Q}$.

Corollary 3.7. *The space $C_0^\infty(\overline{\Omega} \times [0,T))$ is dense in $H^{1,1/2}_{;,0}(Q)$ and $H^{1,1/2}_{;,0}(Q,\mathcal{L}')$.*

The following lemma is essential for the derivation of the jump conditions of the boundary integral operators in Chapter 4.

Lemma 3.8 ([10, Lemma 2.23]). *The combined trace map*

$$(\gamma_0^{int}, \gamma_1^{int}) : u \mapsto (\gamma_0^{int} u, \gamma_1^{int} u)$$

maps $C_0^\infty(\overline{\Omega} \times (0,T])$ onto a dense subspace of $H^{1/2,1/4}(\Sigma) \times H^{-1/2,-1/4}(\Sigma)$.

Remark 3.1. *Lemma 3.8 is also valid if we replace the space $C_0^\infty(\overline{\Omega} \times (0,T])$ with its counterpart $C_0^\infty(\overline{\Omega} \times [0,T))$.*

Recall that $\langle \partial_t \cdot, \cdot \rangle_Q$ denotes the bounded bilinear form on $H^{1,1/2}_{;0,}(Q) \times H^{1,1/2}_{;,0}(Q)$ introduced in Section 3.1.

Theorem 3.9 (Green's first identity). *For $u \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ and $v \in H^{1,1/2}_{;,0}(Q)$ there holds*

$$\alpha \langle \partial_t u, v \rangle_Q + \langle \nabla_x u, \nabla_x v \rangle_{L^2(Q)} = \langle \gamma_1^{int} u, \gamma_0^{int} v \rangle_\Sigma + \langle \mathcal{L} u, v \rangle_{L^2(Q)}.$$

Proof. Let $u \in C_0^\infty(\overline{\Omega} \times (0,T])$. According to (3.14) there holds

$$\langle \mathcal{L}u, v\rangle_{L^2(Q)} = \alpha \langle \partial_t u, v\rangle_{L^2(Q)} + \langle \nabla_x u, \nabla_x v\rangle_{L^2(Q)} - \langle \partial_{n_x} u, v\rangle_{L^2(\Sigma)} \tag{3.16}$$

for all $v \in C_0^\infty(\overline{\Omega} \times [0,T))$. All the terms are continuous with respect to v in the $H^{1,1/2}_{;,0}(Q)$-norm. Hence we can extend (3.16) by continuity to $v \in H^{1,1/2}_{;,0}(Q)$. Whereas for a fixed function $v \in H^{1,1/2}_{;,0}(Q)$ all the terms are continuous with respect to u in the $H^{1,1/2}_{;0,}(Q,\mathcal{L})$-norm. Hence, by applying Lemma 3.6, we can extend (3.16) to $u \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ which concludes the proof. □

Note that Green's first identity remains valid for $u \in H^{1,1/2}_{;0,}(Q)$ with $\mathcal{L}u \in [H^{1,1/2}_{;,0}(Q)]'$ and $v \in H^{1,1/2}_{;,0}(Q)$, see the definiton of the Neumann trace in Section 3.3. The L^2 scalar product $\langle \mathcal{L}u, v\rangle_{L^2(Q)}$ in Theorem 3.9 is then extended to the duality product $\langle \mathcal{L}u, v\rangle_Q$.

Theorem 3.10 (Green's second identity)**.** *For $u \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ and $v \in H^{1,1/2}_{;,0}(Q,\mathcal{L}')$ there holds*

$$\langle \mathcal{L}u, v\rangle_{L^2(Q)} - \langle u, \mathcal{L}'v\rangle_{L^2(Q)} = -\langle \gamma_1^{int} u, \gamma_0^{int} v\rangle_\Sigma + \langle \gamma_0^{int} u, \gamma_1^{int} v\rangle_\Sigma. \tag{3.17}$$

Proof. For $u \in C_0^\infty(\overline{\Omega} \times (0,T])$ and $v \in C_0^\infty(\overline{\Omega} \times [0,T))$ we have

$$\langle \mathcal{L}u, v\rangle_{L^2(Q)} - \langle u, \mathcal{L}'v\rangle_{L^2(Q)} = -\langle \gamma_1^{\text{int}} u, \gamma_0^{\text{int}} v\rangle_{L^2(\Sigma)} + \langle \gamma_0^{\text{int}} u, \gamma_1^{\text{int}} v\rangle_{L^2(\Sigma)}.$$

Similar as in the proof of Theorem 3.9 we can extend this formula to $u \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ and $v \in H^{1,1/2}_{;,0}(Q,\mathcal{L}')$ by applying Lemma 3.6 and Corollary 3.7. □

Again, Green's second identity remains valid for $u \in H^{1,1/2}_{;0,}(Q)$ with $\mathcal{L}u \in [H^{1,1/2}_{;,0}(Q)]'$ and $v \in H^{1,1/2}_{;,0}(Q)$ with $\mathcal{L}'v \in [H^{1,1/2}_{;0,}(Q)]'$. The L^2 scalar products $\langle \mathcal{L}u, v\rangle_{L^2(Q)}$ and $\langle u, \mathcal{L}'v\rangle_{L^2(Q)}$ in Theorem 3.10 are then extended to the duality products $\langle \mathcal{L}u, v\rangle_Q$ and $\langle u, \mathcal{L}'v\rangle_Q$, respectively.

3.5 Non-Homogeneous Initial Datum

The following analysis in the case of a given initial datum and homogeneous Dirichlet boundary conditions is based on [72, Chapter 23] and [12]. In this section we only recall the main results. Let $u_0 \in L^2(\Omega)$ be given. We consider the initial Dirichlet boundary value problem

$$\begin{aligned} \alpha \partial_t u(x,t) - \Delta_x u(x,t) &= 0 && \text{for } (x,t) \in Q, \\ u(x,t) &= 0 && \text{for } (x,t) \in \Sigma, \\ u(x,0) &= u_0(x) && \text{for } x \in \Omega. \end{aligned} \tag{3.18}$$

The analysis of problem (3.18) is done in the space $\mathcal{V}_0(Q)$ defined as [72]

$$\mathcal{V}_0(Q) := L^2(0,T;H_0^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega)).$$

The norm of a function $u \in \mathcal{V}_0(Q)$ is given by

$$\|u\|^2_{\mathcal{V}_0(Q)} := \|u\|^2_{L^2(0,T;H_0^1(\Omega))} + \|\alpha \partial_t u\|^2_{L^2(0,T;H^{-1}(\Omega))},$$

where

$$\|u\|_{L^2(0,T;H_0^1(\Omega))} := \|\nabla_x u\|_{L^2(Q)}$$

and

$$\|\alpha \partial_t u\|_{L^2(0,T;H^{-1}(\Omega))} := \sup_{0 \neq v \in L^2(0,T;H_0^1(\Omega))} \frac{\langle \alpha \partial_t u, v \rangle_Q}{\|v\|_{L^2(0,T;H_0^1(\Omega))}}.$$

Here, $\langle \cdot, \cdot \rangle_Q$ denotes the duality pairing on $L^2(0,T;H^{-1}(\Omega)) \times L^2(0,T;H_0^1(\Omega))$ as extension of the inner product in $L^2(Q)$. Analogously we define the space $\mathcal{V}(Q)$ of functions with non-homogeneous Dirichlet boundary conditions, i.e.

$$\mathcal{V}(Q) := L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))$$

with norm

$$\|u\|^2_{\mathcal{V}(Q)} := \|u\|^2_{L^2(Q)} + \|u\|^2_{\mathcal{V}_0(Q)}.$$

Theorem 3.11 ([72, Theorem 23.A])**.** *For a given initial datum $u_0 \in L^2(\Omega)$ there exists a unique solution $u \in \mathcal{V}_0(Q)$ of problem* (3.18) *satisfying the stability estimate*

$$\|u\|_{\mathcal{V}_0(Q)} \le c_I \|u_0\|_{L^2(\Omega)}.$$

The spaces $\mathcal{V}(Q)$ and $\mathcal{V}_0(Q)$ are dense subspaces of $H^{1,1/2}(Q)$ and $H^{1,1/2}_{0;,}(Q)$, respectively [10, 34]. Moreover, the following norm equivalence holds.

Lemma 3.12. *For $u \in \mathcal{V}(Q)$ with $\mathcal{L}u = 0$ in Q the norms of $\mathcal{V}(Q)$ and $H^{1,1/2}(Q)$ are equivalent, i.e. there exist constants $c_1, c_2 > 0$ such that*

$$\|u\|_{\mathcal{V}(Q)} \le c_1 \|u\|_{H^{1,1/2}(Q)} \le c_2 \|u\|_{\mathcal{V}(Q)}.$$

Proof. Follows the lines of [10, Lemma 2.15]. □

Additionally, if $u \in \mathcal{V}_0(Q)$, i.e. u vanishes on the boundary Σ, we immediately conclude that there exist constants $\tilde{c}_1, \tilde{c}_2 > 0$ such that

$$\|u\|_{\mathcal{V}_0(Q)} \leq \tilde{c}_1 \|u\|_{H^{1,1/2}_{0;,}(Q)} \leq \tilde{c}_2 \|u\|_{\mathcal{V}_0(Q)} \,. \tag{3.19}$$

This follows by using the Poincaré inequality and Lemma 3.12.

An important property of functions $u \in \mathcal{V}(Q)$ is the continuity in time [72], i.e. we have

$$u \in C([0,T]; L^2(\Omega)). \tag{3.20}$$

Hence the initial trace $\tau_0 u := u_{|t=0} \in L^2(\Omega)$ of the solution u of problem (3.18) is well defined.

The unique solution $u \in H^{1,1/2}(Q)$ of the fully non-homogeneous initial boundary value problem (1.1) with Dirichlet boundary conditions $u_{|\Sigma} = g$ is then given as $u = \bar{u}_g + \bar{u}_0$, where $\bar{u}_g \in H^{1,1/2}_{;0,}(Q)$ is the unique solution of problem (3.1) with homogeneous initial conditions and $\bar{u}_0 \in \mathcal{V}_0(Q)$ is the unique solution of problem (3.18). By applying the stability estimate of Theorem 3.2, the Poincaré inequality, estimate (3.19), and Theorem 3.11, we obtain the following stability estimate for the solution $u \in H^{1,1/2}(Q)$,

$$\|u\|_{H^{1,1/2}(Q)} \leq c_R \|f\|_{[H^{1,1/2}_{0;,0}(Q)]'} + c_B \|g\|_{H^{1/2,1/4}(\Sigma)} + c \|u_0\|_{L^2(\Omega)} \,.$$

The initial trace of solutions $u \in H^{1,1/2}(Q)$ of problem (1.1) with Dirichlet boundary conditions is well defined due to the decomposition $u = \bar{u}_g + \bar{u}_0$ with $\bar{u}_g \in H^{1,1/2}_{;0,}(Q)$ and $\bar{u}_0 \in \mathcal{V}_0(Q)$. We set $\tau_0 u := \tau_0 \bar{u}_0 \in L^2(\Omega)$ according to (3.20).

4 BOUNDARY INTEGRAL OPERATORS

In order to express the solution of the initial boundary value problem (1.1) by means of heat potentials as in (1.2), the existence of a fundamental solution is essential. In Section 4.1 we derive the fundamental solution of the heat equation and the related representation formula. In Sections 4.2 - 4.7 we introduce and analyze the heat potentials as well as the resulting (boundary) integral operators. The presented analysis is based on [12].

4.1 Representation Formula for the Heat Equation

In the following section we derive the representation formula (1.2) for the heat equation. Therefore, we consider Green's second identity (3.15) for $u \in C^2(\overline{Q})$. We want the fourth integral on the right hand side to be zero, i.e. we search for a function v which is a solution of the adjoint homogeneous heat equation

$$-\alpha\partial_\tau v(y,\tau) - \Delta_y v(y,\tau) = 0 \quad \text{for } (y,\tau) \in Q.$$

Since we want to find a representation of the solution $u = u(x,t)$ of the model problem (1.1), we define v as

$$v(y,\tau) := U(y-x, t-\tau),$$

where $(x,t) \in Q$ is fixed. In this case we have

$$\partial_\tau v(y,\tau) = \partial_\tau U(y-x,t-\tau) = -\partial_\theta U(y-x,\theta),$$

where $\theta = t - \tau$. Thus

$$\alpha\partial_\theta U(y-x,\theta) - \Delta_y U(y-x,\theta) = 0 \quad \text{for } (y,\theta) \in Q.$$

We assume the function U to be spherically symmetric, i.e. $U(y-x,\theta) = \widetilde{U}(r,\theta)$ with $r = |y-x|$. For $r \neq 0$ we get

$$\alpha\partial_\theta \widetilde{U}(r,\theta) - \partial_{rr}\widetilde{U}(r,\theta) - (n-1)\frac{1}{r}\partial_r \widetilde{U}(r,\theta) = 0. \tag{4.1}$$

With

$$\widetilde{U}(r,\theta) = \theta^\gamma g(z), \quad z = \frac{r}{\sqrt{\theta}}, \quad \gamma \in \mathbb{R}, \quad \theta = t - \tau > 0, \quad \tau < t,$$

we get

$$\begin{aligned}
\partial_\theta \widetilde{U}(r,\theta) &= \gamma\theta^{\gamma-1}g(z) - \frac{1}{2}\theta^{\gamma-1}zg'(z), \\
\partial_r \widetilde{U}(r,\theta) &= g'(z)\theta^{\gamma-\frac{1}{2}}, \\
\partial_{rr}\widetilde{U}(r,\theta) &= g''(z)\theta^{\gamma-1},
\end{aligned}$$

and therefore equation (4.1) becomes

$$\alpha\left[\gamma\theta^{\gamma-1}g(z)-\frac{1}{2}\theta^{\gamma-1}zg'(z)\right]-g''(z)\theta^{\gamma-1}-(n-1)\frac{1}{r}g'(z)\theta^{\gamma-\frac{1}{2}}=0,$$

which is equivalent to

$$\alpha\left[\gamma g(z)-\frac{1}{2}zg'(z)\right]-g''(z)-(n-1)\frac{1}{z}g'(z)=0. \tag{4.2}$$

It remains to solve this ordinary differential equation. First, we consider the one-dimensional case $n=1$, i.e. we have

$$\alpha\gamma g(z)-\alpha\frac{1}{2}zg'(z)-g''(z)=0$$

which can be written as

$$\alpha\left[\gamma+\frac{1}{2}\right]g(z)-\frac{\mathrm{d}}{\mathrm{d}z}\left[\alpha\frac{1}{2}zg(z)+g'(z)\right]=0.$$

By choosing $\gamma=-\frac{1}{2}$ we get

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[\alpha\frac{1}{2}zg(z)+g'(z)\right]=0,$$

and hence

$$\alpha\frac{1}{2}zg(z)+g'(z)=c_0\in\mathbb{R}$$

follows. In particular for $c_0=0$ and by using separation of variables we obtain

$$\ln g=-\alpha\frac{1}{4}z^2+c_1,\quad c_1\in\mathbb{R},$$

and for $c_1=0$ we conclude

$$g(z)=\exp\left(-\frac{\alpha}{4}z^2\right) \tag{4.3}$$

which is a solution of the differential equation (4.2) for $n=1$. Inserting (4.3) into (4.2) for general n yields

$$\begin{aligned}0&=\alpha\left[\gamma\exp\left(-\frac{\alpha}{4}z^2\right)+\frac{\alpha}{4}z^2\exp\left(-\frac{\alpha}{4}z^2\right)\right]+\frac{\alpha}{2}\exp\left(-\frac{\alpha}{4}z^2\right)\\&\quad-\frac{\alpha^2}{4}z^2\exp\left(-\frac{\alpha}{4}z^2\right)+(n-1)\frac{\alpha}{2}\exp\left(-\frac{\alpha}{4}z^2\right)\\&=\exp\left(-\frac{\alpha}{4}z^2\right)\alpha\left[\gamma+\frac{n}{2}\right].\end{aligned}$$

Thus, (4.3) is also a solution in the two- and three-dimensional case if $\gamma = -\frac{n}{2}$. Using the definitions of the functions U and $\widetilde{U}$ leads to

$$U(y-x,t-\tau) = (t-\tau)^{-n/2} \exp\left(-\frac{\alpha|y-x|^2}{4(t-\tau)}\right) \quad \text{for } \tau < t.$$

Due to the singularity of the function U at $(x,t) = (y,\tau)$ we consider the space–time-cylinder $Q_{t-\varepsilon} := \Omega \times (0, t-\varepsilon)$ with $0 < \varepsilon < t$. Analogously to (3.15) we get

$$\begin{aligned}
\alpha \int_\Omega u(y,t-\varepsilon)v(y,t-\varepsilon)\,\mathrm{d}y &= \alpha \int_\Omega u(y,0)v(y,0)\,\mathrm{d}y \\
&+ \int_0^{t-\varepsilon}\int_\Omega \Big[\alpha\partial_\tau u(y,\tau) - \Delta_y u(y,\tau)\Big] v(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau + \int_0^{t-\varepsilon}\int_\Gamma \partial_{n_y} u(y,\tau)v(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau \\
&- \int_0^{t-\varepsilon}\int_\Omega \Big[-\alpha\partial_\tau v(y,\tau) - \Delta_y v(y,\tau)\Big] u(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau - \int_0^{t-\varepsilon}\int_\Gamma \partial_{n_y} v(y,\tau)u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau.
\end{aligned}$$

With $v(y,\tau) = U(y-x,t-\tau)$ we now obtain

$$\begin{aligned}
\alpha \int_\Omega u(y,t-\varepsilon)U(y-x,\varepsilon)\,\mathrm{d}y &= \alpha \int_\Omega u(y,0)U(y-x,t)\,\mathrm{d}y \\
&+ \int_0^{t-\varepsilon}\int_\Omega \Big[\alpha\partial_\tau u(y,\tau) - \Delta_y u(y,\tau)\Big] U(y-x,t-\tau)\,\mathrm{d}y\,\mathrm{d}\tau \\
&+ \int_0^{t-\varepsilon}\int_\Gamma \partial_{n_y} u(y,\tau)U(y-x,t-\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau - \int_0^{t-\varepsilon}\int_\Gamma \partial_{n_y} U(y-x,t-\tau)u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau.
\end{aligned} \tag{4.4}$$

Let us consider the integral on the left hand side, i.e.

$$\alpha \int_\Omega u(y,t-\varepsilon)U(y-x,\varepsilon)\,\mathrm{d}y = \alpha \int_\Omega \varepsilon^{-n/2} u(y,t-\varepsilon) \exp\left(-\frac{\alpha|y-x|^2}{4\varepsilon}\right)\mathrm{d}y.$$

By using the Taylor expansion

$$u(y,t-\varepsilon) = u(x,t) + (y-x)^\top \nabla_x u(\xi_x,\xi_t) - \varepsilon\partial_t u(\xi_x,\xi_t)$$

with

$$\begin{pmatrix}\xi_x \\ \xi_t\end{pmatrix} = \begin{pmatrix} x+\sigma(y-x) \\ t-\sigma\varepsilon\end{pmatrix}, \quad \sigma \in (0,1),$$

we get

$$\begin{aligned}\frac{\alpha}{\varepsilon^{n/2}}\int_{\Omega} u(y,t-\varepsilon)\exp\left(-\frac{\alpha|y-x|^2}{4\varepsilon}\right)\mathrm{d}y &= u(x,t)\frac{\alpha}{\varepsilon^{n/2}}\int_{\Omega}\exp\left(-\frac{\alpha|y-x|^2}{4\varepsilon}\right)\mathrm{d}y \\ &+\frac{\alpha}{\varepsilon^{n/2}}\int_{\Omega}(y-x)^T\nabla_x u(\xi_x,\xi_t)\exp\left(-\frac{\alpha|y-x|^2}{4\varepsilon}\right)\mathrm{d}y \\ &-\frac{\alpha}{\varepsilon^{n/2-1}}\int_{\Omega}\partial_t u(\xi_x,\xi_t)\exp\left(-\frac{\alpha|y-x|^2}{4\varepsilon}\right)\mathrm{d}y.\end{aligned} \tag{4.5}$$

Next we show the convergence of the first integral on the right hand side. First, we consider the spatially one-dimensional case $n=1$, i.e. $\Omega=(a,b)$ with $a,b\in\mathbb{R}$ and $x\in(a,b)$. We have

$$\begin{aligned}A_\varepsilon &:= \frac{\alpha}{\varepsilon^{1/2}}\int_a^b \exp\left(-\frac{\alpha(y-x)^2}{4\varepsilon}\right)\mathrm{d}y \\ &= \frac{\alpha}{\varepsilon^{1/2}}\int_a^x \exp\left(-\frac{\alpha(y-x)^2}{4\varepsilon}\right)\mathrm{d}y+\frac{\alpha}{\varepsilon^{1/2}}\int_x^b \exp\left(-\frac{\alpha(y-x)^2}{4\varepsilon}\right)\mathrm{d}y.\end{aligned}$$

By using the substitution $z=\frac{x-y}{x-a}$ for the first integral and $z=\frac{y-x}{b-x}$ for the second one we get

$$\begin{aligned}A_\varepsilon &= \frac{\alpha}{\varepsilon^{1/2}}(x-a)\int_0^1 \exp\left(-\frac{\alpha(x-a)^2z^2}{4\varepsilon}\right)\mathrm{d}z \\ &\quad+\frac{\alpha}{\varepsilon^{1/2}}(b-x)\int_0^1 \exp\left(-\frac{\alpha(b-x)^2z^2}{4\varepsilon}\right)\mathrm{d}z.\end{aligned}$$

The substitution $\frac{\alpha(x-a)^2z^2}{4\varepsilon}=\eta^2$ for the first and $\frac{\alpha(b-x)^2z^2}{4\varepsilon}=\eta^2$ for the second integral leads to

$$A_\varepsilon = 2\sqrt{\alpha}\int_0^{\frac{(x-a)}{2}\sqrt{\frac{\alpha}{\varepsilon}}}\exp\left(-\eta^2\right)\mathrm{d}\eta+2\sqrt{\alpha}\int_0^{\frac{(b-x)}{2}\sqrt{\frac{\alpha}{\varepsilon}}}\exp\left(-\eta^2\right)\mathrm{d}\eta,$$

and we finally obtain

$$\lim_{\varepsilon\to 0}A_\varepsilon = 4\sqrt{\alpha}\int_0^\infty \exp\left(-\eta^2\right)\mathrm{d}\eta = 2\sqrt{\alpha\pi}.$$

In the two-dimensional case we choose $R>0$ such that $B_R(x)\subset\Omega$ and consider

$$A_\varepsilon := \frac{\alpha}{\varepsilon}\int_{B_R(x)}\exp\left(-\frac{\alpha|y-x|^2}{4\varepsilon}\right)\mathrm{d}y.$$

The integral over $\Omega \setminus B_R(x)$ vanishes as $\varepsilon \to 0$, since

$$\frac{\alpha}{\varepsilon} \exp\left(-\frac{\alpha|y-x|^2}{4\varepsilon}\right) \xrightarrow{\varepsilon\to 0} 0 \quad \text{for } y \neq x.$$

By using polar coordinates we get

$$\begin{aligned} A_\varepsilon &= \frac{\alpha}{\varepsilon} \int_0^R \int_0^{2\pi} \exp\left(-\frac{\alpha r^2}{4\varepsilon}\right) r \,\mathrm{d}\varphi \,\mathrm{d}r = \frac{2\pi\alpha}{\varepsilon} \int_0^R \exp\left(-\frac{\alpha r^2}{4\varepsilon}\right) r \,\mathrm{d}r \\ &= 4\pi \left[1 - \exp\left(-\frac{\alpha R^2}{4\varepsilon}\right)\right] \xrightarrow{\varepsilon\to 0} 4\pi. \end{aligned}$$

In the three-dimensional case we also choose $R > 0$ such that $B_R(x) \subset \Omega$ and consider

$$A_\varepsilon := \frac{\alpha}{\varepsilon^{3/2}} \int_{B_R(x)} \exp\left(-\frac{\alpha|y-x|^2}{4\varepsilon}\right) \mathrm{d}y.$$

As in the two-dimensional case the integral over $\Omega \setminus B_R(x)$ vanishes. By using spherical coordinates we obtain

$$\begin{aligned} A_\varepsilon &= \frac{\alpha}{\varepsilon^{3/2}} \int_0^R \int_0^{2\pi} \int_0^{\pi} \exp\left(-\frac{\alpha r^2}{4\varepsilon}\right) r^2 \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\varphi \,\mathrm{d}r \\ &= \frac{4\pi\alpha}{\varepsilon^{3/2}} \int_0^R \exp\left(-\frac{\alpha r^2}{4\varepsilon}\right) r^2 \,\mathrm{d}r. \end{aligned}$$

The substitution $\eta^2 = \frac{\alpha r^2}{4\varepsilon}$ leads to

$$A_\varepsilon = \frac{32\pi}{\sqrt{\alpha}} \int_0^{\sqrt{\frac{\alpha}{4\varepsilon}}R} \exp\left(-\eta^2\right) \eta^2 \,\mathrm{d}\eta \xrightarrow{\varepsilon\to 0} \frac{32\pi}{\sqrt{\alpha}} \int_0^\infty \exp\left(-\eta^2\right) \eta^2 \,\mathrm{d}\eta = \frac{8\pi^{3/2}}{\sqrt{\alpha}}.$$

The other two integrals in (4.5) vanish as $\varepsilon \to 0$ due to the boundedness of $\nabla_x u$ and $\partial_t u$. We finally get the representation formula by taking the limit $\varepsilon \to 0$ in (4.4), i.e. we have

$$\begin{aligned} u(x,t) &= \int_\Omega u(y,0) U^\star(x-y,t) \,\mathrm{d}y + \frac{1}{\alpha} \int_Q (\mathcal{L}u)(y,\tau) U^\star(x-y,t-\tau) \,\mathrm{d}y \,\mathrm{d}\tau \\ &\quad + \frac{1}{\alpha} \int_\Sigma \partial_{n_y} u(y,\tau) U^\star(x-y,t-\tau) \,\mathrm{d}s_y \,\mathrm{d}\tau \\ &\quad - \frac{1}{\alpha} \int_\Sigma u(y,\tau) \partial_{n_y} U^\star(x-y,t-\tau) \,\mathrm{d}s_y \,\mathrm{d}\tau, \end{aligned}$$

where

$$U^\star(x-y,t-\tau) = \left(\frac{\alpha}{4\pi(t-\tau)}\right)^{n/2} \exp\left(\frac{-\alpha|x-y|^2}{4(t-\tau)}\right) \quad \text{for } \tau < t.$$

The function

$$U^\star(x,t) = \begin{cases} \left(\frac{\alpha}{4\pi t}\right)^{n/2} \exp\left(\frac{-\alpha|x|^2}{4t}\right), & (x,t) \in \mathbb{R}^n \times (0,\infty), \\ 0\,, & \text{else}, \end{cases} \tag{4.6}$$

is called fundamental solution of the heat equation and due to construction, $U^\star$ is a solution of the homogeneous heat equation in $\mathbb{R}^n \times (0,\infty)$, see, e.g., [18], i.e.

$$[\alpha\partial_t - \Delta_x]U^\star(x,t) = 0 \quad \text{for } (x,t) \in \mathbb{R}^n \times (0,\infty).$$

Additionally, the fundamental solution has the following properties.

Lemma 4.1. *For $t > 0$ there holds*

$$\int\limits_{\mathbb{R}^n} U^\star(x,t)\,\mathrm{d}x = 1.$$

Proof. Let $t > 0$. Then

$$\begin{aligned} \int\limits_{\mathbb{R}^n} U^\star(x,t)\,\mathrm{d}x &= \left(\frac{\alpha}{4\pi t}\right)^{n/2} \int\limits_{\mathbb{R}^n} \exp\left(\frac{-\alpha|x|^2}{4t}\right)\mathrm{d}x = \pi^{-n/2} \int\limits_{\mathbb{R}^n} \exp\left(-|z|^2\right)\mathrm{d}z \\ &= \pi^{-n/2} \prod_{i=1}^{n} \int\limits_{\mathbb{R}} \exp\left(-z_i^2\right)\mathrm{d}z_i = 1. \end{aligned}$$

□

Lemma 4.2. *Let $u \in C(\Omega) \cap L^\infty(\Omega)$. For $x \in \Omega$ there holds*

$$\lim_{t\to 0} \int\limits_{\Omega} U^\star(x-y,t)u(y)\,\mathrm{d}y = u(x).$$

Proof. Let $\varepsilon > 0$ and $u \in C(\Omega) \cap L^\infty(\Omega)$. We define the function $\widetilde{u}$ as

$$\widetilde{u}(x) = \begin{cases} u(x) & \text{for } x \in \Omega, \\ 0 & \text{else.} \end{cases}$$

Moreover, let $(x,t) \in \Omega \times (0,\infty)$. Due to Lemma 4.1 and since $U^\star > 0$ on $\mathbb{R}^n \times (0,\infty)$, we have

$$\left| \int_\Omega U^\star(x-y,t)u(y)\,\mathrm{d}y - u(x) \right| = \left| \int_{\mathbb{R}^n} U^\star(x-y,t)[\widetilde{u}(y) - \widetilde{u}(x)]\,\mathrm{d}y \right|$$
$$\leq \int_{\mathbb{R}^n} U^\star(x-y,t)\,|\widetilde{u}(y) - \widetilde{u}(x)|\,\mathrm{d}y.$$

Since u ist continuous on Ω and since $x \in \Omega$, there exists a constant $\delta > 0$ such that $|\widetilde{u}(y) - \widetilde{u}(x)| < \varepsilon/2$ if $|y-x| < \delta$. Thus, we write the last integral as

$$\int_{\mathbb{R}^n} U^\star(x-y,t)\,|\widetilde{u}(y) - \widetilde{u}(x)|\,\mathrm{d}y = \int_{\mathbb{R}^n \setminus B_\delta(x)} U^\star(x-y,t)\,|\widetilde{u}(y) - \widetilde{u}(x)|\,\mathrm{d}y$$
$$+ \int_{B_\delta(x)} U^\star(x-y,t)\,|\widetilde{u}(y) - \widetilde{u}(x)|\,\mathrm{d}y.$$

The second integral can be estimated by

$$\int_{B_\delta(x)} U^\star(x-y,t)\underbrace{|\widetilde{u}(y) - \widetilde{u}(x)|}_{<\varepsilon/2}\,\mathrm{d}y < \frac{\varepsilon}{2}\int_{\mathbb{R}^n} U^\star(x-y,t)\,\mathrm{d}y = \frac{\varepsilon}{2}.$$

For the first integral we obtain, since $u \in L^\infty(\Omega)$,

$$\int_{\mathbb{R}^n \setminus B_\delta(x)} U^\star(x-y,t)\,|\widetilde{u}(y) - \widetilde{u}(x)|\,\mathrm{d}y \leq 2\,\|u\|_{L^\infty(\Omega)} \int_{\mathbb{R}^n \setminus B_\delta(x)} U^\star(x-y,t)\,\mathrm{d}y.$$

The substitution $z = x - y$ yields

$$\begin{aligned}\int_{\mathbb{R}^n \setminus B_\delta(x)} U^\star(x-y,t)\,\mathrm{d}y &= \int_{\mathbb{R}^n \setminus B_\delta(0)} U^\star(z,t)\,\mathrm{d}z \\ &= \left(\frac{\alpha}{4\pi t}\right)^{n/2} \int_{\mathbb{R}^n \setminus B_\delta(0)} \exp\left(\frac{-|z|^2\alpha}{4t}\right)\mathrm{d}z,\end{aligned}$$

and by using polar coordinates we get

$$\int_{\mathbb{R}^n \setminus B_\delta(x)} U^\star(x-y,t)\,\mathrm{d}y \leq Ct^{-n/2}\int_\delta^\infty r^{n-1}\exp\left(\frac{-r^2\alpha}{4t}\right)\mathrm{d}r$$
$$= C' \int_{at^{-1/2}}^\infty \rho^{n-1}\exp\left(-\rho^2\right)\mathrm{d}\rho$$

with suitable constants $C, C' > 0$ and $a = \delta\left(\frac{\alpha}{4}\right)^{1/2}$. The last integral vanishes as $t \to 0$, i.e. for t small enough there holds

$$\int\limits_{\mathbb{R}^n \setminus B_\delta(x)} U^\star(x-y,t)\,|\widetilde{u}(y) - \widetilde{u}(x)|\,\mathrm{d}y < \varepsilon/2.$$

Altogether we obtain

$$\left| \int\limits_\Omega U^\star(x-y,t)u(y)\,\mathrm{d}y - u(x) \right| < \varepsilon$$

for t small enough which concludes the proof. □

One can show that for sufficient regular data $f, \gamma_0^{\mathrm{int}} u, \gamma_1^{\mathrm{int}} u$ and u_0, the solution of the initial boundary value problem (1.1) is given by the representation formula, i.e. for $(x,t) \in Q$ we have

$$\begin{aligned} u(x,t) = &\int\limits_\Omega U^\star(x-y,t)u_0(y)\,\mathrm{d}y + \frac{1}{\alpha}\int\limits_Q U^\star(x-y,t-\tau)f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau \\ &+ \frac{1}{\alpha}\int\limits_\Sigma U^\star(x-y,t-\tau)\gamma_1^{\mathrm{int}} u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau \\ &- \frac{1}{\alpha}\int\limits_\Sigma \partial_{n_y} U^\star(x-y,t-\tau)\gamma_0^{\mathrm{int}} u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau. \end{aligned} \tag{4.7}$$

Due to the given representation (4.7) for the solution of problem (1.1) it suffices to determine, depending on the already given boundary conditions, the unknown Cauchy data to compute the solution in the space–time domain Q. This can be done by applying the trace operators to (4.7) and solving a related boundary integral equation on the space–time boundary Σ. The following sections are devoted to the analysis of the heat potentials in (4.7) and the resulting boundary integral operators.

4.2 Initial Potential

Let $u_0 \in L^2(\Omega)$. The function

$$(\widetilde{M}_0 u_0)(x,t) := \int\limits_\Omega U^\star(x-y,t)u_0(y)\,\mathrm{d}y \quad \text{for } (x,t) \in \mathbb{R}^n \times (0,T)$$

is called initial potential of the heat equation with initial condition u_0.

Lemma 4.3. *For $u_0 \in L^2(\Omega)$ the initial potential $\widetilde{M}_0 u_0$ satisfies the homogeneous heat equation, i.e.*

$$\left[\alpha\partial_t - \Delta_x\right](\widetilde{M}_0 u_0)(x,t) = 0 \quad \textit{for all } (x,t) \in \mathbb{R}^n \times (0,T).$$

Proof. For $(x,t) \in \mathbb{R}^n \times (0,T)$ there exists a compact neighbourhood O of (x,t) such that $O \subset \mathbb{R}^n \times (0,T)$. The restriction of $U^\star(x-y,t)$ to $(x,t) \in O$ and $y \in \Omega$ is bounded and differentiable on O for $y \in \Omega$. Moreover, $U^\star(x-\cdot,t)$ is integrable over Ω. The Leibniz integral rule then implies, that we can interchange differentiation and integration and we obtain

$$\big[\alpha\partial_t - \Delta_x\big](\widetilde{M}_0 u_0)(x,t) = \int\limits_{\Omega} \big[\alpha\partial_t - \Delta_x\big] U^\star(x-y,t) u_0(y)\,\mathrm{d}y.$$

The assertion now follows by using

$$\big[\alpha\partial_t - \Delta_x\big] U^\star(x-y,t) = 0$$

for $(x,t) \in \mathbb{R}^n \times (0,T)$ and $y \in \Omega$. □

Theorem 4.4. *The initial potential $\widetilde{M}_0 : L^2(\Omega) \to \mathcal{V}(Q) \subset H^{1,1/2}(Q)$ is linear and bounded, i.e. there exists a constant $c > 0$ such that*

$$\left\|\widetilde{M}_0 u_0\right\|_{\mathcal{V}(Q)} \le c\,\|u_0\|_{L^2(\Omega)} \quad \textit{for all } u_0 \in L^2(\Omega).$$

Proof. Follows the lines of the proof of [45, Lemma 7.10] with a restriction to the space $\mathcal{V}(Q)$ at the end. □

Due to Lemma 4.3 and the norm equivalence in Lemma 3.12 we conclude that there exists a constant $c_2^M > 0$ such that

$$\left\|\widetilde{M}_0 u_0\right\|_{H^{1,1/2}(Q)} \le c_2^M\,\|u_0\|_{L^2(\Omega)} \quad \text{for all } u_0 \in L^2(\Omega).$$

Lemma 4.3 additionally implies $\widetilde{M}_0 u_0 \in H^{1,1/2}(Q,\mathcal{L})$ for $u_0 \in L^2(\Omega)$. An important property of the initial potential is the continuity in time, i.e. due to (3.20) and Theorem 4.4 we have $\widetilde{M}_0 u_0 \in C([0,T];L^2(\Omega))$. Together with Lemma 4.2 this immediately implies $(\widetilde{M}_0 u_0)(x,0) = u_0(x)$ almost everywhere in Ω. Hence the initial potential satisfies the initial condition.

Due to the mapping properties of the trace operators and Lemma 4.3 we finally conclude that the integral operators

$$\begin{aligned} M_0 &:= \gamma_0^{\mathrm{int}} \widetilde{M}_0 : L^2(\Omega) \to H^{1/2,1/4}(\Sigma), \\ M_1 &:= \gamma_1^{\mathrm{int}} \widetilde{M}_0 : L^2(\Omega) \to H^{-1/2,-1/4}(\Sigma) \end{aligned}$$

are linear and bounded.

4.3 Newton Potential

The Newton potential for a given source term f defined in the space–time domain Q and $(x,t) \in \mathbb{R}^n \times (0,T)$ is defined as

$$(\widetilde{N}_0 f)(x,t) := \frac{1}{\alpha} \int\limits_0^t \int\limits_\Omega U^\star(x-y,t-\tau) f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau.$$

Lemma 4.5. *The function $u(x,t) = (\widetilde{N}_0 f)(x,t)$ for $(x,t) \in \mathbb{R}^n \times (0,T)$ is a generalized solution of the heat equation*

$$\left[\alpha\partial_t - \Delta_x\right] u(x,t) = \begin{cases} f(x,t), & \text{for } (x,t) \in Q, \\ 0, & \text{else.} \end{cases}$$

Proof. First, let $(x,t) \in \Omega \times (0,T)$. Then

$$\left[\alpha\partial_t - \Delta_x\right](\widetilde{N}_0 f)(x,t) = \left[\alpha\partial_t - \Delta_x\right] \left(\lim_{\varepsilon\to 0} \frac{1}{\alpha} \int\limits_0^{t-\varepsilon} \int\limits_\Omega U^\star(x-y,t-\tau) f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau \right).$$

For some fixed $\varepsilon > 0$ an application of the Leibniz integral rule yields

$$\begin{aligned}
&\left[\alpha\partial_t - \Delta_x\right] \frac{1}{\alpha} \int\limits_0^{t-\varepsilon} \int\limits_\Omega U^\star(x-y,t-\tau) f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau \\
&\quad = \int\limits_0^{t-\varepsilon} \int\limits_\Omega \partial_t U^\star(x-y,t-\tau) f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau + \int\limits_\Omega U^\star(x-y,\varepsilon) f(y,t-\varepsilon)\,\mathrm{d}y \\
&\qquad\quad - \frac{1}{\alpha} \int\limits_0^{t-\varepsilon} \int\limits_\Omega \Delta_x U^\star(x-y,t-\tau) f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau \\
&\quad = \frac{1}{\alpha} \int\limits_0^{t-\varepsilon} \int\limits_\Omega [\alpha\partial_t - \Delta_x] U^\star(x-y,t-\tau) f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau \\
&\qquad\quad + \int\limits_\Omega U^\star(x-y,\varepsilon) f(y,t-\varepsilon)\,\mathrm{d}y.
\end{aligned}$$

Since $U^\star(\cdot - y, \cdot - \tau)$ for $(y,\tau) \in \Omega \times (0,t-\varepsilon)$ is a solution of the homogeneous heat equation, the first integral on the right hand side vanishes. Additionally, Lemma 4.2 implies

$$\int\limits_\Omega U^\star(x-y,\varepsilon) f(y,t-\varepsilon)\,\mathrm{d}y \xrightarrow{\varepsilon\to 0} f(x,t).$$

Note that $[\alpha\partial_t - \Delta_x]u(x,t) = 0$ for $x \in \Omega^{\text{ext}} := \mathbb{R}^n \setminus \overline{\Omega}$ follows analogously by considering a ball $B_R \subset \mathbb{R}^n$ with radius $R > 0$ such that $\Omega \cup \{x\} \subset B_R$, and by choosing a zero extension of f in $B_R \setminus \Omega$. □

The following theorem is essential in order to derive the mapping properties of the Newton potential and subsequently of the single and double layer potentials in Sections 4.4 and 4.6. The theorem provides the mapping properties of the convolution with the fundamental solution of the heat equation, see [10, Section 3] and [50, 51].

Theorem 4.6. *The convolution with the fundamental solution $U^\star$*

$$A : \widetilde{H}^{r,r/2}_{\text{comp}}(\mathbb{R}^n \times (0,T)) \to \widetilde{H}^{r+2,r/2+1}_{\text{loc}}(\mathbb{R}^n \times (0,T))$$
$$f \mapsto U^\star * f$$

is linear and continuous for any $r \in \mathbb{R}$.

Here, $\widetilde{H}^{r,r/2}_{\text{comp}}(\mathbb{R}^n \times (0,T))$ denotes the space of functions with compact support in space, whereas the subscript ‘loc’ refers to the local behaviour in the spatial variables, see [10] for a definition of the anisotropic spaces in Theorem 4.6. Hence we immediately get the continuity of the Newton potential

$$\widetilde{N}_0 : [H^{1,1/2}_{;,0}(Q)]' \to \widetilde{H}^{1,1/2}_{\text{loc}}(\mathbb{R}^n \times (0,T)),$$

and by restriction we obtain the following mapping properties.

Theorem 4.7. *The Newton potential $\widetilde{N}_0 : [H^{1,1/2}_{;,0}(Q)]' \to H^{1,1/2}_{;0,}(Q)$ is linear and bounded, i.e. there exists a constant $c_2^N > 0$ such that*

$$\left\|\widetilde{N}_0 f\right\|_{H^{1,1/2}_{;0,}(Q)} \le c_2^N \|f\|_{[H^{1,1/2}_{;,0}(Q)]'} \quad \textit{for all } f \in [H^{1,1/2}_{;,0}(Q)]'.$$

Proof. Follows by applying Theorem 4.6 with $r = -1$ and by restriction to the space–time domain Q. □

The application of the interior Dirichlet trace operator to the Newton potential defines a linear bounded operator

$$N_0 := \gamma_0^{\text{int}} \widetilde{N}_0 : [H^{1,1/2}_{;,0}(Q)]' \to H^{1/2,1/4}(\Sigma)$$

satisfying

$$\|N_0 f\|_{H^{1/2,1/4}(\Sigma)} \le c_2^{N_0} \|f\|_{[H^{1,1/2}_{;,0}(Q)]'} \quad \text{for all } f \in [H^{1,1/2}_{;,0}(Q)]'$$

with some constant $c_2^{N_0} > 0$. Moreover, according to the definition of the Neumann trace in Section 3.3 and Lemma 4.5, the application of the Neumann trace operator yields the bounded operator

$$N_1 := \gamma_1^{\text{int}} \widetilde{N}_0 : [H^{1,1/2}_{;,0}(Q)]' \to H^{-1/2,-1/4}(\Sigma),$$

i.e. there exists a constant $c_2^{N_1} > 0$ such that

$$\|N_1 f\|_{H^{-1/2,-1/4}(\Sigma)} \le c_2^{N_1} \|f\|_{[H^{1,1/2}_{;,0}(Q)]'} \quad \text{for all } f \in [H^{1,1/2}_{;,0}(Q)]'.$$

4.4 Single Layer Potential

We introduce the single layer potential with density $w \in L^1(\Sigma)$ as

$$(\widetilde{V}w)(x,t) := \frac{1}{\alpha} \int_0^t \int_\Gamma U^\star(x-y,t-\tau) w(y,\tau) \,\mathrm{d}s_y \,\mathrm{d}\tau \quad \text{for } (x,t) \in \mathcal{D}_\Gamma, \tag{4.8}$$

where $\mathcal{D}_\Gamma := (\mathbb{R}^n \setminus \Gamma) \times (0,T)$. The fundamental solution $U^\star(x-\cdot,t-\cdot)$ is smooth on Σ for $(x,t) \in \mathcal{D}_\Gamma$, and thus, the single layer potential is well defined for $w \in L^1(\Sigma)$.

Theorem 4.8. *For $w \in L^1(\Sigma)$ the single layer potential $\widetilde{V}w$ satisfies the homogeneous heat equation, i.e.*

$$\big[\alpha\partial_t - \Delta_x\big](\widetilde{V}w)(x,t) = 0 \quad \textit{for all } (x,t) \in \mathcal{D}_\Gamma.$$

Proof. Let $(x,t) \in \mathcal{D}_\Gamma$. Then

$$\big[\alpha\partial_t - \Delta_x\big](\widetilde{V}w)(x,t) = \big[\alpha\partial_t - \Delta_x\big] \left(\lim_{\varepsilon \to 0} \frac{1}{\alpha} \int_0^{t-\varepsilon} \int_\Gamma U^\star(x-y,t-\tau) w(y,\tau) \,\mathrm{d}s_y \,\mathrm{d}\tau \right).$$

Since $(x,t) \in \mathcal{D}_\Gamma$, there exists a compact neighbourhood O of (x,t) such that $O \subset \mathcal{D}_\Gamma$, and thus, $\operatorname{dist}(O,\Sigma) > 0$. Therefore, the restriction of $U^\star(x-y,t-\tau)$ to $(x,t) \in O$ and $(y,\tau) \in \Sigma$ is bounded and differentiable on O for $(y,\tau) \in \Sigma$. Moreover, $U^\star$ is integrable over Σ for $(x,t) \in O$. Hence we can apply the Leibniz integral rule and get

$$\begin{aligned}\big[\alpha\partial_t - \Delta_x\big](\widetilde{V}w)(x,t) =& \frac{1}{\alpha} \int_0^t \int_\Gamma \big[\alpha\partial_t - \Delta_x\big] U^\star(x-y,t-\tau) w(y,\tau) \,\mathrm{d}s_y \,\mathrm{d}\tau \\ &+ \lim_{\varepsilon \to 0} \int_\Gamma U^\star(x-y,\varepsilon) w(y,t-\varepsilon) \,\mathrm{d}s_y.\end{aligned}$$

We then use $[\alpha\partial_t - \Delta_x]U^\star(x-y,t-\tau) = 0$ for $(x,t) \in \mathcal{D}_\Gamma$ and $(y,\tau) \in \Sigma$, and the dominated convergence theorem to conclude

$$\big[\alpha\partial_t - \Delta_x\big](\widetilde{V}w)(x,t) = \lim_{\varepsilon\to 0} \int_\Gamma U^\star(x-y,\varepsilon)w(y,t-\varepsilon)\,\mathrm{d}s_y = 0.$$

□

The explicit representation (4.8) of the operator $\widetilde{V}$ is only suited for $w \in L^1(\Sigma)$. However, the domain of the single layer potential can be extended by using the previously defined convolution operator A in Theorem 4.6. We define the linear and bounded operator

$$\gamma_0' : H^{-1/2,-1/4}(\Sigma) \to \widetilde{H}^{-1,-1/2}_{\mathrm{comp}}(\mathbb{R}^n \times (0,T))$$

by

$$\langle \gamma_0' w, v\rangle = \langle w, \gamma_0^{\mathrm{int}} v\rangle_\Sigma \quad \text{for all } v \in [\widetilde{H}^{-1,-1/2}_{\mathrm{comp}}(\mathbb{R}^n \times (0,T))]'.$$

The single layer potential is then given as

$$\widetilde{V} := A\gamma_0' : H^{-1/2,-1/4}(\Sigma) \to \widetilde{H}^{1,1/2}_{\mathrm{loc}}(\mathbb{R}^n \times (0,T)). \tag{4.9}$$

Since A and γ_0' are bounded, the single layer operator $\widetilde{V} : H^{-1/2,-1/4}(\Sigma) \to H^{1,1/2}_{;0,}(Q)$ is, by restriction, bounded as well, i.e. there exists a constant $c_2^{\widetilde{V}} > 0$ such that

$$\left\| \widetilde{V}w \right\|_{H^{1,1/2}_{;0,}(Q)} \le c_2^{\widetilde{V}} \|w\|_{H^{-1/2,-1/4}(\Sigma)} \quad \text{for all } w \in H^{-1/2,-1/4}(\Sigma).$$

Recall that due to construction the single layer potential is a solution of the homogeneous heat equation in $\mathcal{D}_\Gamma$, i.e. for $w \in H^{-1/2,-1/4}(\Sigma)$ we have

$$\big[\alpha\partial_t - \Delta_x\big]\widetilde{V}w = 0 \quad \text{in } \mathcal{D}_\Gamma.$$

Hence $\widetilde{V}w \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ for $w \in H^{-1/2,-1/4}(\Sigma)$ and therefore the Dirichlet trace as well as the Neumann trace of the single layer potential are well defined. In order to show the jump relations we proceed as follows. Let $B_R \subset \mathbb{R}^n$ be a ball with radius $R > 0$ such that $\Omega \subset B_R$ and set $\Omega^c := B_R \setminus \overline{\Omega}$. Moreover, $Q^c := \Omega^c \times (0,T)$. As before we obtain the continuity of the mapping

$$\widetilde{V} : H^{-1/2,-1/4}(\Sigma) \to H^{1,1/2}_{;0,}(Q^c,\mathcal{L}).$$

Thus, the Dirichlet and Neumann traces are defined from both sides of Σ. Let γ_0^{ext} and γ_1^{ext} denote the exterior Dirichlet trace operator and the exterior Neumann trace operator, respectively. Then the jumps on Σ are defined as

$$[\gamma_0 u] := \gamma_0^{\mathrm{ext}} u - \gamma_0^{\mathrm{int}} u,$$
$$[\gamma_1 u] := \gamma_1^{\mathrm{ext}} u - \gamma_1^{\mathrm{int}} u.$$

Theorem 4.9. *The single layer potential $\widetilde{V}w$ satisfies the jump relations*

$$\left[\gamma_0\widetilde{V}w\right] = 0, \quad \left[\gamma_1\widetilde{V}w\right] = -w, \quad \textit{for all } w \in H^{-1/2,-1/4}(\Sigma).$$

Proof. For a given density $w \in H^{-1/2,-1/4}(\Sigma)$ we have $u := \widetilde{V}w \in H^{1,1/2}_{;0,}(B_R \times (0,T))$ and therefore $\gamma_0^{\text{int}}u = \gamma_0^{\text{ext}}u$. Moreover, we have $[\alpha\partial_t - \Delta_x]u = 0$ in $Q \cup Q^c$. By using Green's second identity (3.17) with a test function $\varphi \in C_0^\infty(B_R \times [0,T))$ we obtain

$$\begin{aligned} -\langle u, [-\alpha\partial_t - \Delta_x]\varphi\rangle_{L^2(Q)} &= \langle \gamma_0^{\text{int}}u, \gamma_1^{\text{int}}\varphi\rangle_\Sigma - \langle \gamma_1^{\text{int}}u, \gamma_0^{\text{int}}\varphi\rangle_\Sigma, \\ -\langle u, [-\alpha\partial_t - \Delta_x]\varphi\rangle_{L^2(Q^c)} &= -\langle \gamma_0^{\text{ext}}u, \gamma_1^{\text{ext}}\varphi\rangle_\Sigma + \langle \gamma_1^{\text{ext}}u, \gamma_0^{\text{ext}}\varphi\rangle_\Sigma. \end{aligned}$$

Adding both equations and using $\gamma_0^{\text{int}}\varphi = \gamma_0^{\text{ext}}\varphi$ as well as $\gamma_1^{\text{int}}\varphi = \gamma_1^{\text{ext}}\varphi$ yields

$$-\langle u, [-\alpha\partial_t - \Delta_x]\varphi\rangle_{L^2(B_R\times(0,T))} = -\langle [\gamma_0 u], \gamma_1^{\text{int}}\varphi\rangle_\Sigma + \langle [\gamma_1 u], \gamma_0^{\text{int}}\varphi\rangle_\Sigma.$$

Since $[\gamma_0 u] = 0$, we conclude

$$-\langle u, [-\alpha\partial_t - \Delta_x]\varphi\rangle_{L^2(B_R\times(0,T))} = \langle [\gamma_1 u], \gamma_0^{\text{int}}\varphi\rangle_\Sigma. \tag{4.10}$$

From the representation (4.9) of the single layer potential $\widetilde{V}$ follows that [10]

$$[\alpha\partial_t - \Delta_x]\widetilde{V}w = [\alpha\partial_t - \Delta_x]A\gamma_0'w = \gamma_0'w$$

holds in $B_R \times (0,T)$ in the distributional sense. Hence we obtain

$$\begin{aligned} \langle u, [-\alpha\partial_t - \Delta_x]\varphi\rangle_{L^2(B_R\times(0,T))} &= \langle [\alpha\partial_t - \Delta_x]u, \varphi\rangle_{B_R\times(0,T)} \\ &= \langle [\alpha\partial_t - \Delta_x]\widetilde{V}w, \varphi\rangle_{B_R\times(0,T)} \\ &= \langle \gamma_0'w, \varphi\rangle_{B_R\times(0,T)} = \langle w, \gamma_0^{\text{int}}\varphi\rangle_\Sigma. \end{aligned}$$

In combination with (4.10) we get

$$\langle [\gamma_1\widetilde{V}w], \gamma_0^{\text{int}}\varphi\rangle_\Sigma = -\langle w, \gamma_0^{\text{int}}\varphi\rangle_\Sigma.$$

The assertion follows since $\gamma_0^{\text{int}}C_0^\infty(B_R \times [0,T))$ is dense in $H^{1/2,1/4}(\Sigma)$. □

The continuity of $\widetilde{V}$ and γ_0^{int} imply that the single layer boundary integral operator

$$V := \gamma_0^{\text{int}}\widetilde{V} : H^{-1/2,-1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma)$$

is linear and bounded, i.e. there exists a constant $c_2^V > 0$ such that

$$\|Vw\|_{H^{1/2,1/4}(\Sigma)} \le c_2^V \|w\|_{H^{-1/2,-1/4}(\Sigma)} \quad \text{for all } w \in H^{-1/2,-1/4}(\Sigma).$$

4.5 Adjoint Double Layer Potential

The adjoint double layer potential $K'w$ with density $w \in H^{-1/2,-1/4}(\Sigma)$ is defined as

$$K'w := \frac{1}{2}\left(\gamma_1^{\text{int}}\widetilde{V}w + \gamma_1^{\text{ext}}\widetilde{V}w\right).$$

Due to the boundedness of the single layer operator $\widetilde{V}$ and the Neumann trace operators, the operator $K' : H^{-1/2,-1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma)$ is bounded as well, i.e. there exists a constant $c_2^{K'} > 0$ such that

$$\left\|K'w\right\|_{H^{-1/2,-1/4}(\Sigma)} \leq c_2^{K'} \left\|w\right\|_{H^{-1/2,-1/4}(\Sigma)} \quad \text{for all } w \in H^{-1/2,-1/4}(\Sigma).$$

For a sufficiently smooth density w we have the representation

$$(K'w)(x,t) = \frac{1}{\alpha}\int_0^t \int_\Gamma \partial_{n_x} U^\star(x-y,t-\tau)w(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau$$

for $(x,t) \in \Sigma$ and Γ smooth in $x \in \Gamma$.

4.6 Double Layer Potential

We introduce the double layer potential with density $v \in L^1(\Sigma)$ as

$$(Wv)(x,t) := \frac{1}{\alpha}\int_0^t \int_\Gamma \partial_{n_y} U^\star(x-y,t-\tau)v(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau \quad \text{for } (x,t) \in \mathcal{D}_\Gamma. \tag{4.11}$$

The fundamental solution $U^\star(x-\cdot,t-\cdot)$ is smooth on Σ for $(x,t) \in \mathcal{D}_\Gamma$, and thus, the double layer potential potential is well defined for $v \in L^1(\Sigma)$.

Theorem 4.10. *For $v \in L^1(\Sigma)$ the double layer potential Wv satisfies the homogeneous heat equation, i.e.*

$$\left[\alpha\partial_t - \Delta_x\right](Wv)(x,t) = 0 \quad \textit{for all } (x,t) \in \mathcal{D}_\Gamma.$$

Proof. Let $(x,t) \in \mathcal{D}_\Gamma$. Then

$$\left[\alpha\partial_t - \Delta_x\right](Wv)(x,t) = \left[\alpha\partial_t - \Delta_x\right]\left(\lim_{\varepsilon\to 0}\frac{1}{\alpha}\int_0^{t-\varepsilon}\int_\Gamma \partial_{n_y} U^\star(x-y,t-\tau)v(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\right).$$

Since $(x,t) \in \mathcal{D}_\Gamma$, there exists a compact neighbourhood O of (x,t) such that $O \subset \mathcal{D}_\Gamma$, and thus, $\operatorname{dist}(O,\Sigma) > 0$. Therefore, the restriction of $\partial_{n_y} U^\star(x-y,t-s)$ to $(x,t) \in O$ and $(y,s) \in \Sigma$ is bounded and differentiable on O for $(y,s) \in \Sigma$. Moreover, $\partial_{n_y} U^\star$ is integrable over Σ for $(x,t) \in O$. Hence we can apply the Leibniz integral rule and additionally interchange the operators $\alpha\partial_t - \Delta_x$ and ∂_{n_y} under the integral sign to obtain

$$\begin{aligned}\big[\alpha\partial_t - \Delta_x\big](Wv)(x,t) = &\frac{1}{\alpha}\int_0^t \int_\Gamma \partial_{n_y}\big[\alpha\partial_t - \Delta_x\big]U^\star(x-y,t-\tau)v(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau \\ &+ \lim_{\varepsilon\to 0}\int_\Gamma \partial_{n_y} U^\star(x-y,\varepsilon)v(y,t-\varepsilon)\,\mathrm{d}s_y.\end{aligned}$$

We then use $[\alpha\partial_t - \Delta_x]U^\star(x-y,t-\tau) = 0$ for $(x,t) \in \mathcal{D}_\Gamma$ and $(y,\tau) \in \Sigma$ and the dominated convergence theorem to conclude

$$[\alpha\partial_t - \Delta_x](Wv)(x,t) = \lim_{\varepsilon\to 0}\int_\Gamma \partial_{n_y} U^\star(x-y,\varepsilon)v(y,t-\varepsilon)\,\mathrm{d}s_y = 0.$$

□

As in the case of the single layer potential $\widetilde{V}$, the representation (4.11) is only valid for $v \in L^1(\Sigma)$, and again, we can extend the domain of the double layer operator W by using the properties of the convolution operator A in Theorem 4.6. For $v \in H^{1/2,1/4}(\Sigma)$ we have the representation $Wv = A\gamma_1' v$. Here, $\gamma_1' v$ is the distribution defined by

$$\langle \gamma_1' v, \varphi\rangle = \langle v, \gamma_1^{\mathrm{int}}\varphi\rangle_\Sigma \quad \text{for all } \varphi \in C_0^\infty(\mathbb{R}^n \times \mathbb{R}).$$

The proof of the continuity of the operator

$$W : H^{1/2,1/4}(\Sigma) \to H^{1,1/2}_{;0,}(Q)$$

follows the lines of [10, Proposition 3.3]. We conclude that there exists a constant $c_2^W > 0$ such that

$$\|Wv\|_{H^{1,1/2}_{;0,}(Q)} \le c_2^W \|v\|_{H^{1/2,1/4}(\Sigma)} \quad \text{for all } v \in H^{1/2,1/4}(\Sigma).$$

The double layer potential Wv for $v \in H^{1/2,1/4}(\Sigma)$ is a solution of the homogeneous heat equation in $\mathcal{D}_\Gamma$, i.e. we have

$$[\alpha\partial_t - \Delta_x]Wv = 0 \quad \text{in } \mathcal{D}_\Gamma.$$

Hence $Wv \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ for $v \in H^{1/2,1/4}(\Sigma)$ and therefore the traces are well defined. Analogously as in the case of the single layer potential, see Section 4.4, we can define the interior and exterior Dirichlet and Neumann traces of Wv and obtain the following jump relations.

Theorem 4.11. *The double layer potential Wv satisfies the jump relations*

$$[\gamma_0 Wv] = v, \quad [\gamma_1 Wv] = 0, \quad \textit{for all } v \in H^{1/2,1/4}(\Sigma).$$

Proof. For a given density $v \in H^{1/2,1/4}(\Sigma)$ we define $u := Wv$ and thus, $[\alpha\partial_t - \Delta_x]u = 0$ in $Q \cup Q^c$. By using Green's second identity (3.17) with a test function $\varphi \in C_0^\infty(B_R \times [0,T))$ we get

$$-\langle u, [-\alpha\partial_t - \Delta_x]\varphi\rangle_{L^2(B_R\times(0,T))} = -\langle [\gamma_0 u], \gamma_1^{\text{int}}\varphi\rangle_\Sigma + \langle [\gamma_1 u], \gamma_0^{\text{int}}\varphi\rangle_\Sigma.$$

From the definition of the double layer potential W follows that [10]

$$[\alpha\partial_t - \Delta_x]Wv = \gamma_1' v$$

holds in $B_R \times (0,T)$ in the distributional sense. Hence we obtain

$$\begin{aligned}
\langle u, [-\alpha\partial_t - \Delta_x]\varphi\rangle_{L^2(B_R\times(0,T))} &= \langle [\alpha\partial_t - \Delta_x]u, \varphi\rangle_{B_R\times(0,T)} \\
&= \langle [\alpha\partial_t - \Delta_x]Wv, \varphi\rangle_{B_R\times(0,T)} \\
&= \langle \gamma_1' v, \varphi\rangle_{B_R\times(0,T)} = \langle v, \gamma_1^{\text{int}}\varphi\rangle_\Sigma
\end{aligned}$$

and conclude

$$\langle [\gamma_1 Wv], \gamma_0^{\text{int}}\varphi\rangle_\Sigma = \langle [\gamma_0 Wv] - v, \gamma_1^{\text{int}}\varphi\rangle_\Sigma. \tag{4.12}$$

Remark 3.1 then implies that each side in (4.12) has to be zero, i.e. $[\gamma_1 Wv] = 0$ and $[\gamma_0 Wv] = v$. □

The double layer boundary integral operator K for $v \in H^{1/2,1/4}(\Sigma)$ is defined as

$$Kv := \frac{1}{2}\left(\gamma_0^{\text{int}} Wv + \gamma_0^{\text{ext}} Wv\right).$$

Due to the boundedness of the double layer potential W and the Dirichlet trace operators, the operator $K : H^{1/2,1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma)$ is bounded as well, i.e. there exists a constant $c_2^K > 0$ such that

$$\|Kv\|_{H^{1/2,1/4}(\Sigma)} \le c_2^K \|v\|_{H^{1/2,1/4}(\Sigma)} \quad \text{for all } v \in H^{1/2,1/4}(\Sigma).$$

4.7 Hypersingular Boundary Integral Operator

The hypersingular operator D defined as

$$D := -\gamma_1^{\text{int}} W : H^{1/2,1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma)$$

is linear and bounded satisfying

$$\|Dv\|_{H^{-1/2,-1/4}(\Sigma)} \le c_2^D \, \|v\|_{H^{1/2,1/4}(\Sigma)} \quad \text{for all } v \in H^{1/2,1/4}(\Sigma)$$

with some constant $c_2^D > 0$. For a sufficiently smooth density v we have the representation

$$(Dv)(x,t) = -\frac{1}{\alpha}\gamma_{1,x}^{\mathrm{int}} \int\limits_0^t \int\limits_\Gamma \gamma_{1,y}^{\mathrm{int}} U^\star(x-y,t-\tau)v(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau$$

for $(x,t) \in \Sigma$. If we assume that the boundary Γ, for $n = 2,3$, is piecewise smooth, we can derive an alternative representation of the bilinear form which is induced by the hypersingular boundary integral operator D, i.e.

$$\langle Du, v\rangle_\Sigma = -\frac{1}{\alpha}\int\limits_\Sigma v(x,t)\gamma_{1,x}^{\mathrm{int}} \int\limits_\Sigma \gamma_{1,y}^{\mathrm{int}} U^\star(x-y,t-\tau)u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t.$$

In this case the bilinear form can be written by means of the single layer boundary integral operator V, i.e. we have weakly singular representations. For $n = 2$, see, e.g., [10, Theorem 6.1], we obtain

$$\begin{aligned}\langle Du,v\rangle_\Sigma = \frac{1}{\alpha}\int\limits_\Sigma \mathrm{curl}_\Gamma\, v(x,t) \int\limits_\Sigma U^\star(x-y,t-\tau)\mathrm{curl}_\Gamma\, u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t \\ -\int\limits_\Sigma \underline{n}^{\mathrm{T}}(x)\,v(x,t)\int\limits_\Sigma \partial_\tau U^\star(x-y,t-\tau)\underline{n}(y)\,u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t,\end{aligned} \tag{4.13}$$

where

$$\mathrm{curl}_\Gamma\, v(x,t) := n_1(x)\frac{\partial}{\partial x_2}v(x,t) - n_2(x)\frac{\partial}{\partial x_1}v(x,t) \quad \text{for } (x,t) \in \Sigma.$$

Whereas for $n = 3$ we have the representation [41, Theorem 2.1]

$$\begin{aligned}\langle Du,v\rangle_\Sigma = \frac{1}{\alpha}\int\limits_\Sigma \underline{\mathrm{curl}}_\Gamma^{\mathrm{T}}\, v(x,t) \int\limits_\Sigma U^\star(x-y,t-\tau)\underline{\mathrm{curl}}_\Gamma\, u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t \\ -\int\limits_\Sigma \underline{n}^{\mathrm{T}}(x)\,v(x,t)\int\limits_\Sigma \partial_\tau U^\star(x-y,t-\tau)\underline{n}(y)\,u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t,\end{aligned} \tag{4.14}$$

with $\underline{\mathrm{curl}}_\Gamma\, v(x,t) := \underline{n}(x) \times \nabla_x v(x,t)$ for $(x,t) \in \Sigma$.

5 BOUNDARY INTEGRAL EQUATIONS

In the following chapter we introduce the Calderón projection operator and deduce related properties of the boundary integral operators defined in the previous chapter, including the definition of the Steklov–Poincaré operator in Section 5.1. In Sections 5.2 - 5.3 we discuss the unique solvability of the model problem (1.1) with different types of boundary conditions by means of analyzing related boundary integral equations. The analysis of exterior boundary value problems and transmission problems is done in Section 5.4 and Section 5.5, respectively. The results in this chapter are mainly based on [10, 12].

The solution $u \in H^{1,1/2}(Q)$ of problem (1.1) with initial datum $u_0 \in L^2(\Omega)$ and source term $f \in [H^{1,1/2}_{;,0}(Q)]'$ is given by the representation formula for the heat equation, i.e. for $(x,t) \in Q$ we have

$$u(x,t) = (\widetilde{V}\gamma_1^{\text{int}}u)(x,t) - (W\gamma_0^{\text{int}}u)(x,t) + (\widetilde{M}_0 u_0)(x,t) + (\widetilde{N}_0 f)(x,t). \tag{5.1}$$

By applying the Dirichlet trace operator to (5.1) and by using the jump relations of the heat potentials we obtain the first boundary integral equation

$$\gamma_0^{\text{int}}u = V\gamma_1^{\text{int}}u + \frac{1}{2}\gamma_0^{\text{int}}u - K\gamma_0^{\text{int}}u + M_0 u_0 + N_0 f \quad \text{on } \Sigma.$$

The application of the Neumann trace operator to (5.1) yields the second boundary integral equation

$$\gamma_1^{\text{int}}u = \frac{1}{2}\gamma_1^{\text{int}}u + K'\gamma_1^{\text{int}}u + D\gamma_0^{\text{int}}u + M_1 u_0 + N_1 f \quad \text{on } \Sigma. \tag{5.2}$$

Together, these equations lead to the so-called Calderón system of boundary integral equations. We have

$$\begin{pmatrix} \gamma_0^{\text{int}}u \\ \gamma_1^{\text{int}}u \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{1}{2}I - K & V \\ D & \frac{1}{2}I + K' \end{pmatrix}}_{=:\,\mathcal{C}} \begin{pmatrix} \gamma_0^{\text{int}}u \\ \gamma_1^{\text{int}}u \end{pmatrix} + \begin{pmatrix} M_0 u_0 \\ M_1 u_0 \end{pmatrix} + \begin{pmatrix} N_0 f \\ N_1 f \end{pmatrix}. \tag{5.3}$$

The operator $\mathcal{C}$ is called the Calderón projection operator.

Lemma 5.1. *$\mathcal{C}$ is a projection, i.e. $\mathcal{C} = \mathcal{C}^2$.*

Proof. Let $(\psi, \varphi) \in H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$. Then the function

$$u := \widetilde{V}\psi - W\varphi$$

is a solution of the homogeneous heat equation. By applying the trace operators we get the boundary integral equations

$$\begin{aligned}\gamma_0^{\text{int}} u &= V\psi + (\frac{1}{2}I - K)\varphi, \\ \gamma_1^{\text{int}} u &= (\frac{1}{2}I + K')\psi + D\varphi.\end{aligned} \tag{5.4}$$

Additionally, u is a solution of the homogeneous heat equation with Cauchy data $\gamma_0^{\text{int}} u, \gamma_1^{\text{int}} u$ and inital condition $u_0 \equiv 0$, i.e. we have

$$\begin{pmatrix}\gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u\end{pmatrix} = \begin{pmatrix}\frac{1}{2}I - K & V \\ D & \frac{1}{2}I + K'\end{pmatrix}\begin{pmatrix}\gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u\end{pmatrix}.$$

Inserting (5.4) yields

$$\begin{pmatrix}\frac{1}{2}I - K & V \\ D & \frac{1}{2}I + K'\end{pmatrix}\begin{pmatrix}\psi \\ \varphi\end{pmatrix} = \begin{pmatrix}\frac{1}{2}I - K & V \\ D & \frac{1}{2}I + K'\end{pmatrix}^2\begin{pmatrix}\psi \\ \varphi\end{pmatrix}.$$

Since the functions ψ, φ were arbitrarily chosen, we conclude $\mathcal{C} = \mathcal{C}^2$. □

As a consequence of the projection property of the Calderón operator $\mathcal{C}$ we obtain the following relations.

Corollary 5.2. *The boundary integral operators satisfy*

$$\begin{aligned}VD &= \left(\frac{1}{2}I + K\right)\left(\frac{1}{2}I - K\right), \\ DV &= \left(\frac{1}{2}I + K'\right)\left(\frac{1}{2}I - K'\right), \\ VK' &= KV, \\ K'D &= DK.\end{aligned}$$

Proof. Follows from $\mathcal{C} = \mathcal{C}^2$. □

Now we state the main theorem of this chapter.

Theorem 5.3 ([10, Corollary 3.10, Theorem 3.11])**.** *The operator*

$$\mathcal{A} : H^{1/2,1/4}(\Sigma) \times H^{-1/2,-1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma) \times H^{-1/2,-1/4}(\Sigma)$$

defined as

$$\mathcal{A} := \begin{pmatrix}-K & V \\ D & K'\end{pmatrix}$$

is an isomorphism and there exists a constant $c_1 > 0$ *such that*

$$\left\langle \begin{pmatrix} \psi \\ \varphi \end{pmatrix}, \begin{pmatrix} V & -K \\ K' & D \end{pmatrix} \begin{pmatrix} \psi \\ \varphi \end{pmatrix} \right\rangle_{\Sigma\times\Sigma} \geq c_1 \left(\|\psi\|^2_{H^{-1/2,-1/4}(\Sigma)} + \|\varphi\|^2_{H^{1/2,1/4}(\Sigma)} \right)$$

for all $(\psi,\varphi) \in H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$.

The ellipticity of the operator in Theorem 5.3 then immediately implies the ellipticity of the single layer boundary integral operator V and the hypersingular operator D.

Lemma 5.4. *The single layer boundary integral operator V defines an isomorphism and there exists a constant* $c_1^V > 0$ *such that*

$$\langle Vw, w\rangle_\Sigma \geq c_1^V \|w\|^2_{H^{-1/2,-1/4}(\Sigma)} \quad \textit{for all } w \in H^{-1/2,-1/4}(\Sigma).$$

Proof. Follows from Theorem 5.3 with $\varphi = 0$. □

Lemma 5.5. *The hypersingular operator D defines an isomorphism and there exists a constant* $c_1^D > 0$ *such that*

$$\langle Dv, v\rangle_\Sigma \geq c_1^D \|v\|^2_{H^{1/2,1/4}(\Sigma)} \quad \textit{for all } v \in H^{1/2,1/4}(\Sigma).$$

Proof. Follows from Theorem 5.3 with $\psi = 0$. □

5.1 Steklov–Poincaré Operator

We consider the system of boundary integral equations (5.3) with source term $f \equiv 0$ and with homogeneous initial conditions, i.e. $u_0 \equiv 0$. Hence

$$\begin{pmatrix} \gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I - K & V \\ D & \frac{1}{2}I + K' \end{pmatrix} \begin{pmatrix} \gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u \end{pmatrix}.$$

By using the first integral equation we can define the Dirichlet to Neumann map

$$\gamma_1^{\text{int}} u = V^{-1}(\frac{1}{2}I + K)\gamma_0^{\text{int}} u. \tag{5.5}$$

The operator

$$S := V^{-1}(\frac{1}{2}I + K) : H^{1/2,1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma)$$

is called Steklov–Poincaré operator for the heat equation. Insertion of (5.5) into the second boundary integral equation yields

$$\gamma_1^{\text{int}} u = \left[D + (\frac{1}{2}I + K')V^{-1}(\frac{1}{2}I + K) \right] \gamma_0^{\text{int}} u.$$

Hence we get a *symmetric* representation of the Steklov–Poincaré operator, i.e.

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

Due to the boundedness of the operators K, K', D and V^{-1}, the operator S is bounded as well.

Lemma 5.6. *The Steklov–Poincaré operator S is elliptic, i.e. there exists a constant $c_1^S > 0$ such that*

$$\langle Sv, v\rangle_\Sigma \geq c_1^S \|v\|^2_{H^{1/2,1/4}(\Sigma)} \quad \textit{for all } v \in H^{1/2,1/4}(\Sigma).$$

Proof. For $v \in H^{1/2,1/4}(\Sigma)$ we define $\psi := V^{-1}\left(\frac{1}{2}I + K\right) v \in H^{-1/2,-1/4}(\Sigma)$ and get

$$\begin{aligned}
&\left\langle \begin{pmatrix} \psi \\ v \end{pmatrix}, \begin{pmatrix} V & -K \\ K' & D \end{pmatrix} \begin{pmatrix} \psi \\ v \end{pmatrix} \right\rangle_{\Sigma\times\Sigma} \\
&\quad = \frac{1}{2}\langle V^{-1}(\frac{1}{2}I + K)v, v\rangle_\Sigma + \langle v, K'V^{-1}(\frac{1}{2}I + K)v + Dv\rangle_\Sigma \\
&\quad = \langle v, (\frac{1}{2}I + K')V^{-1}(\frac{1}{2}I + K)v + Dv\rangle_\Sigma \\
&\quad = \langle v, Sv\rangle_\Sigma.
\end{aligned}$$

The assertion now follows by applying Theorem 5.3. □

5.2 Dirichlet Boundary Value Problem

We consider the initial boundary value problem (1.1) with Dirichlet boundary conditions $g \in H^{1/2,1/4}(\Sigma)$, source term $f \in [H^{1,1/2}_{;,0}(Q)]'$, and initial datum $u_0 \in L^2(\Omega)$, i.e.

$$\begin{aligned}
\alpha\partial_t u(x,t) - \Delta_x u(x,t) &= f(x,t) \qquad \text{for } (x,t) \in Q, \\
\gamma_0^{\text{int}} u(x,t) &= g(x,t) \qquad \text{for } (x,t) \in \Sigma, \\
u(x,0) &= u_0(x) \qquad \text{for } x \in \Omega.
\end{aligned} \tag{5.6}$$

The solution of (5.6) is given by the representation formula

$$u(x,t) = (\widetilde{V}\gamma_1^{\text{int}} u)(x,t) - (Wg)(x,t) + (\widetilde{M}_0 u_0)(x,t) + (\widetilde{N}_0 f)(x,t) \quad \text{for } (x,t) \in Q.$$

It remains to determine the unknown conormal derivative $\gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$. This can be done by solving the first boundary integral equation in (5.3). We have to find $\gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$ such that

$$V\gamma_1^{\text{int}} u = (\frac{1}{2}I + K)g - M_0 u_0 - N_0 f \quad \text{on } \Sigma.$$

The corresponding variational formulation is to find $\gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$ such that

$$\langle V\gamma_1^{\text{int}} u, \tau\rangle_\Sigma = \langle (\frac{1}{2}I + K)g - M_0 u_0 - N_0 f, \tau\rangle_\Sigma \quad \text{for all } \tau \in H^{-1/2,-1/4}(\Sigma). \tag{5.7}$$

Since the boundary integral operators K, M_0, N_0 and V are bounded and V is elliptic, there exists a unique solution $\gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$ according to the Lax–Milgram theorem [62, Theorem 3.4]. The solution $\gamma_1^{\text{int}} u$ then satisfies

$$\begin{aligned}\left\|\gamma_1^{\text{int}} u\right\|_{H^{-1/2,-1/4}(\Sigma)} &\le \frac{1}{c_1^V}\left\|(\frac{1}{2}I + K)g - M_0 u_0 - N_0 f\right\|_{H^{1/2,1/4}(\Sigma)}\\ &\le \frac{1}{c_1^V}\left(\tilde{c}_2^W \|g\|_{H^{1/2,1/4}(\Sigma)} + c_2^{M_0}\|u_0\|_{L^2(\Omega)} + c_2^{N_0}\|f\|_{[H^{1,1/2}_{;,0}(Q)]'}\right).\end{aligned}$$

Another approach is using an indirect formulation with the single layer potential $\widetilde{V}$. A solution of the heat equation with source term f and initial condition u_0 is given by

$$u(x,t) = (\widetilde{V}w)(x,t) + (\widetilde{M}_0 u_0)(x,t) + (\widetilde{N}_0 f)(x,t) \quad \text{for } (x,t) \in Q \tag{5.8}$$

with an unknown density $w \in H^{-1/2,-1/4}(\Sigma)$ to be determined. By applying the Dirichlet trace operator to (5.8) we obtain

$$g = Vw + M_0 u_0 + N_0 f \quad \text{on } \Sigma.$$

Thus, we have to find $w \in H^{-1/2,-1/4}(\Sigma)$ such that

$$Vw = g - M_0 u_0 - N_0 f \quad \text{on } \Sigma.$$

The corresponding variational formulation is to find $w \in H^{-1/2,-1/4}(\Sigma)$ such that

$$\langle Vw, \tau\rangle_\Sigma = \langle g - M_0 u_0 - N_0 f, \tau\rangle_\Sigma \quad \text{for all } \tau \in H^{-1/2,-1/4}(\Sigma). \tag{5.9}$$

As in the case of the direct formulation with the first boundary integral equation, the unique solvability follows with the Lax–Milgram theorem [62, Theorem 3.4].

5.3 Neumann Boundary Value Problem

In this section we consider the initial boundary value problem (1.1) with given Neumann boundary conditions $w \in H^{-1/2,-1/4}(\Sigma)$, source term $f \in [H^{1,1/2}_{;,0}(Q)]'$, and initial datum $u_0 \in L^2(\Omega)$, i.e.

$$\begin{aligned} \alpha\partial_t u(x,t) - \Delta_x u(x,t) &= f(x,t) && \text{for } (x,t) \in Q, \\ \gamma_1^{\text{int}} u(x,t) &= w(x,t) && \text{for } (x,t) \in \Sigma, \\ u(x,0) &= u_0(x) && \text{for } x \in \Omega. \end{aligned} \tag{5.10}$$

The solution of (5.10) is given by

$$u(x,t) = (\widetilde{V} w)(x,t) - (W\gamma_0^{\text{int}} u)(x,t) + (\widetilde{M}_0 u_0)(x,t) + (\widetilde{N}_0 f)(x,t) \quad \text{for } (x,t) \in Q.$$

It remains to determine the unknown Dirichlet datum $\gamma_0^{\text{int}} u \in H^{1/2,1/4}(\Sigma)$. This can be done by solving the second boundary integral equation in (5.3). We have to find $\gamma_0^{\text{int}} u \in H^{1/2,1/4}(\Sigma)$ such that

$$D\gamma_0^{\text{int}} u = (\frac{1}{2}I - K')w - M_1 u_0 - N_1 f \quad \text{on } \Sigma.$$

The corresponding variational formulation is to find $\gamma_0^{\text{int}} u \in H^{1/2,1/4}(\Sigma)$ such that

$$\langle D\gamma_0^{\text{int}} u, v\rangle_\Sigma = \langle (\frac{1}{2}I - K')w - M_1 u_0 - N_1 f, v\rangle_\Sigma \quad \text{for all } v \in H^{1/2,1/4}(\Sigma). \tag{5.11}$$

Since the boundary integral operators K', M_1, N_1 and D are bounded and D is elliptic, there exists a unique solution $\gamma_0^{\text{int}} u \in H^{1/2,1/4}(\Sigma)$ according to the Lax–Milgram theorem [62, Theorem 3.4]. The solution $\gamma_0^{\text{int}} u$ then satisfies

$$\begin{aligned} \left\|\gamma_0^{\text{int}} u\right\|_{H^{1/2,1/4}(\Sigma)} &\le \frac{1}{c_1^D}\left\|(\frac{1}{2}I - K')w - M_1 u_0 - N_1 f\right\|_{H^{-1/2,-1/4}(\Sigma)} \\ &\le \frac{1}{c_1^D}\left(\tilde{c}_2^{\widetilde{V}}\|w\|_{H^{-1/2,-1/4}(\Sigma)} + c_2^{M_1}\|u_0\|_{L^2(\Omega)} + c_2^{N_1}\|f\|_{[H^{1,1/2}_{;,0}(Q)]'}\right). \end{aligned}$$

Another approach is using an indirect formulation with the double layer potential W. A solution of the heat equation with source term f and initial condition u_0 is given by

$$u(x,t) = -(Wg)(x,t) + (\widetilde{M}_1 u_0)(x,t) + (\widetilde{M}_0 f)(x,t) \quad \text{for } (x,t) \in Q \tag{5.12}$$

with an unknown density $g \in H^{1/2,1/4}(\Sigma)$ to be determined. By applying the Neumann trace operator to (5.12) we obtain

$$w = Dg + M_1 u_0 + N_1 f \quad \text{on } \Sigma.$$

Thus, we have to find $g \in H^{1/2,1/4}(\Sigma)$ such that

$$Dg = w - M_1 u_0 - N_1 f \quad \text{on } \Sigma.$$

The corresponding variational formulation is to find $g \in H^{1/2,1/4}(\Sigma)$ such that

$$\langle Dg, v\rangle_\Sigma = \langle w - M_1 u_0 - N_1 f, v\rangle_\Sigma \quad \text{for all } v \in H^{1/2,1/4}(\Sigma). \tag{5.13}$$

Again, the unique solvability follows with the Lax–Milgram theorem [62, Theorem 3.4].

5.4 Exterior Boundary Value Problem

One advantage of boundary element methods is the natural handling of boundary value problems in the exterior domain $Q^{\text{ext}} := \Omega^{\text{ext}} \times (0,T)$ with $\Omega^{\text{ext}} := \mathbb{R}^n \setminus \overline{\Omega}$. We consider the exterior Dirichlet boundary value problem for the heat equation with Dirichlet datum $g \in H^{1/2,1/4}(\Sigma)$, source term $f \equiv 0$ and initial datum $u_0 \equiv 0$, i.e.

$$\begin{aligned} \alpha\partial_t u(x,t) - \Delta_x u(x,t) &= 0 && \text{for } (x,t) \in Q^{\text{ext}}, \\ \gamma_0^{\text{ext}} u(x,t) &= g(x,t) && \text{for } (x,t) \in \Sigma, \\ u(x,0) &= 0 && \text{for } x \in \Omega^{\text{ext}} \end{aligned} \tag{5.14}$$

together with an appropriate radiation condition.

Let $y_0 \in \Omega$ and $B_R(y_0)$ denote a ball with center y_0 and radius $R > 0$, satisfying $\Omega \subset B_R(y_0)$. Using the representation formula (4.7) for $x \in B_R(y_0) \setminus \overline{\Omega}$ and $t \in (0,T)$ yields

$$\begin{aligned} u(x,t) = &-\frac{1}{\alpha}\int\limits_\Sigma U^\star(x-y,t-\tau)\gamma_1^{\text{ext}} u(y,\tau)\mathrm{d}s_y\,\mathrm{d}\tau \\ &+\frac{1}{\alpha}\int\limits_\Sigma \gamma_{1,y}^{\text{ext}} U^\star(x-y,t-\tau)\gamma_0^{\text{ext}} u(y,\tau)\mathrm{d}s_y\,\mathrm{d}\tau \\ &+\frac{1}{\alpha}\int\limits_0^T\int\limits_{\partial B_R(y_0)} U^\star(x-y,t-\tau)\gamma_1^{\text{int}} u(y,\tau)\mathrm{d}s_y\,\mathrm{d}\tau \\ &-\frac{1}{\alpha}\int\limits_0^T\int\limits_{\partial B_R(y_0)} \gamma_{1,y}^{\text{int}} U^\star(x-y,t-\tau)\gamma_0^{\text{int}} u(y,\tau)\mathrm{d}s_y\,\mathrm{d}\tau. \end{aligned}$$

By taking the limit $R \to \infty$ and by using the radiation condition we obtain the representation formula for the exterior boundary value problem, i.e. for $(x,t) \in Q^{\text{ext}}$ we have

$$\begin{aligned} u(x,t) = &-\frac{1}{\alpha} \int\limits_{\Sigma} U^{\star}(x-y,t-\tau)\gamma_1^{\text{ext}} u(y,\tau) \mathrm{d}s_y \, \mathrm{d}\tau \\ &+ \frac{1}{\alpha} \int\limits_{\Sigma} \gamma_{1,y}^{\text{ext}} U^{\star}(x-y,t-\tau)\gamma_0^{\text{ext}} u(y,\tau) \mathrm{d}s_y \, \mathrm{d}\tau. \end{aligned} \tag{5.15}$$

To find the unknown Cauchy data we proceed as follows. The application of the exterior Dirichlet trace operator yields

$$\gamma_0^{\text{ext}} u = -V\gamma_1^{\text{ext}} u + \frac{1}{2}\gamma_0^{\text{ext}} u + K\gamma_0^{\text{ext}} u \quad \text{on } \Sigma,$$

while the application of the exterior Neumann trace operator leads to

$$\gamma_1^{\text{ext}} u = \frac{1}{2}\gamma_1^{\text{ext}} u - K'\gamma_1^{\text{ext}} u - D\gamma_0^{\text{ext}} u \quad \text{on } \Sigma.$$

Together, we obtain the Calderón system of boundary integral equations for the exterior problem, i.e.

$$\begin{pmatrix} \gamma_0^{\text{ext}} u \\ \gamma_1^{\text{ext}} u \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I + K & -V \\ -D & \frac{1}{2}I - K' \end{pmatrix} \begin{pmatrix} \gamma_0^{\text{ext}} u \\ \gamma_1^{\text{ext}} u \end{pmatrix}.$$

These boundary integral equations can be used to solve exterior boundary value problems with different boundary conditions. For the Dirichlet boundary value problem (5.14) we can find the unknown Neumann datum $\gamma_1^{\text{ext}} u \in H^{-1/2,-1/4}(\Sigma)$ by solving the first boundary integral equation for the exterior problem

$$V\gamma_1^{\text{ext}} u = -\frac{1}{2}g + Kg \quad \text{on } \Sigma.$$

Analogously to the interior problem, the unique solvability of the corresponding variational formulation follows from the ellipticity of the operator $V : H^{-1/2,-1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma)$.

5.5 Transmission Problem

Let $\beta_0 \in H^{1/2,1/4}(\Sigma)$ and $\beta_1 \in H^{-1/2,-1/4}(\Sigma)$. We consider the transmission problem

$$\begin{aligned} \alpha \partial_t u(x,t) - \Delta_x u(x,t) &= 0 \quad \text{for } (x,t) \in Q, \\ \partial_t u(x,t) - \Delta_x u(x,t) &= 0 \quad \text{for } (x,t) \in Q^{\text{ext}}, \\ u(x,0) &= 0 \quad \text{for } x \in \mathbb{R}^n \end{aligned} \tag{5.16}$$

with transmission conditions

$$\begin{aligned} \gamma_0^{\text{int}} u(x,t) - \gamma_0^{\text{ext}} u(x,t) &= \beta_0(x,t) \quad \text{for } (x,t) \in \Sigma, \\ \gamma_1^{\text{int}} u(x,t) - \gamma_1^{\text{ext}} u(x,t) &= \beta_1(x,t) \quad \text{for } (x,t) \in \Sigma \end{aligned} \tag{5.17}$$

and assume that the solution satisfies an appropriate radiation condition as $|x| \to \infty$ and $t \in (0,T)$. We define

$$\begin{aligned} u_i &:= \widetilde{V}_\alpha \gamma_1^{\text{int}} u_i - W_\alpha \gamma_0^{\text{int}} u_i, \\ u_e &:= -\widetilde{V} \gamma_1^{\text{ext}} u_e + W \gamma_0^{\text{ext}} u_e \end{aligned}$$

with $u_{|Q} = u_i$, $u_{|Q^{\text{ext}}} = u_e$. Here, the subscript α refers to the integral operators corresponding to the interior problem. Inserting the transmission conditions (5.17) in the second equation yields

$$u_e := -\widetilde{V}(\gamma_1^{\text{int}} u_i - \beta_1) + W(\gamma_0^{\text{int}} u_i - \beta_0).$$

As in (5.3), we obtain the system of boundary integral equations for the interior problem

$$\begin{pmatrix} \gamma_0^{\text{int}} u_i \\ \gamma_1^{\text{int}} u_i \end{pmatrix} = \begin{pmatrix} \frac{1}{2} I - K_\alpha & V_\alpha \\ D_\alpha & \frac{1}{2} I + K_\alpha' \end{pmatrix} \begin{pmatrix} \gamma_0^{\text{int}} u_i \\ \gamma_1^{\text{int}} u_i \end{pmatrix} \tag{5.18}$$

For the exterior problem we get

$$\begin{pmatrix} \gamma_0^{\text{ext}} u_e \\ \gamma_1^{\text{ext}} u_e \end{pmatrix} = \begin{pmatrix} \frac{1}{2} I + K & -V \\ -D & \frac{1}{2} I - K' \end{pmatrix} \begin{pmatrix} \gamma_0^{\text{ext}} u_e \\ \gamma_1^{\text{ext}} u_e \end{pmatrix}. \tag{5.19}$$

By combining (5.18) and (5.19), and by using the transmission conditions (5.17) we finally obtain the system of boundary integral equations for the transmission problem

$$\underbrace{\begin{pmatrix} V_\alpha + V & -K_\alpha - K \\ K_\alpha' + K' & D_\alpha + D \end{pmatrix}}_{=:A} \begin{pmatrix} \gamma_1^{\text{int}} u_i \\ \gamma_0^{\text{int}} u_i \end{pmatrix} = \underbrace{\begin{pmatrix} V_\alpha & \frac{1}{2} I - K_\alpha \\ \frac{1}{2} I + K_\alpha' & D_\alpha \end{pmatrix}}_{=:B} \begin{pmatrix} \beta_1 \\ \beta_0 \end{pmatrix} \tag{5.20}$$

The variational formulation of (5.20) is to find

$$(\gamma_1^{\text{int}} u_i, \gamma_0^{\text{int}} u_i) \in H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$$

such that

$$\left\langle A \begin{pmatrix} \gamma_1^{\text{int}} u_i \\ \gamma_0^{\text{int}} u_i \end{pmatrix}, \begin{pmatrix} \tau \\ v \end{pmatrix} \right\rangle_\Sigma = \left\langle B \begin{pmatrix} \beta_1 \\ \beta_0 \end{pmatrix}, \begin{pmatrix} \tau \\ v \end{pmatrix} \right\rangle_\Sigma \tag{5.21}$$

for all $(\tau, v) \in H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$. Due to the ellipticity and boundedness of the operator A, see Theorem 5.3, and due to the boundedness of the operator B, the variational problem (5.21) is uniquely solvable according to the Lax–Milgram theorem [62, Theorem 3.4].

The coupling of boundary integral equations of different domains represents the basis of so-called multi-trace formulations which are based on the decomposition of the domain into subdomains, e.g. for piecewise constant media, in order to develop domain decomposition solvers or preconditioners, see, e.g., [8, 9, 24] in the case of acoustic and electromagnetic scattering. In the context of multi-trace formulations the ellipticity of related Calderón projection operators as in Theorem 5.3 in the case of the heat equation plays an important role.

6 SPACE–TIME BOUNDARY ELEMENTS

In this chapter we discuss two different space–time discretization techniques in order to compute an approximation of the unknown Cauchy data and derive approximation properties of related space–time boundary element spaces [12]. The first one is the so-called tensor product approach, where we consider separate decompositions of the lateral boundary Γ and the time interval $(0,T)$ and use space–time tensor product spaces to define suitable trial spaces. The second one is using boundary element spaces which are defined with respect to a shape regular triangulation of the whole space–time boundary $\Sigma = \Gamma \times (0,T)$ into boundary elements, allowing us to apply adaptive refinement in space and time simultaneously while maintaining the regularity of the boundary element mesh.

We assume, for $n = 2,3$, that the spatial Lipschitz boundary $\Gamma = \partial\Omega$ is piecewise smooth with $\overline{\Gamma} = \bigcup_{j=1}^{J} \overline{\Gamma}_j$. With $\Sigma_j := \Gamma_j \times (0,T)$, $j = 1,...,J$, we then obtain $\overline{\Sigma} = \bigcup_{j=1}^{J} \overline{\Sigma}_j$. In order to define trial spaces for the Galerkin boundary element discretizations of the variational formulations discussed in Chapter 5 we consider a family $\{\Sigma_N\}_{N\in\mathbb{N}}$ of decompositions $\Sigma_N := \{\sigma_\ell\}_{\ell=1}^{N}$ of the space–time boundary Σ into boundary elements σ_ℓ, i.e. we have

$$\overline{\Sigma} = \bigcup_{\ell=1}^{N} \overline{\sigma}_\ell \,. \tag{6.1}$$

In the following sections we provide information on how to define suitable space–time boundary decompositions in order to obtain Σ_N.

6.1 Decomposition of the Time Interval $(0,T)$

Let $\{I_{N_t}\}_{N_t\in\mathbb{N}}$ be a family of decompositions $I_{N_t} := \{\tau_k\}_{k=1}^{N_t}$ of the time interval $I = (0,T)$ into line segments τ_k, i.e. we have

$$[0,T] = \bigcup_{k=1}^{N_t} \overline{\tau}_k. \tag{6.2}$$

The local mesh size of an element $\tau_k = (t_{k_1}, t_{k_2})$ is then given by $h_{k,t} := t_{k_2} - t_{k_1}$, whereas the global mesh size is defined as $h_t := \max_{k=1,...,N_t} h_{k,t}$. The family $\{I_{N_t}\}_{N_t\in\mathbb{N}}$ of decompositions is said to be globally quasi-uniform if there exists a constant $c_{G,t} \geq 1$ independent of I_{N_t} such that

$$\frac{h_{t,\max}}{h_{t,\min}} \leq c_{G,t}.$$

Trial Spaces

Let $S_h^0(I_{N_t})$ be the space of piecewise constant basis functions which is defined with respect to the decomposition I_{N_t}. Moreover, $S_h^1(I_{N_t})$ denotes the space of piecewise linear and globally continuous basis functions on I_{N_t}. For $p \in \{0,1\}$ we define the L^2 projection $Q_I^p u \in S_h^p(I_{N_t})$ of $u \in L^2(0,T)$ as the unique solution of the variational problem

$$\langle Q_I^p u, v_h \rangle_{L^2(0,T)} = \langle u, v_h \rangle_{L^2(0,T)} \quad \text{for all } v_h \in S_h^p(I_{N_t}). \tag{6.3}$$

The operators $Q_I^p : L^2(0,T) \to L^2(0,T)$ satisfy the trivial stability estimate

$$\left\| Q_I^p u \right\|_{L^2(0,T)} \le \|u\|_{L^2(0,T)} \quad \text{for all } u \in L^2(0,T).$$

By using standard arguments, see, e.g., [10, 17, 45] and the references therein, we obtain the following well known a priori error estimates for the L^2 projections $Q_I^p u$.

Theorem 6.1 ([45, Section 7.1])**.** *Let $u \in H^s(0,T)$ for some $s \in [0, p+1]$. Then there holds the error estimate*

$$\left\| u - Q_I^p u \right\|_{L^2(0,T)} \le c\, h^s |u|_{H^s(0,T)}.$$

Lemma 6.2. *Let $u \in H^s(0,T)$ for some $s \in [0, p+1]$. For $\mu \in [-(p+1), 0]$ there holds the error estimate*

$$\left\| u - Q_I^p u \right\|_{\widetilde{H}^\mu(0,T)} \le c\, h^{s-\mu} |u|_{H^s(0,T)}.$$

Proof. Follows by applying a duality argument and Theorem 6.1. □

Lemma 6.3 ([45, Section 7.1])**.** *Let $\mu \in [0, 1/2)$ and $u \in H^s(0,T)$ for some $s \in [\mu, 1]$. Then there holds the error estimate*

$$\left\| u - Q_I^0 u \right\|_{H^\mu(0,T)} \le c\, h^{s-\mu} \, \|u\|_{H^s(0,T)}\,.$$

Lemma 6.4. *Assume the temporal decomposition* (6.2) *to be globally quasi-uniform. Let $\mu \in [0,1]$ and $u \in H^s(0,T)$ for some $s \in [\mu, 2]$. Then there holds the error estimate*

$$\left\| u - Q_I^1 u \right\|_{H^\mu(0,T)} \le c\, h^{s-\mu} \, \|u\|_{H^s(0,T)}\,.$$

Proof. Follows by using [17, Proposition 1.134] and an interpolation argument. See also [45, Estimate 7.1 ff.] and the references therein. □

Lemma 6.5 (Global inverse inequality [45, Section 7.1])**.** *Assume that the temporal decomposition* (6.2) *is globally quasi-uniform. For $\mu \in [-1, 0]$ there holds the inverse inequality*

$$\|\tau_h\|_{L^2(0,T)} \le c\, h^\mu \, \|\tau_h\|_{\widetilde{H}^\mu(0,T)} \quad \textit{for all } \tau_h \in S_h^0(I_{N_t}).$$

6.2 Decomposition of the Lateral Boundary Γ in 2D and 3D

Let $\{\Gamma_{N_x}\}_{N_x \in \mathbb{N}}$ be, for $n = 2,3$, a family of admissible decompositions $\Gamma_{N_x} := \{\gamma_\ell\}_{\ell=1}^{N_x}$ of the boundary Γ into boundary elements γ_ℓ, i.e. we have

$$\overline{\Gamma} = \bigcup_{\ell=1}^{N_x} \overline{\gamma}_\ell. \tag{6.4}$$

We assume that there are no curved elements and that there is no approximation of the boundary Γ. The boundary elements γ_ℓ are line segments for $n = 2$ and plane triangles for $n = 3$. For each boundary element γ_ℓ there exists $j \in \{1,...,J\}$ such that $\gamma_\ell \subset \Gamma_j$. The boundary elements γ_ℓ can be described as $\gamma_\ell = \chi_\ell(\gamma)$, where γ is some reference element in $\mathbb{R}^{n-1}$. For each boundary element γ_ℓ we define its volume

$$\Delta_\ell := \int_{\gamma_\ell} \mathrm{d}s_x,$$

and its local mesh size

$$h_{\ell,x} := \Delta_\ell^{1/(n-1)}.$$

The global mesh size is then given by

$$h_x := \max_{\ell=1,...,N_x} h_{\ell,x}.$$

Moreover, we define the diameter of the element γ_ℓ as

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

The family $\{\Gamma_{N_x}\}_{N_x \in \mathbb{N}}$ of decompositions is said to be globally quasi-uniform if there exists a constant $c_{G,x} \geq 1$ independent of Γ_{N_x} such that

$$\frac{h_{x,\max}}{h_{x,\min}} \leq c_{G,x}.$$

We assume that the boundary elements γ_ℓ are shape regular, i.e. there exists a constant c_B independent of Γ_{N_x} such that

$$d_{\ell,x} \leq c_B\, h_{\ell,x} \quad \text{for } \ell = 1,...,N_x.$$

Trial Spaces

Let $S_h^0(\Gamma_{N_x})$ be the space of piecewise constant basis functions which is defined with respect to the decomposition Γ_{N_x}. Moreover, $S_h^1(\Gamma_{N_x})$ denotes the space of piecewise linear and globally continuous basis functions on Γ_{N_x}. For $p \in \{0,1\}$ we define the L^2 projection $Q_\Gamma^p u \in S_h^p(\Gamma_{N_x})$ of $u \in L^2(\Gamma)$ as the unique solution of the variational problem

$$\langle Q_\Gamma^p u, v_h \rangle_{L^2(\Gamma)} = \langle u, v_h \rangle_{L^2(\Gamma)} \quad \text{for all } v_h \in S_h^p(\Gamma_{N_x}). \tag{6.5}$$

The operators $Q_\Gamma^p : L^2(\Gamma) \to L^2(\Gamma)$ satisfy the trivial stability estimate

$$\left\| Q_\Gamma^p u \right\|_{L^2(\Gamma)} \le \|u\|_{L^2(\Gamma)} \quad \text{for all } u \in L^2(\Gamma).$$

We then obtain the following approximation properties of the L^2 projection operators Q_Γ^p, see, e.g., [10, 62].

Theorem 6.6 ([62, Theorem 10.2 and Lemma 10.8 ff.]). *Let $u \in H^s(\Gamma)$ with $s \in [0, p+1]$. Then there holds the error estimate*

$$\left\| u - Q_\Gamma^p u \right\|_{L^2(\Gamma)} \le c\, h^s |u|_{H^s(\Gamma)}.$$

Lemma 6.7. *Let $u \in H^s(\Gamma)$ for some $s \in [0, p+1]$. For $\sigma \in [-(p+1), 0]$ there holds the error estimate*

$$\left\| u - Q_\Gamma^p u \right\|_{H^\sigma(\Gamma)} \le c\, h^{s-\sigma} |u|_{H^s(\Gamma)}.$$

Proof. Follows by using a duality argument and Theorem 6.6. □

Lemma 6.8 (Global inverse inequality [62, Lemma 10.10]). *Assume that the boundary decomposition* (6.4) *is globally quasi-uniform. For $\sigma \in [-1, 0]$ there holds the inverse inequality*

$$\|\tau_h\|_{L^2(\Gamma)} \le c\, h^\sigma \, \|\tau_h\|_{H^\sigma(\Gamma)} \quad \textit{for all } \tau_h \in S_h^0(\Gamma_{N_x}).$$

The inverse inequality in [62] was shown for $\sigma = -1/2$. However, the proof utilizes an interpolation argument and can be extended to arbitrary $\sigma \in [-1, 0]$.

Additionally, we assume that for $\sigma \in [0,1]$ and $u \in H^s(\Gamma)$ with $s \in [\sigma, 2]$ the error estimate

$$\left\| u - Q_\Gamma^1 u \right\|_{H^\sigma(\Gamma)} \le c\, h^{s-\sigma} \, \|u\|_{H^s(\Gamma)}$$

holds, which is, e.g., well known for spatial domains Ω with sufficiently smooth boundary Γ, see [10, Section 5] and [45, Chapter 5] and the references therein.

6.3 Decomposition of the Space–Time Boundary Σ

In this section we define suitable boundary decompositions of Σ in order to obtain (6.1), define space–time boundary element spaces and provide approximation properties of related L^2 projection operators.

6.3.1 One-Dimensional Problem

In the spatially one-dimensional case we have $\Omega = (a,b) \subset \mathbb{R}$ with constants $b > a$. Thus, $\Gamma = \{a,b\}$, inducing that $\Sigma = \Sigma_a \cup \Sigma_b$ with $\Sigma_a = \{a\} \times (0,T)$ and $\Sigma_b = \{b\} \times (0,T)$. Hence the boundary elements σ_ℓ are line segments in temporal dimension with fixed spatial coordinate $x_\ell \in \{a,b\}$ as shown in Figure 6.1.

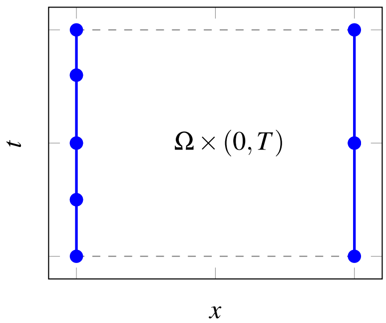


Figure 6.1: Sample BE mesh. We consider an arbitrary decomposition of the space–time boundary Σ. Note that there is no time-stepping scheme involved.

The space–time boundary decomposition (6.1) can be seen as the union of two different decompositions of the time interval $(0,T)$ as described in Section 6.1, one for each boundary point $\{a,b\}$. Note that there is no time-stepping involved, since the decompositions of Σ_a and Σ_b may be different. Let (x_ℓ, t_{ℓ_1}) and (x_ℓ, t_{ℓ_2}) be the nodes of the boundary element σ_ℓ. The local mesh size is then given as $h_\ell := |t_{\ell_2} - t_{\ell_1}|$ while $h := \max_{\ell=1,\dots,N} h_\ell$ is the global mesh size. The family $\{\Sigma_N\}_{N\in\mathbb{N}}$ is said to be globally quasi-uniform if there exists a constant $c_G \geq 1$ independet of Σ_N such that

$$\frac{h_{\max}}{h_{\min}} \leq c_G.$$

Remark 6.1. *In the one-dimensional case the spatial component of the space–time boundary Σ collapses to the points $\{a,b\}$, assuming $\Omega = (a,b)$, and therefore we can identify the anisotropic Sobolev spaces $H^{r,s}(\Sigma)$ with the isotropic version $H^s(\Sigma)$.*

Trial Spaces

Let $S_h^0(\Sigma_N)$ and $S_h^1(\Sigma_N)$ denote the boundary element spaces of piecewise constant and piecewise linear and globally continuous basis functions, respectively, and $Q_\Sigma^p u \in S_h^p(\Sigma_N)$ for $u \in L^2(\Sigma)$ the corresponding L^2 projections defined analogously to Q_I^p in Section 6.1, but for both boundary parts Σ_a and Σ_b. Due to the temporal structure of the space–time decomposition in the spatially one-dimensional case we obtain the same approximation properties for the L^2 projection operators $Q_\Sigma^p : L^2(\Sigma) \to S_h^p(\Sigma_N) \subset L^2(\Sigma)$ as for $Q_I^p : L^2(0,T) \to S_h^p(I_{N_t}) \subset L^2(0,T)$ given in Section 6.1.

6.3.2 Two- and Three-Dimensional Problem

As already mentioned, we consider two different space–time decomposition approaches. The first one is a separate decomposition of the spatial boundary Γ and the time interval $(0,T)$ also employed in, e.g., [21,39,45,49]. We use the resulting tensor product structure to define space–time boundary element spaces, and we derive a priori error estimates for related L^2 projection operators simply by combining the approximation properties of the spatial and temporal discretizations given in Sections 6.1 and 6.2. The second approach is considering an arbitrary triangulation of the full space–time boundary $\Sigma = \Gamma \times (0,T)$ into boundary elements.

Space–Time Tensor Product Decomposition

In order to define space–time tensor product spaces we use the already given decompositions $I_{N_t} = \{\tau_k\}_{k=1}^{N_t}$ and $\Gamma_{N_x} = \{\gamma_\ell\}_{\ell=1}^{N_x}$ introduced in Sections 6.1 and 6.2, respectively. The set $\Sigma_N = \{\sigma_\ell\}_{l=1}^{N}$ of boundary elements σ_ℓ in (6.1) is defined as

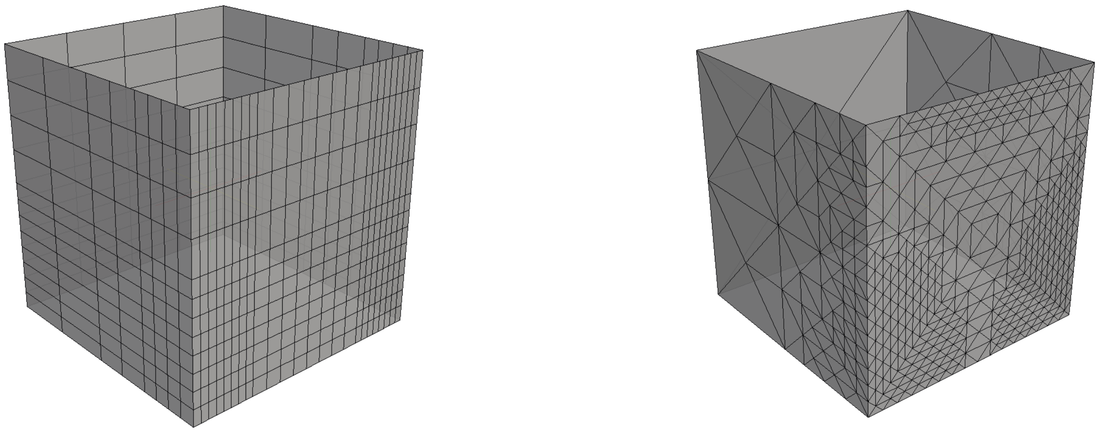
$$\Sigma_N := \left\{\sigma = \gamma_i \times \tau_j, i \in \{1,...,N_x\}, j \in \{1,...,N_t\}\right\} \tag{6.6}$$

with $N = N_x N_t$. The resulting space–time boundary elements are rectangles for $n = 2$ and triangular prisms for $n = 3$. A sample decomposition of the space–time boundary of $Q = (0,1)^3$ is shown in Figure 6.2 (a).

Trial Spaces

Let $p_x, p_t \in \{0,1\}$ denote the polynomial degrees of the basis functions in space and time, respectively. Then the boundary element spaces are given as

$$X_{h_x,h_t}^{p_x,p_t}(\Sigma_N) := S_{h_x}^{p_x}(\Gamma_{N_x}) \otimes S_{h_t}^{p_t}(I_{N_t}),$$



(a) Tensor product decomposition. (b) Triangulation.

Figure 6.2: Sample space–time boundary decompositions of $Q = (0,1)^3$.

where the subscripts h_x and h_t denote the spatial and temporal mesh sizes, respectively. The L^2 projection $Q_\Sigma^{p_x,p_t} u \in X_{h_x,h_t}^{p_x,p_t}(\Sigma_N)$ of $u \in L^2(\Sigma)$ is defined as the unique solution of the variational problem

$$\langle Q_\Sigma^{p_x,p_t} u, v_h \rangle_{L^2(\Sigma)} = \langle u, v_h \rangle_{L^2(\Sigma)} \quad \text{for all } v_h \in X_{h_x,h_t}^{p_x,p_t}(\Sigma_N). \tag{6.7}$$

The L^2 projection operator $Q_\Sigma^{p_x,p_t} : L^2(\Sigma) \to X_{h_x,h_t}^{p_x,p_t}(\Sigma_N) \subset L^2(\Sigma)$ has the representation $Q_\Sigma^{p_x,p_t} = Q_\Sigma^{p_x,\cdot} Q_\Sigma^{\cdot,p_t} = Q_\Sigma^{\cdot,p_t} Q_\Sigma^{p_x,\cdot}$ with

$$\begin{aligned} (Q_\Sigma^{p_x,\cdot} u)(x,t) &:= (Q_\Gamma^{p_x} u(\cdot,t))(x), \\ (Q_\Sigma^{\cdot,p_t} u)(x,t) &:= (Q_I^{p_t} u(x,\cdot))(t) \end{aligned} \tag{6.8}$$

for $u \in L^2(\Sigma)$. Hence we can use the already known approximation properties of the operators $Q_\Gamma^{p_x}$ and $Q_I^{p_t}$ to derive estimates for the L^2 projection $Q_\Sigma^{p_x,p_t} u$ of $u \in L^2(\Sigma)$. The operator $Q_\Sigma^{p_x,p_t}$ satisfies the trivial stability estimate

$$\left\| Q_\Sigma^{p_x,p_t} u \right\|_{L^2(\Sigma)} \le \|u\|_{L^2(\Sigma)} \quad \text{for all } u \in L^2(\Sigma)$$

and we obtain the following approximation properties.

Theorem 6.9. *Let $u \in H^{r,s}(\Sigma)$ for some $r \in [0, p_x + 1]$, $s \in [0, p_t + 1]$. Moreover, let $Q_\Sigma^{p_x,p_t} u \in X_{h_x,h_t}^{p_x,p_t}(\Sigma_N)$ be the L^2 projection of u. Then there holds the error estimate*

$$\left\| u - Q_\Sigma^{p_x,p_t} u \right\|_{L^2(\Sigma)} \le c \, (h_x^r + h_t^s) \, \|u\|_{H^{r,s}(\Sigma)} .$$

Proof. Let $u \in H^{r,s}(\Sigma)$. Inserting intermediate functions and applying the triangle inequality yields

$$\left\| u - Q_\Sigma^{p_x,p_t} u \right\|_{L^2(\Sigma)} \le \left\| u - Q_\Sigma^{p_x,\cdot} u \right\|_{L^2(\Sigma)} + \left\| Q_\Sigma^{p_x,\cdot} (u - Q_\Sigma^{\cdot,p_t} u) \right\|_{L^2(\Sigma)}$$

and the assertion follows by using the definitions (6.8) of the projection operators and by applying the stability of the operator $Q_{\Gamma}^{p_x} : L^2(\Gamma) \to L^2(\Gamma)$, Theorem 6.1 and Theorem 6.6. $\square$

Lemma 6.10. *Let $u \in H^{r,s}(\Sigma)$ for some $r \in [0, p_x+1]$ and $s \in [0, p_t+1]$. Moreover, let $\sigma \in [-(p_x+1), 0]$ and $\mu \in [-(p_t+1), 0]$. Then there holds the error estimate*

$$\left\|u - Q_{\Sigma}^{p_x,p_t} u\right\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \leq c \left(h_x^{-\sigma} + h_t^{-\mu}\right)(h_x^r + h_t^s)\,\|u\|_{H^{r,s}(\Sigma)}.$$

Proof. Let $u \in H^{r,s}(\Sigma)$. By duality and by using (6.7) we obtain

$$\begin{aligned}\left\|u - Q_{\Sigma}^{p_x,p_t} u\right\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} &= \sup_{0 \neq v \in H^{-\sigma,-\mu}(\Sigma)} \frac{\langle u - Q_{\Sigma}^{p_x,p_t} u, v\rangle_{L^2(\Sigma)}}{\|v\|_{H^{-\sigma,-\mu}(\Sigma)}} \\ &= \sup_{0 \neq v \in H^{-\sigma,-\mu}(\Sigma)} \frac{\langle u - Q_{\Sigma}^{p_x,p_t} u, v - Q_{\Sigma}^{p_x,p_t} v\rangle_{L^2(\Sigma)}}{\|v\|_{H^{-\sigma,-\mu}(\Sigma)}}.\end{aligned}$$

An application of the Cauchy–Schwarz inequality and using Theorem 6.9 yields

$$\begin{aligned}\left\|u - Q_{\Sigma}^{p_x,p_t} u\right\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} &\leq \left\|u - Q_{\Sigma}^{p_x,p_t} u\right\|_{L^2(\Sigma)} \sup_{0 \neq v \in H^{-\sigma,-\mu}(\Sigma)} \frac{\left\|v - Q_{\Sigma}^{p_x,p_t} v\right\|_{L^2(\Sigma)}}{\|v\|_{H^{-\sigma,-\mu}(\Sigma)}} \\ &\leq c \left(h_x^{-\sigma} + h_t^{-\mu}\right)(h_x^r + h_t^s)\,\|u\|_{H^{r,s}(\Sigma)}.\end{aligned}$$

$\square$

The following two error estimates in anisotropic Sobolev spaces are to be found in the proof of [10, Proposition 5.3].

Lemma 6.11. *Let $\sigma \in [0,1]$, $\mu \in [0, 1/2)$ and $u \in H^{r,s}(\Sigma)$ for some $r \in [\sigma, 2]$ and $s \in [\mu, 1]$. Then there holds the error estimate*

$$\left\|u - Q_{\Sigma}^{1,0} u\right\|_{H^{\sigma,\mu}(\Sigma)} \leq c \left(h_x^{\beta_1(r,s,\sigma,\mu)} + h_t^{\beta_2(r,s,\sigma,\mu)}\right)\|u\|_{H^{r,s}(\Sigma)}$$

with

$$\beta_1(r,s,\sigma,\mu) := \min\left(r - \sigma, r - \mu \frac{r}{s}\right), \quad \beta_2(r,s,\sigma,\mu) := \min\left(s - \mu, s - \sigma \frac{s}{r}\right). \tag{6.9}$$

Note that for $r\mu = s\sigma$ we obtain the estimate

$$\left\|u - Q_{\Sigma}^{1,0} u\right\|_{H^{\sigma,\mu}(\Sigma)} \leq c \left(h_x^{r-\sigma} + h_t^{s-\mu}\right)\|u\|_{H^{r,s}(\Sigma)}.$$

Lemma 6.12 ([10, Proposition 5.3])**.** *Let $\sigma \in [0,1]$, $\mu \in [0,1]$ and $u \in H^{r,s}(\Sigma)$ for some $r \in [\sigma,2]$ and $s \in [\mu,2]$. Then there holds the error estimate*

$$\left\| u - Q_\Sigma^{1,1} u \right\|_{H^{\sigma,\mu}(\Sigma)} \le c \left(h_x^{\beta_1(r,s,\sigma,\mu)} + h_t^{\beta_2(r,s,\sigma,\mu)} \right) \|u\|_{H^{r,s}(\Sigma)}$$

with β_1, β_2 given by (6.9).

For the setting $r\mu = s\sigma$ we conclude the error estimate

$$\left\| u - Q_\Sigma^{1,1} u \right\|_{H^{\sigma,\mu}(\Sigma)} \le c \left(h_x^{r-\sigma} + h_t^{s-\mu} \right) \|u\|_{H^{r,s}(\Sigma)}.$$

The following inverse inequality is necessary in order to derive an $L^2(\Sigma)$-error estimate for the Galerkin approximation of the unknown Neumann datum w of the initial Dirichlet boundary value problem (5.6).

Lemma 6.13 (Global inverse inequality)**.** *Assume that the decompositions Γ_{N_x} and I_{N_t} are globally quasi-uniform. For $r \in [0,1)$ there holds the global inverse inequality*

$$\|\tau_h\|_{L^2(\Sigma)} \le c \left(h_x^{-r} + h_t^{-r/2} \right) \|\tau_h\|_{\widetilde{H}^{-r,-r/2}(\Sigma)} \quad \textit{for all } \tau_h \in X_{h_x,h_t}^{0,0}(\Sigma_N).$$

Proof. Let $\tau_h \in X_{h_x,h_t}^{0,0}(\Sigma_N)$ and $0 \le r < \frac{1}{2}$. By applying the standard inverse inequalitiy in spatial and temporal dimension [21] we get

$$\begin{aligned}
\|\tau_h\|^2_{H^{r,r/2}(\Sigma)} &\le c \int_\Gamma \|\tau_h(x,\cdot)\|^2_{H^{r/2}(0,T)} \, \mathrm{d}s_x + c \int_0^T \|\tau_h(\cdot,t)\|^2_{H^r(\Gamma)} \, \mathrm{d}t \\
&\le c\, h_t^{-r} \int_\Gamma \|\tau_h(x,\cdot)\|^2_{L^2(0,T)} \, \mathrm{d}s_x + c\, h_x^{-2r} \int_0^T \|\tau_h(\cdot,t)\|^2_{L^2(\Gamma)} \, \mathrm{d}t \\
&\le c \left(h_x^{-2r} + h_t^{-r} \right) \|\tau_h\|^2_{L^2(\Sigma)}.
\end{aligned}$$

This estimate then yields

$$\begin{aligned}
\|\tau_h\|^2_{L^2(\Sigma)} = \langle \tau_h, \tau_h \rangle_{L^2(\Sigma)} &\le \|\tau_h\|_{H^{r,r/2}(\Sigma)} \|\tau_h\|_{\widetilde{H}^{-r,-r/2}(\Sigma)} \\
&\le c \left(h_x^{-r} + h_t^{-r/2} \right) \|\tau_h\|_{L^2(\Sigma)} \|\tau_h\|_{\widetilde{H}^{-r,-r/2}(\Sigma)},
\end{aligned}$$

and we conclude

$$\|\tau_h\|_{L^2(\Sigma)} \le c \left(h_x^{-r} + h_t^{-r/2} \right) \|\tau_h\|_{\widetilde{H}^{-r,-r/2}(\Sigma)} \quad \text{for all } \tau_h \in X_{h_x,h_t}^{0,0}(\Sigma_N).$$

It remains to prove the estimate for $r \in [\frac{1}{2}, 1)$. For $\tau_h \in X^{0,0}_{h_x,h_t}(\Sigma_N)$ we have

$$\|\tau_h\|_{L^2(\Sigma)} \le c\left(h_x^{-r/2} + h_t^{-r/4}\right)\|\tau_h\|_{\widetilde{H}^{-r/2,-r/4}(\Sigma)}. \tag{6.10}$$

By using interpolation results, see, e.g., [34, 35], we get

$$\begin{aligned}\|\tau_h\|^2_{\widetilde{H}^{-r/2,-r/4}(\Sigma)} &\le c\,\|\tau_h\|_{L^2(\Sigma)}\,\|\tau_h\|_{\widetilde{H}^{-r,-r/2}(\Sigma)}\\ &\le c\left(h_x^{-r/2} + h_t^{-r/4}\right)\|\tau_h\|_{\widetilde{H}^{-r/2,-r/4}(\Sigma)}\,\|\tau_h\|_{\widetilde{H}^{-r,-r/2}(\Sigma)},\end{aligned}$$

and together with (6.10) we conclude

$$\|\tau_h\|_{L^2(\Sigma)} \le c\left(h_x^{-r} + h_t^{-r/2}\right)\|\tau_h\|_{\widetilde{H}^{-r,-r/2}(\Sigma)} \quad \text{for all } \tau_h \in X^{0,0}_{h_x,h_t}(\Sigma_N).$$

□

Space–Time Triangulation

Let $\{\Sigma_N\}_{N\in\mathbb{N}}$ be a family of admissible triangulations of the full space–time boundary Σ into boundary elements σ_ℓ given by (6.1). Again, we assume that there are no curved elements and that there is no approximation of the boundary Σ. For each boundary element σ_ℓ there exists exactly one $j \in \{1,\ldots,J\}$ such that $\sigma_\ell \subset \Sigma_j$. The boundary elements σ_ℓ can be described as $\sigma_\ell = \chi_\ell(\sigma)$, where σ is some reference element in $\mathbb{R}^n$. The elements σ_ℓ are plane triangles for $n = 2$ and tetrahedra for $n = 3$. For each boundary element σ_ℓ we define its volume

$$\Delta_\ell := \int_{\sigma_\ell} \mathrm{d}s_x\,\mathrm{d}t$$

and its local mesh size $h_\ell := \Delta_\ell^{1/n}$. The global mesh size is given by $h := \max_{\ell=1,\ldots,N} h_\ell$. The family $\{\Sigma_N\}_{N\in\mathbb{N}}$ of triangulations is said to be globally quasi-uniform if there exists a constant $c_G \ge 1$ independent of Σ_N such that

$$\frac{h_{\max}}{h_{\min}} \le c_G.$$

We consider shape regular boundary elements only, i.e. there exists a constant c_B independent of the boundary decomposition Σ_N such that

$$d_\ell \le c_B\,h_\ell \quad \text{for } \ell = 1,\ldots,N$$

with diameter d_ℓ given by

$$d_\ell := \sup_{(x,t),(y,s)\in\sigma_\ell} |(x,t) - (x,s)|.$$

A sample triangulation of the boundary Σ of the space–time domain $Q = (0,1)^3$ is shown in Figure 6.2 (b).

Trial Spaces

Let $S_h^0(\Sigma_N)$ and $S_h^1(\Sigma_N)$ denote the spaces of piecewise constant and piecewise linear and globally continuous basis functions, respectively, which are defined with respect to the triangulation Σ_N. The L^2 projection $Q_\Sigma^p u \in S_h^p(\Sigma_N)$ of $u \in L^2(\Sigma)$, for $p \in \{0,1\}$, is defined as the unique solution of the variational problem

$$\langle Q_\Sigma^p u, v_h \rangle_{L^2(\Sigma)} = \langle u, v_h \rangle_{L^2(\Sigma)} \quad \text{for all } v_h \in S_h^p(\Sigma_N). \tag{6.11}$$

The operators $Q_\Sigma^p : L^2(\Sigma) \to L^2(\Sigma)$ satisfy the trivial stability estimate

$$\left\| Q_\Sigma^p u \right\|_{L^2(\Sigma)} \le \|u\|_{L^2(\Sigma)} \quad \text{for all } u \in L^2(\Sigma).$$

By using Lemma 2.1 and the well known approximation properties in standard Sobolev spaces, see, e.g., [62], we immediately obtain the following approximation results.

Theorem 6.14. *Let $u \in H^{r,s}(\Sigma)$ for some $r,s \in [0,1]$. Then there hold the error estimates*

$$\begin{aligned} \left\| u - Q_\Sigma^p u \right\|_{L^2(\Sigma)} &\le \|u\|_{L^2(\Sigma)}, \\ \left\| u - Q_\Sigma^p u \right\|_{L^2(\Sigma)} &\le c\, h^{\min(r,s)} \|u\|_{H^{r,s}(\Sigma)}. \end{aligned}$$

Proof. First, let $u \in L^2(\Sigma)$. By using

$$\langle u - Q_\Sigma^p u, v_h \rangle_{L^2(\Sigma)} = 0 \quad \text{for all } v_h \in S_h^0(\Sigma)$$

we obtain

$$\begin{aligned} \left\| u - Q_\Sigma^p u \right\|_{L^2(\Sigma)}^2 &= \langle u - Q_\Sigma^p u, u - Q_\Sigma^p u \rangle_{L^2(\Sigma)} = \langle u - Q_\Sigma^p u, u \rangle_{L^2(\Sigma)} \\ &\le \left\| u - Q_\Sigma^p u \right\|_{L^2(\Sigma)} \|u\|_{L^2(\Sigma)} \end{aligned}$$

and we conclude the first error estimate. For $u \in H^{r,s}(\Sigma)$ with $r,s \in [0,1]$ and $m := \min(r,s)$ we argue as follows. Analogously to [62, Theorem 10.2 and Estimate 10.12] we get

$$\left\| u - Q_\Sigma^p u \right\|_{L^2(\Sigma)} \le c\, h^m \|u\|_{H^m(\Sigma)}. \tag{6.12}$$

According to Lemma 2.1 we have $H^{r,s}(\Sigma) \hookrightarrow H^m(\Sigma)$ and we therefore conclude

$$\left\| u - Q_\Sigma^p u \right\|_{L^2(\Sigma)} \le c\, h^m \|u\|_{H^{r,s}(\Sigma)}.$$

□

Note that estimate (6.12) in the proof of Theorem 6.14 is also valid for $m \in (1,2]$, i.e. $r,s \in (1,2]$, and $p = 1$. However, the embedding $H^{r,s}(\Sigma) \hookrightarrow H^m(\Sigma)$ does not hold for that particular choice of r and s and therefore it is not possible to extend the result in Theorem 6.14 to $r,s \in (1,2]$ and $p = 1$.

Lemma 6.15. *Let $u \in H^{r,s}(\Sigma)$ for some $r,s \in [0,1]$ and $\sigma,\mu \in [-1,0]$. Then there holds the error estimate*

$$\left\|u - Q_\Sigma^p u\right\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \le c\, h^{\min(r,s)+\min(-\sigma,-\mu)} \|u\|_{H^{r,s}(\Sigma)}.$$

Proof. Let $u \in H^{r,s}(\Sigma)$. Using (6.11) yields

$$\begin{aligned}\left\|u - Q_\Sigma^p u\right\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} &= \sup_{0\neq v\in H^{-\sigma,-\mu}(\Sigma)} \frac{\langle u - Q_\Sigma^p u, v\rangle_{L^2(\Sigma)}}{\|v\|_{H^{-\sigma,-\mu}(\Sigma)}} \\ &= \sup_{0\neq v\in H^{-\sigma,-\mu}(\Sigma)} \frac{\langle u - Q_\Sigma^p u, v - Q_\Sigma^p v\rangle_{L^2(\Sigma)}}{\|v\|_{H^{-\sigma,-\mu}(\Sigma)}}.\end{aligned}$$

By applying the Cauchy–Schwarz inequality and Theorem 6.14 we obtain

$$\begin{aligned}\left\|u - Q_\Sigma^p u\right\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} &\le \left\|u - Q_\Sigma^p u\right\|_{L^2(\Sigma)} \sup_{0\neq v\in H^{-\sigma,-\mu}(\Sigma)} \frac{\left\|v - Q_\Sigma^p v\right\|_{L^2(\Sigma)}}{\|v\|_{H^{-\sigma,-\mu}(\Sigma)}} \\ &\le c\, h^{\min(r,s)} h^{\min(-\sigma,-\mu)} \|u\|_{H^{r,s}(\Sigma)}.\end{aligned}$$

□

Since we consider shape regular boundary elements, the following inverse inequality holds.

Lemma 6.16 (Global inverse inequality)**.** *For a globally quasi-uniform boundary decomposition Σ_N and $\sigma,\mu \in [0,1]$ there holds*

$$\|\tau_h\|_{L^2(\Sigma)} \le c\, h^{-\max(\sigma,\mu)} \|\tau_h\|_{\widetilde{H}^{-\sigma,-\mu}(\Sigma)} \quad \textit{for all } \tau_h \in S_h^0(\Sigma_N).$$

Proof. Let $\tau_h \in S_h^0(\Sigma_N)$. Application of the standard inverse inequality [62, Section 10.2] yields

$$\|\tau_h\|_{L^2(\Sigma)} \le c\, h^{-\max(\sigma,\mu)} \|\tau_h\|_{\widetilde{H}^{-\max(\sigma,\mu)}(\Sigma)}. \tag{6.13}$$

Since $H^{\max(\sigma,\mu)}(\Sigma) \hookrightarrow H^{\sigma,\mu}(\Sigma)$, see Lemma 2.1, we obtain

$$\begin{aligned}\|\tau_h\|_{\widetilde{H}^{-\max(\sigma,\mu)}(\Sigma)} &= \sup_{0\neq v\in H^{\max(\sigma,\mu)}(\Sigma)} \frac{\langle \tau_h, v\rangle_\Sigma}{\|v\|_{H^{\max(\sigma,\mu)}(\Sigma)}} \\ &\le c \sup_{0\neq v\in H^{\sigma,\mu}(\Sigma)} \frac{\langle \tau_h, v\rangle_\Sigma}{\|v\|_{H^{\sigma,\mu}(\Sigma)}} = c\, \|\tau_h\|_{\widetilde{H}^{-\sigma,-\mu}(\Sigma)},\end{aligned} \tag{6.14}$$

and the assertion follows from combining (6.13) and (6.14). □

Note that for $\sigma = 1/2$ and $\mu = 1/4$ we have $\widetilde{H}^{-1/2,-1/4}(\Sigma) = H^{-1/2,-1/4}(\Sigma)$ and therefore

$$\|\tau_h\|_{L^2(\Sigma)} \le c\,h^{-1/2}\,\|\tau_h\|_{H^{-1/2,-1/4}(\Sigma)} \quad \text{for all } \tau_h \in S_h^0(\Sigma_N).$$

For $\sigma \in [0,1]$ we define the $H^\sigma(\Sigma)$-projection $Q_\Sigma^{1,\sigma} u \in S_h^1(\Sigma_N)$ of $u \in H^\sigma(\Sigma)$ as the unique solution of the variational problem

$$\langle Q_\Sigma^{1,\sigma} u, v_h\rangle_{H^\sigma(\Sigma)} = \langle u, v_h\rangle_{H^\sigma(\Sigma)} \quad \text{for all } v_h \in S_h^1(\Sigma_N)$$

and obtain the following error estimate for functions u with additional regularity, see, e.g., [62, Section 9.3 and Section 10.2]. For $\sigma \in [0,1]$ and $u \in H^r(\Sigma)$ with $r \in [\sigma, 2]$ there holds the error estimate

$$\left\| u - Q_\Sigma^{1,\sigma} u \right\|_{H^\sigma(\Sigma)} \le c\,h^{r-\sigma}\,\|u\|_{H^r(\Sigma)}. \tag{6.15}$$

We therefore conclude the following approximation properties in anisotropic Sobolev spaces.

Corollary 6.17. *Let $\sigma, \mu \in [0,1]$ and $u \in H^r(\Sigma)$ for some $r \in [\nu, 2]$ with $\nu := \max(\sigma, \mu)$. Then there holds the error estimate*

$$\left\| u - Q_\Sigma^{1,\nu} u \right\|_{H^{\sigma,\mu}(\Sigma)} \le c\,h^{r-\nu}\,\|u\|_{H^r(\Sigma)}.$$

Proof. Let $u \in H^r(\Sigma)$ and define $\nu := \max(\sigma, \mu)$. According to Lemma 2.1 we have $H^\nu(\Sigma) \hookrightarrow H^{\sigma,\mu}(\Sigma)$ and therefore

$$\left\| u - Q_\Sigma^{1,\nu} u \right\|_{H^{\sigma,\mu}(\Sigma)} \le c \left\| u - Q_\Sigma^{1,\nu} u \right\|_{H^\nu(\Sigma)}.$$

The assertion then follows by applying estimate (6.15). □

As already mentioned, the extension of Corollary 6.17 to functions $u \in H^{r,s}(\Sigma)$ with $r, s \in [1,2]$ is in general not possible, see the remarks after Theorem 6.14. However, if $u \in H^{r,s}(\Sigma)$ for some $r, s \in [\nu, 1]$ with $\nu := \max(\sigma, \mu)$ we obtain the estimate

$$\left\| u - Q_\Sigma^{1,\nu} u \right\|_{H^{\sigma,\mu}(\Sigma)} \le c\,h^{\min(r,s)-\nu}\,\|u\|_{H^{r,s}(\Sigma)}, \tag{6.16}$$

which is a direct consequence of Corollary 6.17 and Lemma 2.1.

7 BOUNDARY ELEMENT METHODS

In this chapter we discuss Galerkin discretizations of space–time integral equations related to the model problem (1.1) with different types of boundary conditions, see Chapter 5, and we derive a priori error estimates for the Galerkin approximations of the unknown Cauchy data [12].

Here and in the following chapters, X_h and Y_h denote conforming boundary element spaces of $H^{-1/2,-1/4}(\Sigma)$ and $H^{1/2,1/4}(\Sigma)$, respectively, which were introduced in the previous chapter. We only consider shape regular boundary element meshes Σ_N, both for an arbitrary triangulation of Σ as well as for a tensor product decomposition, since we want to compare the theoretical and practical results of the two discretization techniques. In the following, h denotes the mesh size of the space–time boundary elements of Σ_N. Hence for the tensor product approach we choose $h \sim h_t \sim h_x$. A priori error estimates and numerical experiments for a different refinement strategy, e.g. $h_t \sim h_x^2$, can be found in, e.g., [10,45].

7.1 Dirichlet Boundary Value Problem

In this section we discretize the variational formulation (5.7) in order to compute an approximation of the unknown Neumann datum $w = \gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$ by using the previously introduced boundary element spaces and derive a priori error estimates for the Galerkin approximation, see Subsection 7.1.1. The numerical analysis of the discretized indirect formulation (5.9) follows exactly the same path. In Subsection 7.1.2 we prove error estimates for the related approximation of the solution u in the space–time domain Q, and we provide numerical experiments in order to evaluate the theoretical findings in Subsection 7.1.3. The numerical analysis in this section is based on [12].

For the discretization of the variational formulation (5.7) we consider the space of piecewise constant basis functions $X_h \in \left\{ X_{h,h}^{0,0}(\Sigma_N), S_h^0(\Sigma_N) \right\}$ which is defined with respect to a shape regular boundary element mesh Σ_N as introduced in Chapter 6. The Galerkin–Bubnov variational formulation of (5.7) is to find $w_h \in X_h$ such that

$$\langle V w_h, \tau_h \rangle_\Sigma = \langle (\frac{1}{2} I + K) g - M_0 u_0 - N_0 f, \tau_h \rangle_\Sigma \quad \text{for all } \tau_h \in X_h. \tag{7.1}$$

Due to the ellipticity of the single layer boundary integral operator V and the boundedness of the integral operators, problem (7.1) admits a unique solution.

7.1.1 Error Estimates

Let $w \in H^{-1/2,-1/4}(\Sigma)$ be the unique solution of the variational problem (5.7). Since the operator V is elliptic and bounded, we can apply Cea's Lemma [62, Theorem 8.1] to conclude quasi-optimality of the Galerkin approximation $w_h \in X_h$, i.e. we have

$$\|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)} \leq \frac{c_2^V}{c_1^V} \inf_{\tau_h \in X_h} \|w - \tau_h\|_{H^{-1/2,-1/4}(\Sigma)} .$$

Hence we can use the approximation properties of the boundary element space X_h to derive error estimates for the solution w_h of (7.1). Recall that Γ is assumed to be piecewise smooth, i.e. we have the representation $\overline{\Sigma} = \bigcup_{j=1}^{J} \overline{\Sigma}_j$ with $\Sigma_j = \Gamma_j \times (0,T)$ for $j = 1, ..., J$. Due to the local definition of the trial space X_h and by applying Lemma 2.5 we obtain

$$\|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)} \leq \frac{c_2^V}{c_1^V} \sum_{j=1}^{J} \inf_{\tau_h^j \in X_{h|\Sigma_j}} \left\| w_{|\Sigma_j} - \tau_h^j \right\|_{\widetilde{H}^{-1/2,-1/4}(\Sigma_j)} . \tag{7.2}$$

Note that all the approximation properties shown in the previous chapter also hold for an open part $\Sigma_j \subset \Sigma$ of the space–time boundary Σ, i.e. we can replace the space $H^{r,s}(\Sigma)$ with the larger space $H^{r,s}_{\mathrm{pw}}(\Sigma)$ and we still get the same error estimates in the appropriate norms.

One-Dimensional Problem

Recall that in the one-dimensional case we identify the Sobolev spaces $H^{r,s}(\Sigma)$ with $H^s(\Sigma)$. Moreover, we have $\Sigma = \Sigma_a \cup \Sigma_b$.

Theorem 7.1. *Let $w_h \in S_h^0(\Sigma_N)$ be the unique solution of the Galerkin variational problem* (7.1). *For $w \in H^s_{pw}(\Sigma)$ with $s \in [0,1]$ there holds the error estimate*

$$\|w - w_h\|_{H^{-1/4}(\Sigma)} \leq c\, h^{s+1/4} |w|_{H^s_{pw}(\Sigma)}.$$

Proof. Follows by applying Lemma 6.2 for $p = 0$ in (7.2) for both boundary parts Σ_a and Σ_b. □

Moreover, we can derive an error estimate in the $L^2(\Sigma)$-norm, assuming that the family of boundary decompositions $\{\Sigma_N\}_{N\in\mathbb{N}}$ is globally quasi-uniform.

Theorem 7.2. *Let $w_h \in S_h^0(\Sigma_N)$ be the unique solution of the Galerkin variational problem* (7.1). *For $w \in H^s_{pw}(\Sigma)$ with $s \in [0,1]$ there holds*

$$\|w - w_h\|_{L^2(\Sigma)} \leq c\, h^s |w|_{H^s_{pw}(\Sigma)}.$$

Proof. By using the triangle inequality, Theorem 6.1 and Lemma 6.5 we get

$$\begin{aligned}\|w-w_h\|_{L^2(\Sigma)} &\leq \left\|w-Q_\Sigma^0 w\right\|_{L^2(\Sigma)}+\left\|Q_\Sigma^0 w-w_h\right\|_{L^2(\Sigma)} \\ &\leq c\,h^s|w|_{H^s_{\mathrm{pw}}(\Sigma)}+c\,h^{-1/4}\left\|Q_\Sigma^0 w-w_h\right\|_{H^{-1/4}(\Sigma)}.\end{aligned}$$

The assertion follows with

$$\left\|Q_\Sigma^0 w-w_h\right\|_{H^{-1/4}(\Sigma)} \leq \left\|Q_\Sigma^0 w-w\right\|_{H^{-1/4}(\Sigma)}+\|w-w_h\|_{H^{-1/4}(\Sigma)},$$

Theorem 7.1 and Lemma 6.2 with $p=0$. □

Two- and Three-Dimensional Problem

Theorem 7.3. *Let $w_h \in X_h$ be the unique solution of the Galerkin–Bubnov variational formulation* (7.1). *For $w \in H^{r,s}_{pw}(\Sigma)$ with $r,s \in [0,1]$ there holds*

$$\|w-w_h\|_{H^{-1/2,-1/4}(\Sigma)} \leq c\,h^{\min(r,s)+1/4}\,\|w\|_{H^{r,s}_{pw}(\Sigma)}.$$

Proof. The assertion follows by applying Lemma 6.10 with $p_x=p_t=0$ for $X_h=X^{0,0}_{h,h}(\Sigma_N)$, and Lemma 6.15 with $p=0$ for $X_h=S^0_h(\Sigma_N)$ in (7.2). □

Theorem 7.4. *Assume that the boundary decomposition Σ_N is globally quasi-uniform. Let $w_h \in X_h$ be the unique solution of the Galerkin–Bubnov variational problem* (7.1). *For $w \in H^{r,s}_{pw}(\Sigma)$ with $r,s \in [1/4,1]$ there holds*

$$\|w-w_h\|_{L^2(\Sigma)} \leq c\,h^{\min(r,s)-1/4}\,\|w\|_{H^{r,s}_{pw}(\Sigma)}.$$

Proof. By using the triangle inequality, Theorem 6.9 with $p_x=p_t=0$ and Lemma 6.13 for $X_h=X^{0,0}_{h,h}(\Sigma_N)$, Theorem 6.14 with $p=0$ and Lemma 6.16 for $X_h=S^0_h(\Sigma_N)$, we get

$$\begin{aligned}\|w-w_h\|_{L^2(\Sigma)} &\leq \|w-Q_\Sigma w\|_{L^2(\Sigma)}+\|Q_\Sigma w-w_h\|_{L^2(\Sigma)} \\ &\leq c\,h^{\min(r,s)}\,\|w\|_{H^{r,s}_{\mathrm{pw}}(\Sigma)}+c\,h^{-1/2}\,\|Q_\Sigma w-w_h\|_{H^{-1/2,-1/4}(\Sigma)}.\end{aligned}$$

Here, Q_Σ is either the L^2 projection onto $X^{0,0}_{h,h}(\Sigma_N)$ or $S^0_h(\Sigma_N)$. The assertion follows with

$$\|Q_\Sigma w-w_h\|_{H^{-1/2,-1/4}(\Sigma)} \leq \|Q_\Sigma w-w\|_{H^{-1/2,-1/4}(\Sigma)}+\|w-w_h\|_{H^{-1/2,-1/4}(\Sigma)},$$

Theorem 7.3, Lemma 6.10 with $p_x=p_t=0$ for $X_h=X^{0,0}_{h,h}(\Sigma_N)$, and Lemma 6.15 with $p=0$ for $X_h=S^0_h(\Sigma_N)$. □

Hence we can prove the same convergence rates for $X_h = X_{h,h}^{0,0}(\Sigma_N)$ and $X_h = S_h^0(\Sigma_N)$ of the Galerkin approximation w_h in the energy norm as well as in the $L^2(\Sigma)$-norm, assuming that the boundary element mesh Σ_N is shape regular. However, the numerical results in Subsection 7.1.3 show that the $L^2(\Sigma)$-error estimate in Theorem 7.4 is not optimal. This is due to the application of the inverse inequality in Theorem 7.4. One possible way to show an optimal $L^2(\Sigma)$-error estimate for the Galerkin approximation w_h is to consider the integral equation in $H^{1,1/2}(\Sigma)$ and prove a related discrete stability condition which then immediately implies an $L^2(\Sigma)$-error estimate.

7.1.2 Domain Error Estimates

Let $w_h \in X_h$ be the unique solution of the Galerkin variational problem (7.1). We obtain an approximate solution of the initial Dirichlet boundary value problem (5.6) by using the representation formula (5.1) with the approximation w_h, i.e for $(x,t) \in Q$ we have

$$\tilde{u}(x,t) = (\widetilde{V} w_h)(x,t) - (Wg)(x,t) + (\widetilde{M}_0 u_0)(x,t) + (\widetilde{N}_0 f)(x,t).$$

For the related error we obtain for $(x,t) \in Q$

$$\begin{aligned} |u(x,t) - \tilde{u}(x,t)| &= \left| (\widetilde{V}(w - w_h))(x,t) \right| \\ &= \frac{1}{\alpha} \left| \int_{\Sigma} U^\star(x - y, t - \tau)(w - w_h)(y,\tau)\, \mathrm{d}s_y\, \mathrm{d}\tau \right|. \end{aligned}$$

Since $(x,t) \in Q$, the fundamental solution $U^\star(x - \cdot, t - \cdot)$ is smooth for $(y,\tau) \in \Sigma$ and we therefore conclude $U^\star(x - \cdot, t - \cdot) \in H^{-\sigma,-\sigma/2}(\Sigma)$ for any $\sigma \in \mathbb{R}$. Hence

$$|u(x,t) - \tilde{u}(x,t)| \le \frac{1}{\alpha} \|U^\star(x - \cdot, t - \cdot)\|_{H^{-\sigma,-\sigma/2}(\Sigma)} \|w - w_h\|_{\widetilde{H}^{\sigma,\sigma/2}(\Sigma)}. \tag{7.3}$$

Thus, in order to derive an error estimate for the pointwise error $|u(x,t) - \tilde{u}(x,t)|$, $(x,t) \in Q$, we need an error estimate for $\|w - w_h\|_{\widetilde{H}^{\sigma,\sigma/2}(\Sigma)}$ where $\sigma \in \mathbb{R}$ is minimal. In the following, $Q_\Sigma : L^2(\Sigma) \to X_h \subset L^2(\Sigma)$ denotes the L^2 projection onto the space X_h.

Theorem 7.5 (Aubin–Nitsche Trick)**.** *Let $w \in H_{pw}^{r,s}(\Sigma)$ for some $r,s \in [0,1]$ be the unique solution of* (5.7)*, and let $w_h \in X_h$ be the unique solution of the Galerkin variational problem* (7.1)*. Assume that the adjoint single layer operator*

$$V^* : H^{-1-\sigma,-1/2-\mu}(\Sigma) \to H^{-\sigma,-\mu}(\Sigma)$$

is continuous and bijective for some $-2 \le \sigma \le -1$ and $\mu = \sigma/2$. Then there holds the error estimate

$$\|w - w_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \le c\, h^{\min(r,s) - \mu} \|w\|_{H_{pw}^{r,s}(\Sigma)}.$$

Proof. For $\sigma \leq -1$ and $\mu = \sigma/2$ we have

$$\|w - w_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} = \sup_{0 \neq v \in H^{-\sigma,-\mu}(\Sigma)} \frac{\langle w - w_h, v\rangle_\Sigma}{\|v\|_{H^{-\sigma,-\mu}(\Sigma)}}.$$

By assumption, the adjoint single layer operator

$$V^* : H^{-1-\sigma,-1/2-\mu}(\Sigma) \to H^{-\sigma,-\mu}(\Sigma)$$

is continuous and bijective. Hence for $v \in H^{-\sigma,-\mu}(\Sigma)$ there exists a unique density $z \in H^{-1-\sigma,-1/2-\mu}(\Sigma)$ such that $v = V^* z$. Therefore, and by applying the Galerkin orthogonality

$$\langle V(w - w_h), \tau_h\rangle_\Sigma = 0 \quad \text{for all } \tau_h \in X_h,$$

we obtain

$$\begin{aligned}
\|w - w_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} &= \sup_{0 \neq z \in H^{-1-\sigma,-1/2-\mu}(\Sigma)} \frac{\langle w - w_h, V^* z\rangle_\Sigma}{\|V^* z\|_{H^{-\sigma,-\mu}(\Sigma)}} \\
&= \sup_{0 \neq z \in H^{-1-\sigma,-1/2-\mu}(\Sigma)} \frac{\langle V(w - w_h), z - Q_\Sigma z\rangle_\Sigma}{\|V^* z\|_{H^{-\sigma,-\mu}(\Sigma)}}.
\end{aligned}$$

Since V^* is bijective, there exists a constant $c > 0$ such that [17, Lemma A.40]

$$\|V^* z\|_{H^{-\sigma,-\mu}(\Sigma)} \geq c\, \|z\|_{H^{-1-\sigma,-1/2-\mu}(\Sigma)} \quad \text{for all } z \in H^{-1-\sigma,-1/2-\mu}(\Sigma).$$

Thus, by using the boundedness of the operator $V : H^{-1/2,-1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma)$ we conclude

$$\begin{aligned}
&\|w - w_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \\
&\quad \leq \tilde{c}\, \|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)} \sup_{0 \neq z \in H^{-1-\sigma,-1/2-\mu}(\Sigma)} \frac{\|z - Q_\Sigma z\|_{H^{-1/2,-1/4}(\Sigma)}}{\|z\|_{H^{-1-\sigma,-1/2-\mu}(\Sigma)}}.
\end{aligned}$$

When considering $-1 - \sigma \leq 1$, i.e. $\sigma \geq -2$, we obtain from the approximation properties of the operator Q_Σ the error estimate

$$\|w - w_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \leq \hat{c}\, h^{-1/4-\mu}\, \|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)},$$

and the assertion follows by applying the error estimate for the Galerkin approximation w_h in the energy norm. $\square$

Hence in the one-dimensional case we obtain the optimal error estimate

$$\|w - w_h\|_{\widetilde{H}^{\mu}(\Sigma)} \leq c\, h^{s-\mu}\, \|w\|_{H^s_{\mathrm{pw}}(\Sigma)}$$

for $w \in H^s(\Sigma)$ with $s \in [0,1]$ and $-1 \le \mu \le -1/2$.

Note that the estimate in Theorem 7.5 may be extended to $-1 \le \sigma \le -1/2$. The proof follows exactly the same path but utilizes approximation properties of the L^2 projection operators for functions $w \in \widetilde{H}^{r,s}(\Sigma)$ with $r,s < 0$, see [10, 45, 62].

Now assume that the solution w of the variational formulation (5.7) is sufficiently smooth, i.e. $w \in H^{1,1}_{\mathrm{pw}}(\Sigma)$. From estimate (7.3) and by choosing $\sigma = -2$ in Theorem (7.5) we get, for $(x,t) \in Q$, the optimal pointwise error estimate

$$\begin{aligned} |u(x,t) - \tilde{u}(x,t)| &\le \tilde{c}\, \|U^\star(x-\cdot, t-\cdot)\|_{H^{2,1}(\Sigma)}\, \|w - w_h\|_{\widetilde{H}^{-2,-1}(\Sigma)} \\ &\le c\, h^2\, \|U^\star(x-\cdot, t-\cdot)\|_{H^{2,1}(\Sigma)}\, \|w\|_{H^{1,1}_{\mathrm{pw}}(\Sigma)}. \end{aligned} \tag{7.4}$$

Next we consider problem (3.1) with source term $f \equiv 0$. To estimate the global error $\|u - \tilde{u}\|_{H^{1,1/2}_{;0,}(Q)}$ we proceed as follows. We first consider the Dirichlet trace of the discretized representation formula (7.17), i.e. we have

$$\hat{g} := V w_h + \frac{1}{2} g - K g.$$

Moreover, the first boundary integral equation in (5.3) gives

$$g = V w + \frac{1}{2} g - K g,$$

and we therefore conclude the relation

$$g - \hat{g} = V(w - w_h). \tag{7.5}$$

Theorem 7.6 (Domain error estimate)**.** *Let $u \in H^{1,1/2}_{;0,}(Q)$ be the unique solution of the Dirichlet boundary value problem* (3.1) *with source term $f \equiv 0$, and let $\tilde{u} \in H^{1,1/2}_{;0,}(Q)$ be the corresponding approximation given by* (7.17) *with $f \equiv 0$ and $u_0 \equiv 0$. Then there holds the error estimate*

$$\|u - \tilde{u}\|_{H^{1,1/2}_{;0,}(Q)} \le c\, \|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)}.$$

Proof. The solution $u = \bar{u} + \mathcal{E}_0 g \in H^{1,1/2}_{;0,}(Q)$ of problem (3.1) with homogeneous source term is given as the unique solution of the variational problem

$$a(\bar{u}, v) = -a(\mathcal{E}_0 g, v) \quad \text{for all } v \in H^{1,1/2}_{0;,0}(Q).$$

For the approximation $\tilde{u}$ we consider the decomposition $\tilde{u} = \hat{u} + \mathcal{E}_0 \hat{g} \in H^{1,1/2}_{;0,}(Q)$ which satisfies

$$a(\hat{u}, v) = -a(\mathcal{E}_0 \hat{g}, v) \quad \text{for all } v \in H^{1,1/2}_{0;,0}(Q).$$

By subtracting the last two equations we obtain

$$a(\bar{u}-\hat{u},v) = a(\mathcal{E}_0(\hat{g}-g),v) \quad \text{for all } v \in H^{1,1/2}_{0;,0}(Q).$$

Since $\bar{u}-\hat{u} \in H^{1,1/2}_{0;0,}(Q)$, we can apply the stability estimate (3.6) to get

$$\begin{aligned}
\frac{1}{2}\,\|\bar{u}-\hat{u}\|_{H^{1,1/2}_{0;0,}(Q)} &\leq \sup_{0\neq v\in H^{1,1/2}_{0;,0}(Q)} \frac{a(\bar{u}-\hat{u},v)}{\|v\|_{H^{1,1/2}_{0;,0}(Q)}} \\
&= \sup_{0\neq v\in H^{1,1/2}_{0;,0}(Q)} \frac{a(\mathcal{E}_0(\hat{g}-g),v)}{\|v\|_{H^{1,1/2}_{0;,0}(Q)}} \leq c\,\|\mathcal{E}_0(\hat{g}-g)\|_{H^{1,1/2}_{;0,}(Q)}\,.
\end{aligned}$$

Hence, by using the triangle inequality, the Poincaré inequality and the boundedness of the inverse trace operator $\mathcal{E}_0$, we obtain

$$\begin{aligned}
\|u-\tilde{u}\|_{H^{1,1/2}_{;0,}(Q)} &\leq \|\bar{u}-\hat{u}\|_{H^{1,1/2}_{;0,}(Q)} + \|\mathcal{E}_0(\hat{g}-g)\|_{H^{1,1/2}_{;0,}(Q)} \\
&\leq \tilde{c}\,\|\bar{u}-\hat{u}\|_{H^{1,1/2}_{0;0,}(Q)} + \|\mathcal{E}_0(\hat{g}-g)\|_{H^{1,1/2}_{;0,}(Q)} \\
&\leq \hat{c}\,\|\mathcal{E}_0(\hat{g}-g)\|_{H^{1,1/2}_{;0,}(Q)} \leq \bar{c}\,\|\hat{g}-g\|_{H^{1/2,1/4}(\Sigma)}\,,
\end{aligned}$$

and the assertion follows with the relation (7.5). □

Note that for $w \in H^{1,1}_{\mathrm{pw}}(\Sigma)$ we finally conclude the optimal error estimate

$$\|u-\tilde{u}\|_{H^{1,1/2}_{;0,}(Q)} \leq c\,h^{5/4}\,\|w\|_{H^{1,1}_{\mathrm{pw}}(\Sigma)}\,.$$

7.1.3 Numerical Results

We consider the initial Dirichlet boundary value problem (5.6) with boundary conditions $g \in H^{1/2,1/4}(\Sigma)$, homogeneous source term $f \equiv 0$, time horizon $T = 1$, and with the heat capacity constant $\alpha = 10$. We present examples for the spatially one- and two-dimensional case and compare the tensor product decomposition with a triangulation of the space–time boundary Σ. All of the following examples refer to a shape regular boundary decomposition Σ_N.

The Galerkin boundary element discretization of the variational formulation (5.7) is done by using piecewise constant basis functions $X_h = \operatorname{span}\{\varphi^0_\ell\}_{\ell=1}^N$, defined with respect to the boundary decomposition Σ_N. For the approximation of the Dirichlet datum g we consider a conforming boundary element space $Y_h = \operatorname{span}\{\psi_i\}_{i=1}^{M_\Sigma} \subset H^{1/2,1/4}(\Sigma)$ introduced in the previous chapter, while the initial datum u_0 is discretized by using the space of piecewise linear and globally continuous functions $S_h^1(\Omega_{N_\Omega}) = \operatorname{span}\left\{\varphi_j^1\right\}_{j=1}^{M_\Omega}$, which is defined with respect to a given triangulation $\Omega_{N_\Omega} := \{\omega_i\}_{i=1}^{N_\Omega}$ of the domain Ω. This leads to the system of linear equations

$$\mathsf{V}_h \boldsymbol{w} = (\frac{1}{2}\mathsf{M}_h + \mathsf{K}_h)\boldsymbol{g} - \mathsf{M}_h^0 \boldsymbol{u}_0 \tag{7.6}$$

where

$$\mathsf{V}_h[\ell,k] := \frac{1}{\alpha} \int_{\sigma_\ell} \int_{\sigma_k} U^\star(x-y,t-\tau)\, \mathrm{d}s_y\, \mathrm{d}\tau\, \mathrm{d}s_x\, \mathrm{d}t, \tag{7.7}$$

$$\mathsf{K}_h[\ell,i] := \frac{1}{\alpha} \int_{\sigma_\ell} \int_{\Sigma} \partial_{n_y} U^\star(x-y,t-\tau)\, \psi_i(y,\tau)\, \mathrm{d}s_y\, \mathrm{d}\tau\, \mathrm{d}s_x\, \mathrm{d}t, \tag{7.8}$$

$$\mathsf{M}_h^0[\ell,j] := \int_{\sigma_\ell} \int_{\Omega} U^\star(x-y,t)\, \varphi_j^1(y)\, \mathrm{d}y\, \mathrm{d}s_x\, \mathrm{d}t, \tag{7.9}$$

and

$$\mathsf{M}_h[\ell,i] := \int_{\sigma_\ell} \int_{\Sigma} \psi_i(y,\tau)\, \mathrm{d}s_y\, \mathrm{d}\tau\, \mathrm{d}s_x\, \mathrm{d}t. \tag{7.10}$$

The vectors $\boldsymbol{w} \in \mathbb{R}^N$, $\boldsymbol{g} \in \mathbb{R}^{M_\Sigma}$ and $\boldsymbol{u}_0 \in \mathbb{R}^{M_\Omega}$ in (7.6) represent the coefficients of the trial function $w_h := \sum_{\ell=1}^N w_\ell \varphi_\ell^0$, and the given approximations $g_h := \sum_{i=1}^{M_\Sigma} g_i \psi_i$ and $u_h^0 := \sum_{i=1}^{M_\Omega} u_i^0 \varphi_i^1$ of the Dirichlet datum g and the initial datum u_0, respectively. Due to the ellipticity of the single layer operator V, the matrix V_h is positive definite and therefore (7.6) is uniquely solvable. The system is solved by using the GMRES method with a relative accuracy of 10^{-8} as stopping criteria.

By using the representation formula (5.1) with the approximations w_h, g_h and u_h^0 we can compute an approximation $\tilde{u}$ of u, i.e. for $(x,t) \in Q$ we obtain

$$\tilde{u}(x,t) = \sum_{i=1}^{M_\Omega} u_i^0 (\widetilde{M}_0 \varphi_i^1)(x,t) + \sum_{\ell=1}^{N} w_\ell (\widetilde{V} \varphi_\ell^0)(x,t) - \sum_{i=1}^{M_\Sigma} g_i (W \psi_i)(x,t). \tag{7.11}$$

Computation of Matrix Entries

In this paragraph we comment on the stable computation of the matrix entries (7.7), (7.8),(7.9) and (7.10), and on the stable evaluation of the representation formula (7.11) based on [14]. Due to the singularity of the fundamental solution at $(x,t) = (y,s)$ we have to deal with weakly singular integrands. For the assembly of the boundary element matrices V_h, K_h and M_h^0 we use an element-based strategy, i.e. we loop over all pairs of boundary elements for V_h and K_h, and over boundary elements and finite elements of the initial mesh Ω_h for M_h^0. Depending on the mutual position of the two elements we use different integration routines.

In the one-dimensional case we can compute all matrix entries analytically and therefore we skip the discussion of the 1D problem. The situation is different in the two-dimensional case. In what follows, we will discuss the integration routines for a tensor product decomposition of Σ, i.e. we choose $X_h = X^{0,0}_{h_x,h_t}(\Sigma_N)$ and $Y_h \in \left\{X^{1,0}_{h_x,h_t}(\Sigma_N), X^{1,1}_{h_x,h_t}(\Sigma_N)\right\}$. The results can be extended to boundary element spaces defined with respect to a triangulation of the space–time boundary Σ with just a few slight modifications.

Let us first consider the matrix V_h. In Fig. 7.1a the integration routines for the computation of the matrix entries $\mathsf{V}_h[\ell,\cdot]$ are shown. The grid represents a part of the space–time boundary element mesh Σ_N. The element σ_ℓ is fixed and depending on where the element σ_k is located, we distinguish between the following integration routines:

A – analytic integration,

N – fully numerical integration,

S – semi-analytic integration, i.e. numerical in space and analytical in time,

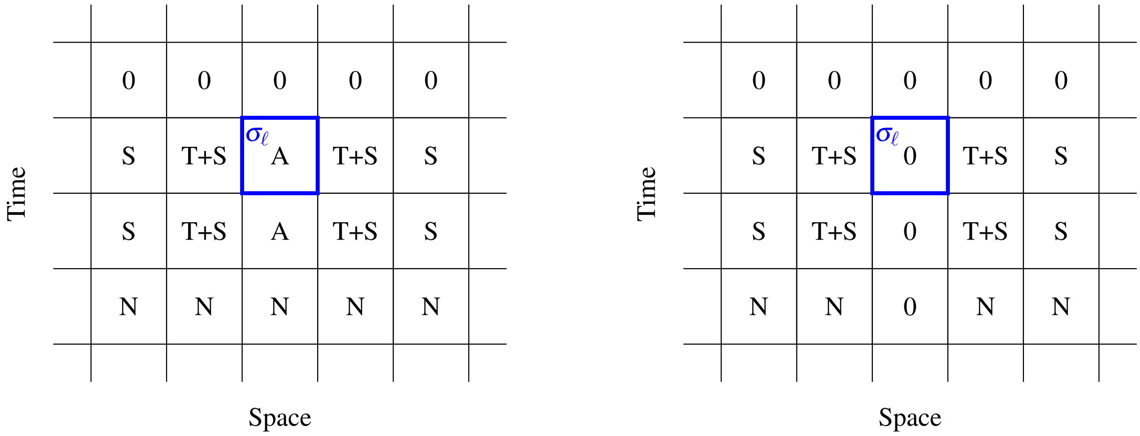
T – transformation of the integral to get rid of the weak singularity.

We give a sketch of the overall situation in Fig. 7.1a. For the computation of the matrix entries corresponding to the elements marked with N, i.e. if two elements σ_ℓ and σ_k are well separated, we use numerical integration in space and time. The computation of these entries takes most of the computational time, but the evaluation of these integrals can be vectorized [14]. The integrands corresponding to the elements marked with T have a singularity at the shared space-vertex. In these cases we transform the integrals with respect to the spatial dimensions to get rid of the weak singularity [25, 53] and then apply semi-analytic integration, i.e. numerical integration in space and analytical integration in time [57]. If the element σ_k is located above the element σ_ℓ, the value of the integral is zero due to the causality of the fundamental solution (4.6).

The situation is quite the same for the matrix K_h. The only difference is that the value of the integral is zero if the elements σ_ℓ and σ_k share the same spatial element γ, see Fig. 7.1b.

For the computation of the matrix entries of M^0_h, where we assemble a local matrix corresponding to a boundary element and a triangular element of the initial mesh, we proceed as follows. For the integral over the triangle we use the seven-point rule [52], and for the integral over the boundary element we apply semi-analytic integration, i.e. analytical in time and numerical in space. In this case we do not have to handle weakly singular integrands separately. The sparse matrix M_h can be assembled from local mass matrices in a standard way.

Similar integration techniques are used for the evaluation of the representation formula (7.11). However, since we evaluate (7.11) for $(x,t) \in Q$, we do not have to handle weakly singular integrands.



(a) Computation of V_h. (b) Computation of K_h.

Figure 7.1: Computation of the matrix entries $\mathsf{V}_h[\ell,\cdot]$ and $\mathsf{K}_h[\ell,\cdot]$ for a fixed boundary element σ_ℓ and varying element σ_k.

One-Dimensional problem

First we provide numerical experiments for the simple one-dimensional problem. We consider the spatial domain $\Omega = (0,1)$ and homogeneous Dirichlet conditions $g \equiv 0$. Recall that the boundary elements are line segments in temporal dimension.

Uniform Refinement. The first example corresponds to the initial datum

$$u_0(x) = \sin(2\pi x) \quad \text{for } x \in \Omega = (0,1)$$

and a globally uniform boundary element mesh of mesh size $h = 2^{-L}$. Table 7.1 shows the error $\|w - w_h\|_{L_2(\Sigma)}$ and the estimated order of convergence (eoc), which is linear as expected according to Theorem 7.2, assuming that $w \in H^1_{\mathrm{pw}}(\Sigma)$. Moreover, the iteration numbers of the GMRES method are given.

Adaptive Refinement. For the second example we consider the initial datum

$$u_0(x) = 5\exp(-10x)\sin(\pi x) \quad \text{for } x \in \Omega = (0,1),$$

which motivates the use of a locally quasi-uniform boundary element mesh resulting from some adaptive refinement strategy. The Galerkin approximation w_h is shown in Figure 7.2. In Figure 7.3 the convergence history of the approximation for uniform and adaptive refinement is given.

L	N	$\|w-w_h\|_{L_2(\Sigma)}$	eoc	It.
5	64	$7.950\cdot10^{-2}$	1.01	31
6	128	$3.959\cdot10^{-2}$	1.01	41
7	256	$1.976\cdot10^{-2}$	1.00	50
8	512	$9.872\cdot10^{-3}$	1.00	59
9	1 024	$4.929\cdot10^{-3}$	1.00	70
10	2 048	$2.468\cdot10^{-3}$	1.00	82
11	4 096	$1.233\cdot10^{-3}$	1.00	96

Table 7.1: $L^2(\Sigma)$-error and convergence rate of the Galerkin approximation w_h, and iteration numbers of the GMRES method (It.) in the case of uniform refinement in 1D. The parameter N denotes the number of boundary elements on level L.

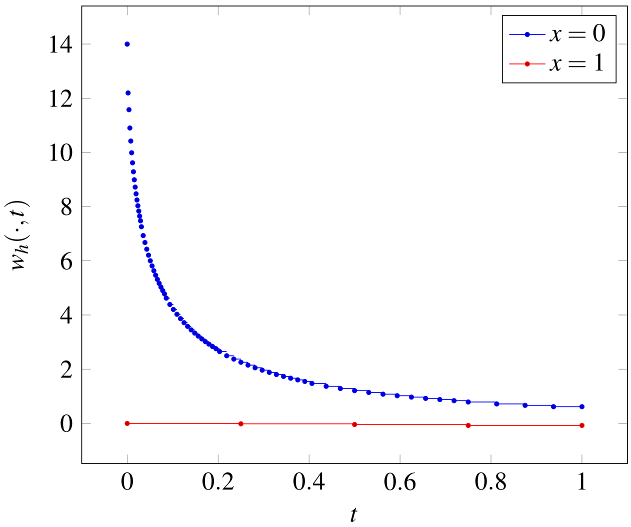


Figure 7.2: Galerkin approximation w_h on the two boundary parts Σ_0 and Σ_1 in the case of adaptive refinement in 1D.

Two-Dimensional Problem

For the numerical experiments for the spatially two-dimensional problem we choose the spatial domain $\Omega=(0,1)^2$, i.e. $Q=(0,1)^3$.

Uniform Refinement. We consider the exact solution

$$u(x,t)=\exp\left(-\frac{t}{\alpha}\right)\sin\left(x_1\cos\frac{\pi}{8}+x_2\sin\frac{\pi}{8}\right)\quad\text{for }(x,t)=(x_1,x_2,t)\in Q,$$

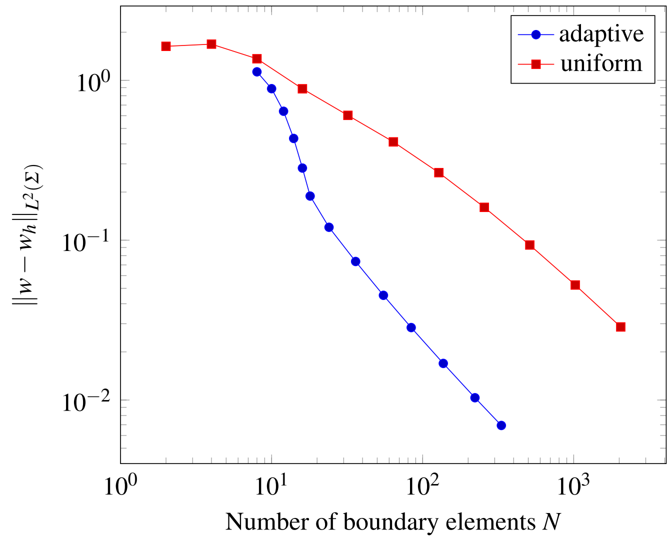


Figure 7.3: Convergence history of the Galerkin approximation w_h for uniform and adaptive refinement in 1D.

and determine the Dirichlet datum g and the initial datum u_0 accordingly. We use a globally quasi-uniform boundary element mesh with mesh size $h = \mathcal{O}(2^{-L})$, both for the tensor product approach as well as for a triangulation of the space–time boundary Σ. Table 7.2 and Table 7.3 show the error $\|w - w_h\|_{L^2(\Sigma)}$ of the Galerkin approximation w_h as well as the pointwise error $|(u - \tilde{u})(x,t)|$ in $x = (0.5, 0.5)$, $t = 0.5$, and the corresponding convergence rates (eoc). Additionally, the iteration numbers of the GMRES method are listed. While the convergence rate of the pointwise error is quadratic and therefore in line with the theoretical findings (7.4), we obtain linear convergence of the Galerkin approximation w_h in the $L^2(\Sigma)$-norm, which is, according to Theorem 7.4, better than expected, see the discussion at the end of Subsection 7.1.1.

As already mentioned before, we consider shape regular boundary elements only, i.e. in case of the tensor product approach we choose $h_x \sim h_t$. Although the relation $h_t \sim h_x^2$ is recommended in order to obtain optimal convergence results of the Galerkin approximation w_h in the energy norm [10, 45], we get linear convergence of the approximation in the $L^2(\Sigma)$-norm in our experiments. Note that numerical results in [10, Section 6] indicate that the relation $h_t \sim h_x^2$ is not necessary for an optimal convergence rate in the $L^2(\Sigma)$-norm.

Adaptive Refinement. As a second example we consider the initial datum

$$u_0(x_1, x_2) = 40 \exp\left(-10(x_1 + x_2)\right) \sin\left(\pi x_1\right) \sin\left(\pi x_2\right) \quad \text{for } (x_1, x_2) \in \Omega,$$

see Figure 7.4, and we use a globally quasi-uniform as well as a locally quasi-uniform triangulation of the space–time boundary resulting from some adaptive refinement strat-

L	N	$\|w-w_h\|_{L_2(\Sigma)}$	eoc	$\|(u-\tilde{u})(x,t)\|$	eoc	It.
0	4	$2.795\cdot10^{-1}$	-	$2.598\cdot10^{-2}$	-	2
1	16	$1.413\cdot10^{-1}$	0.98	$5.544\cdot10^{-3}$	2.23	9
2	64	$6.882\cdot10^{-2}$	1.04	$9.146\cdot10^{-4}$	2.60	14
3	256	$3.353\cdot10^{-2}$	1.04	$2.485\cdot10^{-4}$	1.88	18
4	1 024	$1.650\cdot10^{-2}$	1.02	$6.315\cdot10^{-5}$	1.98	24
5	4 096	$8.172\cdot10^{-3}$	1.01	$1.563\cdot10^{-5}$	2.01	35
6	16 384	$4.066\cdot10^{-3}$	1.01	$3.748\cdot10^{-6}$	2.06	50
7	65 536	$2.030\cdot10^{-3}$	1.00	$8.468\cdot10^{-7}$	2.15	67

Table 7.2: Error and convergence rates of the Galerkin approximation w_h and of the approximated solution $\tilde{u}$ in the interior, and iteration numbers of the GMRES method (It.) in the case of uniform refinement for a tensor product decomposition of Σ in 2D. The parameter N denotes the number of boundary elements on level L.

L	N	$\|w-w_h\|_{L_2(\Sigma)}$	eoc	$\|(u-\widetilde{u})(x,t)\|$	eoc	It.
0	16	$1.588\cdot10^{-1}$	-	$2.046\cdot10^{-2}$	-	9
1	64	$6.326\cdot10^{-2}$	1.33	$5.395\cdot10^{-3}$	1.92	16
2	256	$2.502\cdot10^{-2}$	1.34	$1.337\cdot10^{-3}$	2.01	23
3	1 024	$1.084\cdot10^{-2}$	1.21	$3.336\cdot10^{-4}$	2.00	32
4	4 096	$5.040\cdot10^{-3}$	1.11	$8.348\cdot10^{-5}$	2.00	44
5	16 384	$2.447\cdot10^{-3}$	1.04	$2.093\cdot10^{-5}$	2.00	62
6	65 536	$1.233\cdot10^{-3}$	0.99	$5.265\cdot10^{-6}$	1.99	85

Table 7.3: Error and convergence rates of the Galerkin approximation w_h and of the approximated solution $\tilde{u}$ in the interior, and iteration numbers of the GMRES method (It.) in the case of uniform refinement for a triangulation of Σ in 2D. The parameter N denotes the number of boundary elements on level L.

egy. In Figure 7.6 the convergence history of the approximation for uniform and adaptive refinement is given, while the resulting boundary element mesh is shown in Figure 7.5.

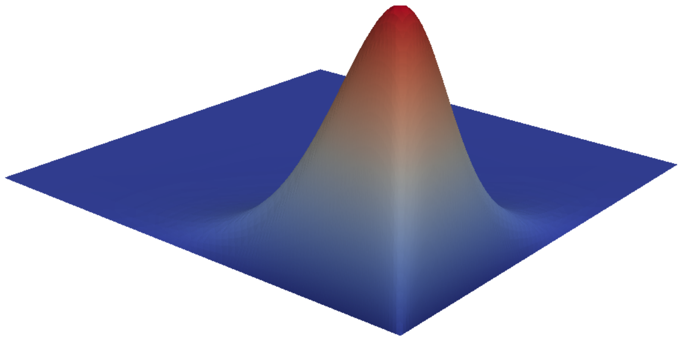


Figure 7.4: Initial datum u_0 for the sample Dirichlet boundary value problem in 2D.

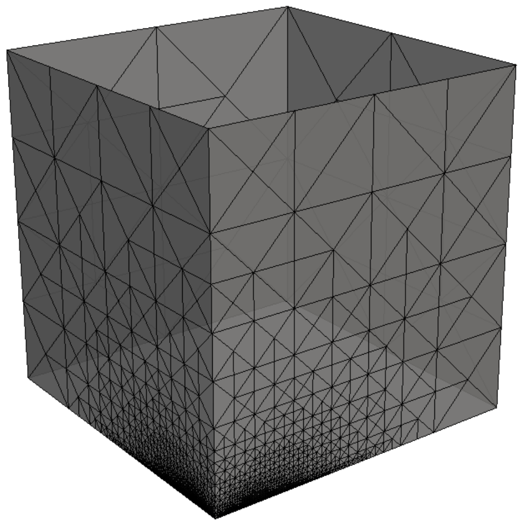


Figure 7.5: Triangular boundary element mesh in the case of adaptive refinement in 2D.

7.2 Neumann Boundary Value Problem

In this section we discretize the variational formulation (5.11) in order to compute an approximation of the unknown Dirichlet datum $g = \gamma_0^{\text{int}} u \in H^{1/2,1/4}(\Sigma)$ by using the introduced space–time boundary element spaces and derive a priori error estimates for the Galerkin approximation in Subsection 7.2.1. The numerical analysis of the discretized indirect formulation (5.13) follows exactly the same path. In Subsection 7.2.2 we prove error estimates for the related approximation of the solution u in the space–time domain Q, and we provide numerical experiments in Subsection 7.2.3.

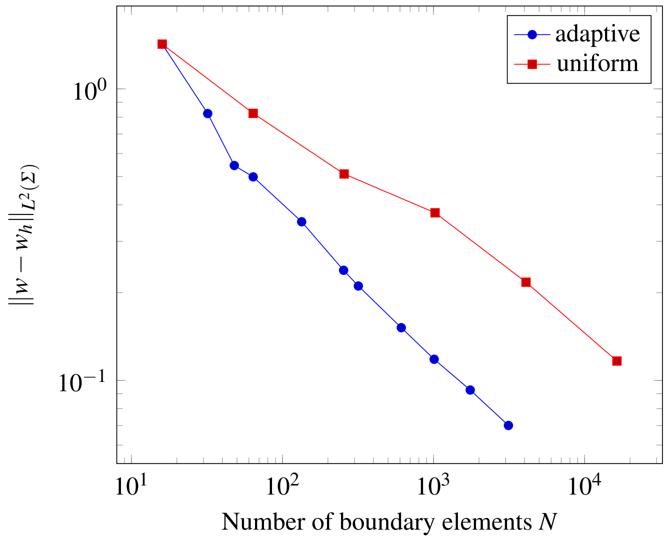


Figure 7.6: Convergence of the Galerkin approximation w_h for uniform and adaptive refinement in 2D.

For the discretization of the variational formulation (5.11) we consider a conforming boundary element space $Y_h \subset H^{1/2,1/4}(\Sigma)$ defined with respect to a shape regular boundary element mesh Σ_N as introduced in Chapter 6. The Galerkin–Bubnov variational formulation of (5.11) is to find $g_h \in Y_h$ such that

$$\langle D g_h, v_h \rangle_\Sigma = \langle (\frac{1}{2} I - K') w - M_1 u_0 - N_1 f, v_h \rangle_\Sigma \quad \text{for all } v_h \in Y_h. \tag{7.12}$$

Due to the ellipticity of the hypersingular integral operator D and the boundedness of the integral operators, problem (7.12) is uniquely solvable.

7.2.1 Error Estimates

Let $g \in H^{1/2,1/4}(\Sigma)$ be the unique solution of the variational problem (5.11). Since the operator D is elliptic and bounded we can apply Cea's Lemma [62, Theorem 8.1] to conclude quasi-optimality of the Galerkin approximation $g_h \in Y_h$, i.e. we have

$$\|g - g_h\|_{H^{1/2,1/4}(\Sigma)} \leq \frac{c_2^D}{c_1^D} \inf_{v_h \in Y_h} \|g - v_h\|_{H^{1/2,1/4}(\Sigma)} \,. \tag{7.13}$$

Hence we can use the approximation properties of the boundary element space Y_h to derive error estimates for the discrete solution g_h of (7.12).

One-Dimensional Problem

Recall that in the one-dimensional case we have $\Sigma = \Sigma_a \cup \Sigma_b$. Moreover, we can identify the Sobolev spaces $H^{r,s}(\Sigma)$ with $H^s(\Sigma)$. Therefore, we can either use $S_h^0(\Sigma_N)$ or $S_h^1(\Sigma_N)$ for the approximation of g, since $S_h^p(\Sigma_N) \subset H^{1/4}(\Sigma)$ for $p \in \{0,1\}$.

Theorem 7.7. *Let $g_h \in S_h^p(\Sigma_N)$ be the unique solution of the Galerkin variational problem* (7.12). *For $g \in H^s(\Sigma)$ with $s \in [1/4, p+1]$ there holds the error estimate*

$$\|g - g_h\|_{H^{1/4}(\Sigma)} \le c\, h^{s-1/4}\, \|g\|_{H^s(\Sigma)}\,.$$

Proof. Follows by applying Lemma 6.3 for $p = 0$ and Lemma 6.4 for $p = 1$ in (7.13) for both boundary parts Σ_a and Σ_b. □

Moreover, we can derive an error estimate in weaker norms by using the Aubin–Nitsche Trick.

Theorem 7.8 (Aubin–Nitsche Trick)**.** *Let $g \in H^s(\Sigma)$ for some $s \in [1/4, p+1]$ be the unique solution of the variational problem* (5.11)*, and let $g_h \in S_h^p(\Sigma_N)$ be the unique solution of the Galerkin variational problem* (7.12)*. Assume that the adjoint hypersingular layer operator*

$$D^* : H^{1/2-\mu}(\Sigma) \to H^{-\mu}(\Sigma)$$

is continuous and bijective for some $-1/2 \le \mu \le 1/4$. Then there holds the error estimate

$$\|g - g_h\|_{\widetilde{H}^{\mu}(\Sigma)} \le c\, h^{s-\mu}\, \|g\|_{H^s(\Sigma)}\,.$$

Proof. For $-1/2 \le \mu \le 1/4$ we have

$$\|g - g_h\|_{\widetilde{H}^{\mu}(\Sigma)} = \sup_{0 \ne v \in H^{-\mu}(\Sigma)} \frac{\langle g - g_h, v\rangle_\Sigma}{\|v\|_{H^{-\mu}(\Sigma)}}.$$

By assumption, the adjoint hypersingular operator

$$D^* : H^{1/2-\mu}(\Sigma) \to H^{-\mu}(\Sigma)$$

is continuous and bijective. Hence for $v \in H^{-\mu}(\Sigma)$ there exists a unique $z \in H^{1/2-\mu}(\Sigma)$ such that $v = D^* z$. Therefore, and by applying the Galerkin orthogonality

$$\langle D(g - g_h), v_h\rangle_\Sigma = 0 \quad \text{for all } v_h \in S_h^p(\Sigma_N),$$

we obtain

$$\begin{aligned}
\|g - g_h\|_{\widetilde{H}^{\mu}(\Sigma)} &= \sup_{0 \ne z \in H^{1/2-\mu}(\Sigma)} \frac{\langle g - g_h, D^* z\rangle_\Sigma}{\|D^* z\|_{H^{-\mu}(\Sigma)}} \\
&= \sup_{0 \ne z \in H^{1/2-\mu}(\Sigma)} \frac{\langle D(g - g_h), z - Q_\Sigma^p z\rangle_\Sigma}{\|D^* z\|_{H^{-\mu}(\Sigma)}}.
\end{aligned}$$

Since D^* is bijective, there exists a constant $c > 0$ such that [17, Lemma A.40]

$$\|D^* z\|_{H^{-\mu}(\Sigma)} \geq c\, \|z\|_{H^{1/2-\mu}(\Sigma)} \quad \text{for all } z \in H^{1/2-\mu}(\Sigma).$$

Thus, by using the boundedness of the operator $D : H^{1/4}(\Sigma) \to H^{-1/4}(\Sigma)$ we conclude

$$\|g - g_h\|_{\widetilde{H}^{\mu}(\Sigma)} \leq \tilde{c}\, \|g - g_h\|_{H^{1/4}(\Sigma)} \sup_{0 \neq z \in H^{1/2-\mu}(\Sigma)} \frac{\|z - Q_\Sigma^p z\|_{H^{1/4}(\Sigma)}}{\|z\|_{H^{1/2-\mu}(\Sigma)}}.$$

From the approximation properties of the operator Q_Σ^p we obtain the error estimate

$$\|g - g_h\|_{\widetilde{H}^{\mu}(\Sigma)} \leq \hat{c}\, h^{1/4-\mu}\, \|g - g_h\|_{H^{1/4}(\Sigma)},$$

and the assertion follows by applying the error estimate for the Galerkin approximation g_h in the energy norm. $\square$

By using Theorem 7.8 with $\mu = 0$ we conclude the optimal $L^2(\Sigma)$-error estimate

$$\|g - g_h\|_{L^2(\Sigma)} \leq c\, h^s\, \|g\|_{H^s(\Sigma)}.$$

for the Galerkin approximation $g_h \in S_h^p(\Sigma_N)$ of $g \in H^s(\Sigma)$ with $s \in [1/4, p+1]$. Hence for a sufficiently smooth Dirichlet datum, i.e. $g \in H^{p+1}(\Sigma)$, we obtain

$$\|g - g_h\|_{L^2(\Sigma)} \leq c\, h^{p+1}\, \|g\|_{H^{p+1}(\Sigma)}. \tag{7.14}$$

Two- and Three-Dimensional Problem

Here we have to distinguish between the boundary element spaces $Y_h = X_{h,h}^{1,p_t}(\Sigma_N)$ and $Y_h = S_h^1(\Sigma_N)$ due to the different regularity assumptions that are necessary in order to obtain the approximation properties of the related L^2 projection operators, see Chapter 6. In the following, p_t denotes the polynomial degree of the tensor product boundary element spaces in temporal dimension.

Theorem 7.9. *Let $g_h \in X_{h,h}^{1,p_t}(\Sigma_N)$ be the unique solution of the Galerkin–Bubnov variational formulation* (7.12). *For $g \in H^{r,s}(\Sigma)$ with $r \in [1/2, 2]$ and $s \in [1/4, p_t + 1]$ there holds the error estimate*

$$\|g - g_h\|_{H^{1/2,1/4}(\Sigma)} \leq c\, h^{\beta(r,s)}\, \|g\|_{H^{r,s}(\Sigma)}$$

with

$$\beta(r,s) := \min\left(\beta_1(r,s,1/2,1/4), \beta_2(r,s,1/2,1/4)\right) \tag{7.15}$$

and β_1, β_2 given by (6.9).

Proof. Follows by applying Lemma 6.11 for $p_t = 0$ and Lemma 6.12 for $p_t = 1$ in (7.13). $\square$

For a triangulation of the boundary Σ we conclude the following convergence rates of the Galerkin approximation g_h.

Theorem 7.10. *Let $g_h \in S_h^1(\Sigma_N)$ be the unique solution of the Galerkin–Bubnov variational formulation* (7.12)*. For $g \in H^r(\Sigma)$ with $r \in [1/2, 2]$ there holds*

$$\|g - g_h\|_{H^{1/2,1/4}(\Sigma)} \leq c\, h^{r-1/2} \, \|g\|_{H^r(\Sigma)} \, .$$

Proof. The assertion follows by applying Corollary 6.17 in (7.13). $\square$

Moreover, for $u \in H^{r,s}(\Sigma)$ with $r, s \in [1/2, 1]$ estimate (6.16) yields

$$\|g - g_h\|_{H^{1/2,1/4}(\Sigma)} \leq c\, h^{\min(r,s)-1/2} \, \|g\|_{H^{r,s}(\Sigma)} \, .$$

Again, we can derive error estimates in weaker norms by using the Aubin–Nitsche Trick in the case of the tensor product approach.

Theorem 7.11 (Aubin–Nitsche Trick)**.** *Let $g \in H^{r,s}(\Sigma)$ for some $r \in [1/2, 2]$ and some $s \in [1/4, p_t + 1]$ be the unique solution of the variational problem* (5.11)*, and let $g_h \in X_{h,h}^{1,p_t}(\Sigma_N)$ be the unique solution of the Galerkin variational problem* (7.12)*. Assume that the adjoint hypersingular operator*

$$D^* : H^{1-\sigma,1/2-\mu}(\Sigma) \to H^{-\sigma,-\mu}(\Sigma)$$

is continuous and bijective for some $-1 \leq \sigma \leq 1/2$ and $\mu = \sigma/2$. Then there holds the error estimate

$$\|g - g_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \leq c\, h^{\beta(r,s)+1/4-\mu} \, \|g\|_{H^{r,s}(\Sigma)}$$

with β given by (7.15)*.*

Proof. For $-1 \leq \sigma \leq 1/2$ and $\mu = \sigma/2$ we have

$$\|g - g_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} = \sup_{0 \neq v \in H^{-\sigma,-\mu}(\Sigma)} \frac{\langle g - g_h, v\rangle_\Sigma}{\|v\|_{H^{-\sigma,-\mu}(\Sigma)}} .$$

By assumption, the adjoint hypersingular operator

$$D^* : H^{1-\sigma,1/2-\mu}(\Sigma) \to H^{-\sigma,-\mu}(\Sigma)$$

is continuous and bijective. Hence for a given function $v \in H^{-\sigma,-\mu}(\Sigma)$ there exists a uniquely defined density $z \in H^{1-\sigma,1/2-\mu}(\Sigma)$ such that $v = D^*z$. Therefore, and by applying the Galerkin orthogonality

$$\langle D(g-g_h), v_h\rangle_\Sigma = 0 \quad \text{for all } v_h \in X_{h,h}^{1,p_t}(\Sigma_N),$$

we obtain

$$\begin{aligned} \|g-g_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} &= \sup_{0\neq z\in H^{1-\sigma,1/2-\mu}(\Sigma)} \frac{\langle g-g_h, D^*z\rangle_\Sigma}{\|D^*z\|_{H^{-\sigma,-\mu}(\Sigma)}} \\ &= \sup_{0\neq z\in H^{1-\sigma,1/2-\mu}(\Sigma)} \frac{\langle D(g-g_h), z-Q_\Sigma^{1,p_t}z\rangle_\Sigma}{\|D^*z\|_{H^{-\sigma,-\mu}(\Sigma)}}. \end{aligned}$$

Since D^* is bijective, there exists a constant $c>0$ such that [17, Lemma A.40]

$$\|D^*z\|_{H^{-\sigma,-\mu}(\Sigma)} \geq c\,\|z\|_{H^{1-\sigma,1/2-\mu}(\Sigma)} \quad \text{for all } z\in H^{1-\sigma,1/2-\mu}(\Sigma).$$

Thus, by using the boundedness of the operator $D : H^{1/2,1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma)$ we conclude

$$\|g-g_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \leq \tilde{c}\,\|g-g_h\|_{H^{1/2,1/4}(\Sigma)} \sup_{0\neq z\in H^{1-\sigma,1/2-\mu}(\Sigma)} \frac{\left\|z-Q_\Sigma^{1,p_t}z\right\|_{H^{1/2,1/4}(\Sigma)}}{\|z\|_{H^{1-\sigma,1/2-\mu}(\Sigma)}}.$$

When considering $1/2 \leq 1-\sigma \leq 2$, i.e. $-1\leq\sigma\leq 1/2$, we obtain from the approximation properties of the operator Q_Σ^{1,p_t} the error estimate

$$\|g-g_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \leq \hat{c}\,h^{1/4-\mu}\,\|g-g_h\|_{H^{1/2,1/4}(\Sigma)},$$

and the assertion follows by applying the error estimate for the Galerkin approximation g_h in the energy norm. □

By using Theorem 7.11 with $\sigma=0$ we conclude the $L^2(\Sigma)$-error estimate

$$\|g-g_h\|_{L^2(\Sigma)} \leq c\,h^{\beta(r,s)+1/4}\,\|g\|_{H^{r,s}(\Sigma)}.$$

for the Galerkin approximation $g_h \in X_{h,h}^{1,p_t}(\Sigma_N)$ of $g\in H^{r,s}(\Sigma)$ with regularity $r\in[1/2,2]$ and $s\in[1/4,p_t+1]$. Hence for sufficiently smooth Dirichlet data, i.e. $g\in H^{2,p_t+1}(\Sigma)$, we obtain

$$\|g-g_h\|_{L^2(\Sigma)} \leq c\,h^{1+3/4\,p_t}\,\|g\|_{H^{2,p_t+1}(\Sigma)}. \tag{7.16}$$

Finally, let $g_h\in S_h^1(\Sigma_N)$ be the unique solution of the Galerkin variational problem (7.12), i.e. the approximation defined with respect to a triangulation of the space–time boundary

Σ. Due to the regularity assumption in Corollary 6.17 and the following remarks, Theorem 7.11 is only applicable for $g \in H^{r,s}(\Sigma)$ with $r,s \in [1/2,1]$, $\sigma \in [0,1/2]$ and $\mu = \sigma/2$. Analogously to the proof of Theorem 7.11 with an application of estimate 6.16 we obtain

$$\|g - g_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \leq c\, h^{\min(r,s)-1/4-\mu} \, \|g\|_{H^{r,s}(\Sigma)} \,.$$

Hence for $\sigma = 0$ we conclude the error estimate

$$\|g - g_h\|_{L^2(\Sigma)} \leq c\, h^{\min(r,s)-1/4} \, \|g\|_{H^{r,s}(\Sigma)} \,.$$

Note that the $L^2(\Sigma)$-error estimates for the two- and three-dimensional problem are not optimal. As in the case of the Dirichlet boundary value problem one may consider the integral equation in a different setting, i.e. in $H^{-1,-1/2}(\Sigma)$, and derive a related discrete stability condition in order to prove an optimal $L^2(\Sigma)$-error estimate.

7.2.2 Domain Error Estimates

Let $g_h \in Y_h$ be the unique solution of the Galerkin variational problem (7.12). We obtain an approximate solution of the initial Neumann boundary value problem (5.10) by using the representation formula (5.1) with the approximation g_h, i.e. for $(x,t) \in Q$ we have

$$\tilde{u}(x,t) = (\widetilde{V}w)(x,t) - (W g_h)(x,t) + (\widetilde{M}_0 u_0)(x,t) + (\widetilde{N}_0 f)(x,t). \qquad (7.17)$$

For the related error we obtain for $(x,t) \in Q$

$$\begin{aligned} |u(x,t) - \tilde{u}(x,t)| &= |(W(g-g_h))(x,t)| \\ &= \frac{1}{\alpha} \left| \int_\Sigma \partial_{n_y} U^\star(x-y,t-\tau)(g-g_h)(y,\tau)\, \mathrm{d}s_y\, \mathrm{d}\tau \right| . \end{aligned}$$

Since $(x,t) \in Q$, the normal derivative of the fundamental solution $\partial_{n_y} U^\star(x-\cdot,t-\cdot)$ is smooth for $(y,\tau) \in \Sigma$ and we therefore conclude $\partial_{n_y} U^\star(x-\cdot,t-\cdot) \in H^{-\sigma,-\sigma/2}(\Sigma)$ for any $\sigma \in \mathbb{R}$. Hence

$$|u(x,t) - \tilde{u}(x,t)| \leq \frac{1}{\alpha} \left\| \partial_{n_y} U^\star(x-\cdot,t-\cdot) \right\|_{H^{-\sigma,-\sigma/2}(\Sigma)} \|g - g_h\|_{\widetilde{H}^{\sigma,\sigma/2}(\Sigma)} \,.$$

Thus, we can use the previously shown error estimates for $\|g - g_h\|_{\widetilde{H}^{\sigma,\sigma/2}(\Sigma)}$ in order to derive an error estimate for the pointwise error $|u(x,t) - \tilde{u}(x,t)|$, $(x,t) \in Q$.

In the one-dimensional case we obtain the estimate

$$|u(x,t) - \tilde{u}(x,t)| \leq c\, h^{s+1/2} \, \|g\|_{H^s(\Sigma)}$$

for $(x,t) \in Q$ by using Theorem 7.8 with $\mu = -1/2$ and $s \in [1/4, p+1]$, where p denotes the polynomial degree of the trial space $S_h^p(\Sigma_N)$. Hence for sufficiently smooth data, i.e. $g \in H^{p+1}(\Sigma)$, we get the estimate

$$|u(x,t) - \tilde{u}(x,t)| \le c\, h^{p+3/2}\, \|g\|_{H^{p+1}(\Sigma)}$$

for $(x,t) \in Q$.

If the discretization of the variational problem (5.11) in the two- or three-dimensional case is done with respect to the trial space $Y_h = X_{h,h}^{1,p_t}(\Sigma_N)$, we obtain the error estimate

$$|u(x,t) - \tilde{u}(x,t)| \le c\, h^{\beta(r,s)+3/4}\, \|g\|_{H^{r,s}(\Sigma)}$$

for $(x,t) \in Q$ by applying Theorem 7.11 with $\sigma = -1$, $r \in [1/2, 2]$ and $s \in [1/4, p_t+1]$. Hence for $(x,t) \in Q$ and sufficiently smooth data, i.e. $g \in H^{2,p_t+1}(\Sigma)$, we get

$$|u(x,t) - \tilde{u}(x,t)| \le c\, h^{3/2+3/4\,p_t}\, \|g\|_{H^{2,p_t+1}(\Sigma)}\,.$$

7.2.3 Numerical Results

We consider the Neumman boundary value problem (5.10) with given Neumann datum $w \in H^{-1/2,-1/4}(\Sigma)$, homogeneous source term $f \equiv 0$, time horizon $T = 1$, and with the heat capacity constant $\alpha = 10$. We present examples for the one- and two-dimensional case with respect to a shape regular boundary decomposition.

The Galerkin boundary element discretization of the variational formulation (5.11) is done by using the trial space $Y_h = S_h^0(\Sigma_N)$ for the spatially one-dimensional problem and $Y_h = X_{h,h}^{1,0}(\Sigma_N)$ in the two-dimensional case. We write $Y_h = \operatorname{span}\{\psi_i\}_{i=1}^{M_\Sigma}$. For the approximation of the Neumann datum $w = \gamma_1^{\mathrm{int}} u \in H^{-1/2,-1/4}(\Sigma)$ we consider the space of piecewise constant basis functions $X_h = \operatorname{span}\left\{\varphi_\ell^0\right\}_{\ell=1}^{N} \subset H^{-1/2,-1/4}(\Sigma)$ defined with respect to the decomposition Σ_N, while the initial datum u_0 is discretized by using the space of piecewise linear and globally continuous functions $S_h^1(\Omega_{N_\Omega}) = \operatorname{span}\left\{\varphi_j^1\right\}_{j=1}^{M_\Omega}$, which is defined with respect to a given triangulation $\Omega_{N_\Omega} := \{\omega_i\}_{i=1}^{N_\Omega}$ of the domain Ω. This leads to the system of linear equations

$$\mathsf{D}_h \boldsymbol{g} = (\frac{1}{2}\mathsf{M}_h - \mathsf{K}_h')\boldsymbol{w} - \mathsf{M}_h^1 \boldsymbol{u}_0 \tag{7.18}$$

where

$$\mathsf{D}_h[i,k] := -\frac{1}{\alpha} \int\limits_\Sigma \psi_i(x,t)\gamma_{1,x}^{\mathrm{int}} \int\limits_\Sigma \gamma_{1,y}^{\mathrm{int}} U^\star(x-y, t-\tau)\, \psi_k(y,\tau)\, \mathrm{d}s_y\, \mathrm{d}\tau\, \mathrm{d}s_x\, \mathrm{d}t, \tag{7.19}$$

$$\mathsf{K}_h'[i,\ell] := \frac{1}{\alpha} \int\limits_{\Sigma} \psi_i(x,t) \int\limits_{\sigma_\ell} \partial_{n_x} U^\star(x-y,t-\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t, \tag{7.20}$$

$$\mathsf{M}_h^1[i,j] := \int\limits_{\Sigma} \psi_i(x,t) \int\limits_{\Omega} \partial_{n_x} U^\star(x-y,t)\varphi_j^1(y)\,\mathrm{d}y\,\mathrm{d}s_x\,\mathrm{d}t, \tag{7.21}$$

and

$$\mathsf{M}_h[i,\ell] := \int\limits_{\Sigma} \int\limits_{\sigma_\ell} \psi_i(x,t)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t. \tag{7.22}$$

Again, the vectors $\boldsymbol{g} \in \mathbb{R}^{M_\Sigma}$, $\boldsymbol{w} \in \mathbb{R}^N$ and $\boldsymbol{u}_0 \in \mathbb{R}^{M_\Omega}$ denote the coefficients of the trial functions g_h, w_h, and u_h^0, respectively, see Subsection 7.1.3. Due to the ellipticity of the hypersingular operator D, the matrix D_h is positive definite and therefore (7.18) is uniquely solvable. The system is solved by using the GMRES method with a relative accuracy of 10^{-8} as stopping criteria. The approximation $\tilde{u}$ of the solution u in the space–time domain Q is given by the discrete representation formula (7.11).

The computation of the matrix entries (7.19), (7.20), (7.21) and (7.22) follows the same scheme as described in Subsection 7.1.3 for the Dirichlet boundary value problem. For the assembly of the matrix D_h in the two-dimensional case we use the alternative representation of the bilinear form (4.13). In the spatially one-dimensional case the matrix entries were computed analytically.

One-Dimensional Problem

For the numerical experiments in the spatially one-dimensional case we choose the domain $\Omega = (0,1)$. Recall that the boundary elements are line segments in temporal dimension.

We consider the exact solution

$$u(x,t) = \exp\left(-4\pi^2 \frac{t}{\alpha}\right)\cos(2\pi x) \quad \text{for } (x,t) \in Q,$$

and determine the Neumann datum w and the initial datum u_0 accordingly. We use a globally uniform boundary element mesh of mesh size $h = 2^{-L}$ and the space of piecewise constant basis functions $S_h^0(\Sigma_N)$ for the discretization of the Dirichlet datum g. Table 7.4 shows the error $\|g - g_h\|_{L_2(\Sigma)}$ and the estimated order of convergence (eoc), which is linear as expected according to (7.14), assuming that $g \in H^1(\Sigma)$. Moreover, the iteration numbers of the GMRES method are given.

L	N	$\|g-g_h\|_{L_2(\Sigma)}$	eoc	It.
5	64	$5.885\cdot 10^{-2}$	0.74	31
6	128	$3.077\cdot 10^{-2}$	0.94	44
7	256	$1.529\cdot 10^{-2}$	1.01	58
8	512	$7.500\cdot 10^{-3}$	1.03	75
9	1 024	$3.682\cdot 10^{-3}$	1.03	95
10	2 048	$1.815\cdot 10^{-3}$	1.02	120
11	4 096	$8.990\cdot 10^{-4}$	1.01	152

Table 7.4: $L^2(\Sigma)$-error and convergence rate of the Galerkin approximation g_h, and iteration numbers of the GMRES method (It.) in the case of uniform refinement in 1D. The parameter N denotes the number of boundary elements on level L.

Two-Dimensional Problem

We choose $\Omega = (0,1)^2$, i.e. $Q = (0,1)^3$, and consider the exact solution

$$u(x,t) = \exp\left(-\frac{t}{\alpha}\right)\sin\left(x_1\cos\frac{\pi}{8} + x_2\sin\frac{\pi}{8}\right) \quad \text{for } (x,t) = (x_1,x_2,t) \in Q.$$

We determine the Neumann datum w and the initial datum u_0 accordingly. We use a globally quasi-uniform boundary element mesh with mesh size $h = \mathcal{O}(2^{-L})$ and the tensor product space $X_{h,h}^{1,0}(\Sigma_N)$ for the approximation of the Dirichlet datum $g = \gamma_0^{\text{int}}u$. Table 7.5 shows the error $\|g-g_h\|_{L^2(\Sigma)}$ of the Galerkin approximation g_h as well as the pointwise error $|(u-\tilde{u})(x,t)|$ in $x = (0.5,0.5)$, $t = 0.5$, and the corresponding convergence rates (eoc). Additionally, the iteration numbers of the GMRES method are listed.

We obtain linear convergence of the Galerkin approximation g_h in the $L^2(\Sigma)$-norm, which is in line with estimate (7.16). For the pointwise error we obtain linear convergence as well. However, due to the given regularity of the solution we expected a rate of at least $3/2$ according to the theoretical findings in Subsection 7.2.2. This gap may be due to the additional approximation of the right hand side, i.e. we have computed a piecewise constant approximation w_h of the given Neumann datum w. Thus, an application of the Strang theorem [62, Theorem 8.2] is necessary in order to obtain adjusted convergence rates.

L	N	$\|g-g_h\|_{L_2(\Sigma)}$	eoc	$\|(u-\tilde{u})(x,t)\|$	eoc	It.
0	4	$1.564 \cdot 10^{-1}$	-	$3.351 \cdot 10^{-2}$	-	3
1	16	$8.274 \cdot 10^{-2}$	0.92	$6.466 \cdot 10^{-3}$	2.37	11
2	64	$4.325 \cdot 10^{-2}$	0.94	$2.672 \cdot 10^{-3}$	1.27	12
3	256	$1.897 \cdot 10^{-2}$	1.19	$1.330 \cdot 10^{-3}$	1.01	14
4	1 024	$8.733 \cdot 10^{-3}$	1.12	$6.021 \cdot 10^{-4}$	1.14	22
5	4 096	$4.131 \cdot 10^{-3}$	1.08	$2.740 \cdot 10^{-4}$	1.14	36
6	16 384	$1.987 \cdot 10^{-3}$	1.06	$1.282 \cdot 10^{-4}$	1.10	54
7	65 536	$9.709 \cdot 10^{-4}$	1.03	$6.143 \cdot 10^{-5}$	1.06	80

Table 7.5: Error and convergence rates of the Galerkin approximation g_h and the approximated solution $\tilde{u}$ in the interior, and iteration numbers of the GMRES method (It.) in the case of uniform refinement for a tensor product decomposition of Σ in 2D. The parameter N denotes the number of boundary elements on level L.

7.3 Transmission Problem

In this section we discuss the discretization of the variational formluation (5.21) in order to find an approximation of the unknown Cauchy data

$$(w,g) = \left(\gamma_1^{\text{int}} u_i, \gamma_0^{\text{int}} u_i\right) \in H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$$

of the transmission problem (5.16). Related error estimates are given in Subsection 7.3.1. In Subsection 7.3.2 we provide numerical experiments for the spatially two-dimensional problem.

Let $X_h \subset H^{-1/2,-1/4}(\Sigma)$ and $Y_h \subset H^{1/2,1/4}(\Sigma)$ be conforming boundary element spaces which are defined with respect to a shape regular boundary element mesh Σ_N introduced in Section 6.3. The Galerkin–Bubnov variational formulation of (5.21) is to find $(w_h, g_h) \in X_h \times Y_h$ such that

$$\left\langle A \begin{pmatrix} w_h \\ g_h \end{pmatrix}, \begin{pmatrix} \tau_h \\ v_h \end{pmatrix} \right\rangle_\Sigma = \left\langle B \begin{pmatrix} \beta_1 \\ \beta_0 \end{pmatrix}, \begin{pmatrix} \tau_h \\ v_h \end{pmatrix} \right\rangle_\Sigma \tag{7.23}$$

for all $(\tau_h, v_h) \in X_h \times Y_h$. Due to the ellipticity of the operator A and the boundedness of A and B, problem (7.23) admits a unique solution.

7.3.1 Error Estimates

Let $(w,g) \in H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$ be the unique solution of the variational problem (5.21). Since the operator A is elliptic and bounded, we can apply Cea's Lemma [62, Theorem 8.1] to obtain an error estimate for the Galerkin approximation $(w_h, g_h) \in X_h \times Y_h$, i.e. we conclude

$$\begin{aligned} &\|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)} + \|g - g_h\|_{H^{1/2,1/4}(\Sigma)} \\ &\quad \leq c_w \inf_{\tau_h \in X_h} \|w - \tau_h\|_{H^{-1/2,-1/4}(\Sigma)} + c_g \inf_{v_h \in Y_h} \|g - v_h\|_{H^{1/2,1/4}(\Sigma)} \end{aligned} \tag{7.24}$$

with some constants $c_w, c_g > 0$. Hence we can use the approximation properties of the boundary element spaces X_h and Y_h to derive error estimates for the solution (w_h, g_h) of (7.23).

One-Dimensional Problem

For the spatially one-dimensional problem we consider the trial spaces $X_h = S_h^0(\Sigma_N)$ and $Y_h = S_h^p(\Sigma_N)$ for the approximation of the Cauchy data (w, g). Recall that we can identify the Sobolev spaces $H^{r,s}(\Sigma)$ with $H^s(\Sigma)$.

Theorem 7.12. *Let $(w_h, g_h) \in X_h \times Y_h$ be the unique solution of the Galerkin variational problem* (7.23). *For $(w, g) \in H^s(\Sigma) \times H^\nu(\Sigma)$ with $s \in [0,1]$ and $\nu \in [1/4, p+1]$ there holds the error estimate*

$$\|w - w_h\|_{H^{-1/4}(\Sigma)} + \|g - g_h\|_{H^{1/4}(\Sigma)} \leq c_1 \, h^{s+1/4} |w|_{H^s(\Sigma)} + c_2 \, h^{\nu - 1/4} \, \|g\|_{H^\nu(\Sigma)} \, .$$

Proof. We use (7.24) and estimate the first term by applying Lemma 2.5 and Lemma 6.2 with $p = 0$. For the estimation of the error of the Dirichlet datum we apply Lemma 6.3 for $p = 0$ and Lemma 6.4 for $p = 1$. □

Two- and Three-Dimensional Problem

Similar to the initial Neumann boundary value problem we distinguish between the tensor product decomposition and the triangulation of the space–time boundary Σ.

Theorem 7.13. *Let $(w_h, g_h) \in X_{h,h}^{0,0}(\Sigma_N) \times X_{h,h}^{1,p_t}(\Sigma_N)$ be the unique solution of the Galerkin variational problem* (7.23). *For $(w, g) \in H_{pw}^{r,s}(\Sigma) \times H^{\rho,\nu}(\Sigma)$ with $r, s \in [0,1]$, $\rho \in [1/2, 2]$ and $\nu \in [1/4, p_t + 1]$ there holds the error estimate*

$$\begin{aligned} &\|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)} + \|g - g_h\|_{H^{1/2,1/4}(\Sigma)} \\ &\quad \leq c_1 \, h^{\min(r,s)+1/4} \, \|w\|_{H_{pw}^{r,s}(\Sigma)} + c_2 \, h^{\beta(\rho,\nu)} \, \|g\|_{H^{\rho,\mu}(\Sigma)} \end{aligned}$$

with β given by (7.15).

Proof. According to (7.24) we have

$$\begin{aligned}&\|w-w_h\|_{H^{-1/2,-1/4}(\Sigma)}+\|g-g_h\|_{H^{1/2,1/4}(\Sigma)}\\&\quad\le c_w\left\|w-Q_\Sigma^{0,0}w\right\|_{H^{-1/2,-1/4}(\Sigma)}+c_g\left\|g-Q_\Sigma^{1,p_t}g\right\|_{H^{1/2,1/4}(\Sigma)}.\end{aligned}$$

The first term on the right hand side can be estimated by applying Lemma 2.5 and Lemma 6.10 with $p_x=p_t=0$. For the estimation of the second term we use Lemma 6.11 for $p_t=0$ and Lemma 6.12 for $p_t=1$. □

If the discretization (7.23) is done with respect to a triangulation of the space–time boundary Σ we obtain the following result.

Theorem 7.14. *Let $(w_h,g_h)\in S_h^0(\Sigma_N)\times S_h^1(\Sigma_N)$ be the unique solution of the Galerkin variational problem* (7.23)*. For $(w,g)\in H_{pw}^{r,s}(\Sigma)\times H^\rho(\Sigma)$ with $r,s\in[0,1]$ and $\rho\in[1/2,2]$ there holds the error estimate*

$$\begin{aligned}&\|w-w_h\|_{H^{-1/2,-1/4}(\Sigma)}+\|g-g_h\|_{H^{1/2,1/4}(\Sigma)}\\&\quad\le c_1\,h^{\min(r,s)+1/4}\,\|w\|_{H_{pw}^{r,s}(\Sigma)}+c_2\,h^{\rho-1/2}\,\|g\|_{H^\rho(\Sigma)}.\end{aligned}$$

Proof. According to (7.24) we have

$$\begin{aligned}&\|w-w_h\|_{H^{-1/2,-1/4}(\Sigma)}+\|g-g_h\|_{H^{1/2,1/4}(\Sigma)}\\&\quad\le c_w\left\|w-Q_\Sigma^{0}w\right\|_{H^{-1/2,-1/4}(\Sigma)}+c_g\left\|g-Q_\Sigma^{1,\nu}g\right\|_{H^{1/2,1/4}(\Sigma)}\end{aligned}$$

with $\nu=1/2$ and the assertion follows by applying Lemma 6.15 and Corollary 6.17. □

7.3.2 Numerical Results

We consider the transmission problem (5.16) with given jump terms $\beta_1\in H^{-1/2,-1/4}(\Sigma)$ and $\beta_0\in H^{1/2,1/4}(\Sigma)$. The Galerkin boundary element discretization of the variational problem (5.21) is done by using piecewise constant basis functions $X_h=\operatorname{span}\{\varphi_\ell^0\}_{\ell=1}^N\subset H^{-1/2,-1/4}(\Sigma)$ for the approximation w and a conforming boundary element space $Y_h=\operatorname{span}\{\psi_i\}_{i=1}^M\subset H^{1/2,1/4}(\Sigma)$ for the approximation of g, which are defined with respect to a shape regular decomposition Σ_N. The spaces X_h and Y_h are also used for the discretization of the jump terms β_1 and β_0, respectively. This leads to the system of linear equations

$$\begin{pmatrix}\mathsf{V}_{h,\alpha}+\mathsf{V}_h & -\mathsf{K}_{h,\alpha}-\mathsf{K}_h\\ \mathsf{K}'_{h,\alpha}+\mathsf{K}'_h & \mathsf{D}_{h,\alpha}+\mathsf{D}_h\end{pmatrix}\begin{pmatrix}\boldsymbol{w}\\ \boldsymbol{g}\end{pmatrix}=\begin{pmatrix}\mathsf{V}_h & \frac12\mathsf{M}_h-\mathsf{K}_h\\ \frac12\mathsf{M}_h^{\mathrm T}+\mathsf{K}'_h & \mathsf{D}_h\end{pmatrix}\begin{pmatrix}\boldsymbol{\beta}_1\\ \boldsymbol{\beta}_0\end{pmatrix} \tag{7.25}$$

where

$$\mathsf{V}_{h,\alpha}[\ell,k] := \langle V_\alpha \varphi_k^0, \varphi_\ell^0\rangle_\Sigma, \quad \mathsf{K}_{h,\alpha}[\ell,i] := \langle K_\alpha \psi_i, \varphi_\ell^0\rangle_\Sigma, \quad \mathsf{M}_h[\ell,i] := \langle \psi_i, \varphi_\ell^0\rangle_\Sigma$$

$$\mathsf{D}_{h,\alpha}[i,j] := \langle D_\alpha \psi_j, \psi_i\rangle_\Sigma, \quad \mathsf{K}'_{h,\alpha}[i,\ell] := \langle K'_\alpha \varphi_\ell^0, \psi_i\rangle_\Sigma$$

for $\ell,k = 1,...,N$ and $i,j = 1,...M$. The matrices $\mathsf{V}_h, \mathsf{D}_h, \mathsf{K}_h, \mathsf{K}'_h$ for the exterior problem are defined analogously. For an explicit representation of the matrix entries and for a discussion of the integration routines used for the assembly of the matrices see Subsection 7.1.3 and Subsection 7.2.3. Here, the vectors $\boldsymbol{w}, \boldsymbol{\beta}_1 \in \mathbb{R}^N$ and $\boldsymbol{g}, \boldsymbol{\beta}_0 \in \mathbb{R}^M$ denote the coefficients of the corresponding trial functions.

In the following numerical experiment we choose the time horizon $T = 1$ and set the heat capacity constant in the interior domain to $\alpha = 10$. The system (7.25) is solved by using the GMRES method with a relative accuracy of 10^{-8} as stopping criteria.

We can describe a reference solution of the transmission problem by picking a heat source point $x_p \in \mathbb{R}^n$ outside the domain Ω and by defining

$$u_p(x,t) := \left(\frac{\alpha}{4\pi t}\right)^{n/2} \exp\left(-\frac{\alpha|x-x_p|^2}{4t}\right) \quad \text{for } (x,t) \in \mathbb{R}^n \times (0,T).$$

Then u with $u_{|Q} = u_i = u_{p|Q}$ and $u_{|Q^{\text{ext}}} = u_e = 0$ is a solution of the homogeneous heat equation in the interior and exterior domain. We determine the jump terms according to

$$\begin{aligned}\beta_0 &:= \gamma_0^{\text{int}} u - \gamma_0^{\text{ext}} u = \gamma_0^{\text{int}} u_i = \gamma_0^{\text{int}} u_p,\\ \beta_1 &:= \gamma_1^{\text{int}} u - \gamma_1^{\text{ext}} u = \gamma_1^{\text{int}} u_i = \gamma_1^{\text{int}} u_p.\end{aligned}$$

Two-Dimensional Problem

We consider $Q = (0,1)^3$ and choose a heat source point $x_p = (1.5, 1.6)$. We use a globally quasi-uniform, shape regular boundary element mesh with mesh size $h = \mathcal{O}(2^{-L})$ and the tensor product spaces $X_h = X_{h,h}^{0,0}(\Sigma_N)$ and $Y_h = X_{h,h}^{1,0}(\Sigma_N)$ for the discretization of the variational problem (5.21). Table 7.6 shows the errors $\|w - w_h\|_{L^2(\Sigma)}$ and $\|g - g_h\|_{L^2(\Sigma)}$ of the Galerkin approximations w_h and g_h, respectively, as well as the corresponding convergence rates (eoc) and the iteration numbers of the GMRES method. We obtain linear convergence in the $L^2(\Sigma)$-norm for both approximations which is reasonable due to the constant approximation in time for both the Neumann and the Dirichlet datum. The observed convergence rates are also in line with the rates we obtained for the Dirichlet and Neumann boundary value problem in Subsection 7.1.3 and Subsection 7.2.3, respectively.

L	N	$\|w - w_h\|_{L_2(\Sigma)}$	eoc	$\|g - g_h\|_{L^2(\Sigma)}$	eoc	It.
0	4	$1.071 \cdot 10^{-1}$	-	$4.896 \cdot 10^{-2}$	-	6
1	16	$8.524 \cdot 10^{-2}$	0.33	$4.431 \cdot 10^{-2}$	0.14	18
2	64	$6.550 \cdot 10^{-2}$	0.38	$3.141 \cdot 10^{-2}$	0.50	42
3	256	$4.817 \cdot 10^{-2}$	0.44	$1.365 \cdot 10^{-2}$	1.20	83
4	1 024	$2.194 \cdot 10^{-2}$	1.13	$6.648 \cdot 10^{-3}$	1.04	171
5	4 096	$1.127 \cdot 10^{-2}$	0.96	$3.427 \cdot 10^{-3}$	0.96	345
6	16 384	$5.506 \cdot 10^{-3}$	1.03	$1.706 \cdot 10^{-3}$	1.01	701
7	65 536	$2.712 \cdot 10^{-3}$	1.02	$8.591 \cdot 10^{-4}$	0.99	1375

Table 7.6: Error and convergence rates of the Galerkin approximations w_h and g_h, and iteration numbers of the GMRES method (It.) in the case of uniform refinement for a tensor product decomposition of Σ in 2D. The parameter N denotes the number of boundary elements on level L.

8 OPERATOR PRECONDITIONING

In this chapter we describe a space–time preconditioning technique for discretized boundary integral equations of the time-dependent heat equation. The presented strategy is based on using boundary integral operators of opposite order, referred to as Calderon preconditioning [64] or operator preconditioning [23]. We consider the initial boundary value problem for the heat equation with given Dirichlet or Neumann datum and determine the unknown Cauchy datum by solving a related boundary integral equation. Based on the mapping properties of the single layer boundary integral operator and the hypersingular boundary integral operator we establish robust preconditioning strategies for the discretized integral equations. The theoretical results are confirmed by numerical tests for the spatially one- and two-dimensional problem.

The presented preconditioning strategy was introduced and analyzed in [64] for the Laplace equation, where the involved integral operators are in general self adjoint. The results were extended to a more abstract setting in [23]. In the following sections we introduce and analyze this method for space–time integral equations, see also [11, 13].

First we give a brief introduction of the preconditioning strategy based on [23]. Let X and Y be two reflexive Banach spaces. We consider continuous bilinear forms $a : X \times X \to \mathbb{R}$ and $b : Y \times Y \to \mathbb{R}$. Moreover, let $X_h := \operatorname{span}\{\varphi_\ell\}_\ell^N \subset X$ and $Y_h := \operatorname{span}\{\psi_\ell\}_\ell^N \subset Y$ be finite-dimensional subspaces of the same dimension N satisfying

$$\begin{aligned} \sup_{0 \neq \tau_h \in X_h} \frac{a(w_h, \tau_h)}{\|\tau_h\|_X} &\geq c_A \|w_h\|_X \quad \text{for all } w_h \in X_h, \\ \sup_{0 \neq v_h \in Y_h} \frac{b(u_h, v_h)}{\|v_h\|_Y} &\geq c_B \|u_h\|_Y \quad \text{for all } u_h \in Y_h. \end{aligned} \tag{8.1}$$

We assume that there exists a continuous bilinear form $m : X \times Y \to \mathbb{R}$ such that

$$\sup_{0 \neq v_h \in Y_h} \frac{m(w_h, v_h)}{\|v_h\|_Y} \geq c_M \|w_h\|_X \quad \text{for all } w_h \in X_h. \tag{8.2}$$

The corresponding Galerkin matrices are given as

$$\mathsf{A}_h[\ell,k] := a(\varphi_k, \varphi_\ell), \quad \mathsf{B}_h[\ell,k] := b(\psi_k, \psi_\ell), \quad \mathsf{M}_h[\ell,k] := m(\varphi_k, \psi_\ell) \quad \text{for } \ell, k = 1, \ldots, N.$$

Note that Y_h has the same dimension as the finite-dimensional subspace X_h and thus, M_h is a square matrix. Additionally, we require the matrix M_h to be invertible. In this case we obtain the following result.

Theorem 8.1 ([23, Theorem 2.1])**.** *Assume that* (8.1) - (8.2) *holds. Then*

$$\kappa(\mathsf{M}_h^{-1}\mathsf{B}_h\mathsf{M}_h^{-\mathsf{T}}\mathsf{A}_h) \leq \frac{\|a\| \, \|b\| \, \|m\|^2}{c_A c_B c_M^2},$$

where $\kappa(\cdot)$ denotes the spectral condition number of a square matrix.

Now let us assume that the bilinear forms $a(\cdot,\cdot)$ and $b(\cdot,\cdot)$ are induced by elliptic operators $A : X \to X'$ and $B : X' \to X$, i.e.

$$\begin{aligned} a(u,v) &:= \langle Au, v\rangle_{X'\times X} \quad \text{for all } u,v \in X, \\ b(u,v) &:= \langle Bu, v\rangle_{X\times X'} \quad \text{for all } u,v \in X'. \end{aligned}$$

Then the stability estimates (8.1) are trivially satisfied for any finite-dimensional subspaces $X_h \subset X$ and $Y_h \subset X'$. Hence, for a given trial space X_h we have to find Y_h with the same dimension N and a continuous bilinear form $m : X \times X' \to \mathbb{R}$ such that (8.2) holds.

8.1 Dirichlet Boundary Value Problem

We consider the Dirichlet boundary value problem (5.6) with source term $f \in [H^{1,1/2}_{;,0}(Q)]'$, Dirichlet datum $g \in H^{1/2,1/4}(\Sigma)$ and initial datum $u_0 \in L^2(\Omega)$. We use the direct formulation (5.7) in order to compute the unknown Neumann datum $w = \gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$ of the solution $u \in H^{1,1/2}(Q)$. Hence we have to find $w \in H^{-1/2,-1/4}(\Sigma)$ such that

$$\langle Vw, \tau\rangle_\Sigma = \langle (\frac{1}{2}I + K)g - M_0 u_0 - N_0 f, \tau\rangle_\Sigma \quad \text{for all } \tau \in H^{-1/2,-1/4}(\Sigma). \tag{8.3}$$

The ellipticity of the single layer operator $V : H^{-1/2,-1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma)$ ensures unique solvability of (8.3).

For the discretization of (8.3) we consider the space of piecewise constant basis functions $X_h = \operatorname{span}\{\varphi_\ell^0\}_\ell^N \subset L^2(\Sigma)$ which is defined with respect to an admissible, shape regular boundary element mesh Σ_N as introduced in Section 6.3. This could either be a tensor product decomposition or an arbitrary triangulation of Σ. Thus, we obtain the system of linear equations $\mathsf{V}_h \boldsymbol{w} = \boldsymbol{f}$ with

$$\mathsf{V}_h[\ell,k] := \langle V\varphi_k^0, \varphi_\ell^0\rangle_\Sigma, \quad \boldsymbol{f}[\ell] := \langle (\frac{1}{2}I + K)g - M_0 u_0 - N_0 f, \varphi_\ell^0\rangle_\Sigma \quad \text{for } \ell,k = 1,\ldots,N.$$

The boundary element discretization is done with respect to the whole space–time boundary Σ and since we want to solve $\mathsf{V}_h \boldsymbol{w} = \boldsymbol{f}$ without an application of time-stepping schemes to make use of parallelization in time, we need to develop an efficient iterative solution technique. The linear system with the positive definite but non-symmetric matrix V_h can be solved with a preconditioned GMRES method. Here we will apply the previously introduced operator preconditioning technique.

The single layer boundary integral operator $V : H^{-1/2,-1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma)$ and the hypersingular operator $D : H^{1/2,1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma)$ are both elliptic and the composition $DV : H^{-1/2,-1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma)$ defines an operator of order zero. Hence the stability estimates (8.1) are satisfied and thus, the Galerkin discretization of D allows the construction of a suitable preconditioner for V_h. While the discretization of the single layer operator V is done with respect to X_h, for the Galerkin discretization of the hypersingular operator D we need to use a conforming trial space $Y_h = \operatorname{span}\{\psi_\ell\}_{\ell=1}^N \subset H^{1/2,1/4}(\Sigma)$, see also [11, 13]. The continuous bilinear form $m(\cdot,\cdot)$ in (8.2) is chosen to be the duality product on $H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$ and thus, for subspaces $X_h, Y_h \subset L^2(\Sigma)$ we have $m(\tau_h, v_h) = \langle \tau_h, v_h \rangle_{L^2(\Sigma)}$, yielding the following theorem.

Theorem 8.2. *Assume that the discrete stability condition*

$$\sup_{0 \neq v_h \in Y_h} \frac{\langle \tau_h, v_h \rangle_{L^2(\Sigma)}}{\|v_h\|_{H^{1/2,1/4}(\Sigma)}} \geq c_1^M \|\tau_h\|_{H^{-1/2,-1/4}(\Sigma)} \quad \text{for all } \tau_h \in X_h \tag{8.4}$$

holds. Then there exists a constant $c_\kappa \geq 1$ such that

$$\kappa\left(\mathsf{M}_h^{-1}\mathsf{D}_h\mathsf{M}_h^{-\top}\mathsf{V}_h\right) \leq c_\kappa$$

where, for $k, \ell = 1, \ldots, N$,

$$\mathsf{V}_h[\ell,k] = \langle V\varphi_k^0, \varphi_\ell^0 \rangle_\Sigma\,, \quad \mathsf{D}_h[\ell,k] = \langle D\psi_k, \psi_\ell \rangle_\Sigma\,, \quad \mathsf{M}_h[\ell,k] = \langle \varphi_k^0, \psi_\ell \rangle_{L^2(\Sigma)}\,.$$

Proof. Apply Theorem 8.1 with the bilinear forms

$$a(w,\tau) := \langle Vw, \tau \rangle_\Sigma, \quad b(u,v) := \langle Du, v \rangle_\Sigma, \quad m(\tau,v) := \langle \tau, v \rangle_\Sigma$$

for $w, \tau \in H^{-1/2,-1/4}(\Sigma)$ and $u, v \in H^{1/2,1/4}(\Sigma)$. □

Thus, we can use $\mathsf{C}_\mathsf{V}^{-1} := \mathsf{M}_h^{-1}\mathsf{D}_h\mathsf{M}_h^{-\top}$ as a preconditioner for V_h. For the computation of the matrix D_h in the spatially two- and three-dimensional case we use the alternative representations (4.13) and (4.14) of the associated bilinear form which is attained by applying integration by parts. Note that the boundary element space Y_h is chosen to have the same dimension as X_h and thus, M_h is a square matrix. It remains to define a suitable boundary element space Y_h such that the mass matrix M_h is invertible and that the stability condition (8.4) is satisfied.

In order to prove the stability condition (8.4) we establish the $H^{1/2,1/4}(\Sigma)$-stability of the L^2 projection operator $Q_\Sigma : L^2(\Sigma) \to Y_h \subset L^2(\Sigma)$ defined by the variational problem

$$\langle Q_\Sigma u, \tau_h \rangle_{L^2(\Sigma)} = \langle u, \tau_h \rangle_{L^2(\Sigma)} \quad \text{for all } \tau_h \in X_h. \tag{8.5}$$

Depending on the boundary element spaces X_h and Y_h this could either be a Galerkin–Bubnov or a Galerkin–Petrov variational formulation. We assume that the variational problem (8.5) is uniquely solvable, i.e. the boundary element spaces X_h and Y_h satisfy the stability condition

$$\sup_{0\neq\tau_h\in X_h} \frac{\langle v_h, \tau_h\rangle_{L^2(\Sigma)}}{\|\tau_h\|_{L^2(\Sigma)}} \geq c\,\|v_h\|_{L^2(\Sigma)} \quad \text{for all } v_h \in Y_h \tag{8.6}$$

which is trivial for $Y_h = X_h$, i.e. in the case of a Galerkin–Bubnov variational problem. Then the $H^{1/2,1/4}(\Sigma)$-stability of the operator Q_Σ immediately implies the stability condition (8.4).

Theorem 8.3. *Let X_h and Y_h be given boundary element spaces satisfying* (8.6). *Moreover, let the L^2 projection operator Q_Σ defined by* (8.5) *be $H^{1/2,1/4}(\Sigma)$-stable, i.e. there exists a constant $c_S > 0$ such that*

$$\|Q_\Sigma u\|_{H^{1/2,1/4}(\Sigma)} \leq c_S\,\|u\|_{H^{1/2,1/4}(\Sigma)} \quad \textit{for all } u \in H^{1/2,1/4}(\Sigma).$$

Then the stability condition (8.4) *holds.*

Proof. Let $\tau_h \in X_h$. By using the definition (8.5) of the operator Q_Σ and its $H^{1/2,1/4}(\Sigma)$-stability we get by duality

$$\begin{aligned}\|\tau_h\|_{H^{-1/2,-1/4}(\Sigma)} &= \sup_{0\neq v\in H^{1/2,1/4}(\Sigma)} \frac{\langle \tau_h, v\rangle_{L^2(\Sigma)}}{\|v\|_{H^{1/2,1/4}(\Sigma)}} = \sup_{0\neq v\in H^{1/2,1/4}(\Sigma)} \frac{\langle \tau_h, Q_\Sigma v\rangle_{L^2(\Sigma)}}{\|v\|_{H^{1/2,1/4}(\Sigma)}} \\ &\leq c_S \sup_{0\neq v\in H^{1/2,1/4}(\Sigma)} \frac{\langle \tau_h, Q_\Sigma v\rangle_{L^2(\Sigma)}}{\|Q_\Sigma v\|_{H^{1/2,1/4}(\Sigma)}} = c_S \sup_{0\neq v_h\in Y_h} \frac{\langle \tau_h, v_h\rangle_{L^2(\Sigma)}}{\|v_h\|_{H^{1/2,1/4}(\Sigma)}}.\end{aligned}$$

□

Hence, according to Theorem 8.2, the condition number $\kappa(\mathsf{C}_\mathsf{V}^{-1}\mathsf{V}_h)$ with $\mathsf{C}_\mathsf{V}^{-1} = \mathsf{M}_h^{-1}\mathsf{D}_h\mathsf{M}_h^{-\top}$ is bounded. In what follows we will discuss possible choices of the boundary element space Y_h for given X_h such that the stability estimate in Theorem 8.3 is satsified.

Note that for a globally quasi-uniform boundary element mesh the $H^{1/2,1/4}(\Sigma)$-stability may follow directly with the approximation properties of related L^2 projection operators. However, this is not applicable for meshes generated by an application of adaptive refinement strategies, e.g. for locally quasi-uniform meshes.

8.1.1 One-Dimensional Problem

Recall that in the spatially one-dimensional case the spatial component of the space–time boundary Σ collapses to the points $\{a,b\}$, assuming $\Omega = (a,b)$, and therefore we identify the Sobolev spaces $H^{r,s}(\Sigma)$ with $H^s(\Sigma)$. We use the space $X_h = S_h^0(\Sigma_N)$ of piecewise constant basis functions for the discretization of the weakly singular integral equation (8.3) which is defined with respect to an arbitrary decomposition of the space–time boundary $\Sigma = \Sigma_a \cup \Sigma_b$. The decompositions of Σ_a and Σ_b may be different as shown in Fig. 6.1.

Piecewise Constant Basis Functions

Since the boundary element space $S_h^0(\Sigma_N)$ also satisfies $S_h^0(\Sigma_N) \subset H^{1/4}(\Sigma)$ in the 1D case, we can choose $Y_h = S_h^0(\Sigma_N)$ for the discretization of the hypersingular operator D as well. Then M_h becomes diagonal and is therefore easily invertible. According to Theorem 8.3 we need to establish the $H^{1/4}(\Sigma)$-stability of the L^2 projection operator $Q_\Sigma^0 : L^2(\Sigma) \to S_h^0(\Sigma_N) \subset L^2(\Sigma)$ defined by

$$\langle Q_\Sigma^0 v, \tau_h \rangle_{L^2(\Sigma)} = \langle v, \tau_h \rangle_{L^2(\Sigma)} \quad \text{for all } \tau_h \in S_h^0(\Sigma_N) \tag{8.7}$$

in order to conclude the boundedness of the condition number in Theorem 8.2. Note that (8.7) is a Galerkin–Bubnov variational formulation and thus, uniquely solvable.

Since $\Sigma = \Sigma_a \cup \Sigma_b$ with $\Sigma_a := \{a\} \times (0,T)$ and $\Sigma_b := \{b\} \times (0,T)$, it suffices to prove the stability estimate for the boundary part Σ_a. W.l.o.g. we choose $a = 0$. In this case we can identify Σ_a with the time interval $I = (0,T)$ and consider a decomposition I_{N_t} of I into line segments $\tau_\ell = (t_{\ell_1}, t_{\ell_2})$ as given by (6.2). For $\ell = 1,\dots,N_t$ we define $J(\ell)$ to be the index set containing the indices of the element τ_ℓ and all its adjacent elements. We assume the decomposition I_{N_t} to be locally quasi-uniform, i.e. there exists a constant $c_L \geq 1$ such that

$$\frac{1}{c_L} \leq \frac{h_\ell}{h_k} \leq c_L \quad \text{for all } k \in J(\ell) \text{ and } \ell = 1,\dots,N_t.$$

The L^2 projection $Q_I^0 u \in S_h^0(I_{N_t})$ for $u \in L^2(0,T)$, where $S_h^0(I_{N_t}) = \operatorname{span}\{\varphi_\ell^0\}_{\ell=1}^{N_t}$ is the space of piecewise constant basis functions on I_{N_T}, is defined as the unique solution of the variational problem

$$\langle Q_I^0 u, \tau_h \rangle_{L^2(0,T)} = \langle u, \tau_h \rangle_{L^2(0,T)} \quad \text{for all } \tau_h \in S_h^0(I_{N_t}). \tag{8.8}$$

For $u \in L^2(0,T)$ we have $(Q_I^0 u)(t) = \sum_{\ell=1}^{N_t} u_\ell \varphi_\ell^0(t)$ with

$$u_\ell = \frac{1}{h_\ell} \int\limits_{\tau_\ell} u(\tau)\mathrm{d}\tau \quad \text{for } \ell = 1,\dots,N_t.$$

Lemma 8.4. *Let the decomposition I_{N_t} be locally quasi-uniform. Then there exists a constant $c_S^0 > 0$ such that*

$$\left\| Q_I^0 u \right\|_{H^{1/4}(0,T)} \leq c_S^0 \left\| u \right\|_{H^{1/4}(0,T)} \quad \textit{for all } u \in H^{1/4}(0,T).$$

Proof. Let $u \in H^{1/4}(0,T)$. Then we have

$$\begin{aligned} \left\| Q_I^0 u \right\|^2_{H^{1/4}(0,T)} &= \left\| Q_I^0 u \right\|^2_{L^2(0,T)} + |Q_I^0 u|^2_{H^{1/4}(0,T)} \\ &\leq \|u\|^2_{L^2(0,T)} + |Q_I^0 u|^2_{H^{1/4}(0,T)}. \end{aligned}$$

The second term can be written as

$$|Q_I^0 u|^2_{H^{1/4}(0,T)} = \int_0^T \int_0^T \frac{[(Q_I^0 u)(t) - (Q_I^0 u)(s)]^2}{|t-s|^{3/2}} \mathrm{d}s\,\mathrm{d}t$$
$$= \sum_{\ell=1}^N \sum_{k=1}^N \underbrace{\int_{\tau_\ell} \int_{\tau_k} \frac{[(Q_I^0 u)(t) - (Q_I^0 u)(s)]^2}{|t-s|^{3/2}} \mathrm{d}s\,\mathrm{d}t}_{=:\, c_{\ell k}}.$$

For $\ell = k$ we have $(Q_I^0 u)(t) = (Q_I^0 u)(s)$ for $(t,s) \in \tau_\ell \times \tau_\ell$ and therefore

$$c_{\ell\ell} = 0 \leq \int_{\tau_\ell} \int_{\tau_\ell} \frac{[u(t) - u(s)]^2}{|t-s|^{3/2}} \mathrm{d}s\,\mathrm{d}t.$$

For $\ell \neq k$ we obtain

$$c_{\ell k} = \int_{\tau_\ell} \int_{\tau_k} \frac{1}{|t-s|^{3/2}} \left[\frac{1}{h_\ell} \int_{\tau_\ell} u(\tau)\mathrm{d}\tau - \frac{1}{h_k} \int_{\tau_k} u(\eta)\mathrm{d}\eta \right]^2 \mathrm{d}s\,\mathrm{d}t$$
$$= \frac{1}{h_\ell^2 h_k^2} \underbrace{\left[\int_{\tau_\ell} \int_{\tau_k} \frac{1}{|t-s|^{3/2}} \mathrm{d}s\,\mathrm{d}t \right]}_{=:\, \alpha_{\ell k}} \left[\int_{\tau_\ell} \int_{\tau_k} \frac{u(\tau) - u(\eta)}{|\tau-\eta|^{3/4}} |\tau-\eta|^{3/4} \mathrm{d}\eta\,\mathrm{d}\tau \right]^2.$$

By applying the Cauchy–Schwarz inequality we get

$$c_{\ell k} \leq \frac{\alpha_{\ell k}}{h_\ell^2 h_k^2} \underbrace{\left[\int_{\tau_\ell} \int_{\tau_k} |\tau-\eta|^{3/2} \mathrm{d}\eta\,\mathrm{d}\tau \right]}_{=:\, \beta_{\ell k}} \left[\int_{\tau_\ell} \int_{\tau_k} \frac{[u(\tau) - u(\eta)]^2}{|\tau-\eta|^{3/2}} \mathrm{d}\eta\,\mathrm{d}\tau \right]$$

and it remains to estimate the coefficients $\alpha_{\ell k}$ and $\beta_{\ell k}$. First we examine non-adjacent elements. We write $\tau_\ell = (t_{\ell_1}, t_{\ell_2})$, $\tau_k = (t_{k_1}, t_{k_2})$ and assume w.l.o.g. that $t_{k_1} > t_{\ell_2}$. We have

$$\beta_{\ell k} = \int_{\tau_\ell} \int_{\tau_k} |\tau-\eta|^{3/2} \mathrm{d}\tau\,\mathrm{d}\eta \leq \int_{\tau_\ell} \int_{\tau_k} (t_{k_2} - t_{\ell_1})^{3/2} \mathrm{d}\tau\,\mathrm{d}\eta = (t_{k_2} - t_{\ell_1})^{3/2} h_\ell h_k.$$

Since $|t-s| \geq t_{k_1} - t_{\ell_2}$ for $(t,s) \in \tau_\ell \times \tau_k$, we have

$$\frac{1}{|t-s|^{3/2}} \leq \frac{1}{(t_{k_1} - t_{\ell_2})^{3/2}}$$

and therefore

$$\alpha_{\ell k} = \int\limits_{\tau_\ell}\int\limits_{\tau_k} \frac{1}{|t-s|^{3/2}} \mathrm{d}s\,\mathrm{d}t \le \frac{1}{(t_{k_1}-t_{\ell_2})^{3/2}} h_\ell h_k.$$

Together, we obtain

$$\alpha_{\ell k}\beta_{\ell k} \le h_\ell^2 h_k^2 \left(\frac{t_{k_2}-t_{\ell_1}}{t_{k_1}-t_{\ell_2}}\right)^{3/2}.$$

Due to the assumption that the decomposition I_{N_t} is locally quasi-uniform we have

$$\frac{t_{k_2}-t_{\ell_1}}{t_{k_1}-t_{\ell_2}} = \frac{h_k}{t_{k_1}-t_{\ell_2}} + \frac{h_\ell}{t_{k_1}-t_{\ell_2}} + 1 \le 1 + 2c_L$$

and conclude

$$c_{\ell k} \le (1+2c_L)^{3/2} \int\limits_{\tau_\ell}\int\limits_{\tau_k} \frac{[u(\tau)-u(\eta)]^2}{|\tau-\eta|^{3/2}} \mathrm{d}\eta\,\mathrm{d}\tau.$$

Next we want to find an estimate for adjacent elements τ_ℓ, τ_k. We assume w.l.o.g. that $t_{k_1} = t_{\ell_2}$. Then

$$\begin{aligned}\alpha_{\ell k} &= \int\limits_{\tau_\ell}\int\limits_{\tau_k} \frac{1}{|t-s|^{3/2}} \mathrm{d}s\,\mathrm{d}t = 4\left[(t_{k_2}-t_{\ell_2})^{1/2} - (t_{k_2}-t_{\ell_1})^{1/2} + (t_{\ell_2}-t_{\ell_1})^{1/2}\right] \\ &= 4\left[h_k^{1/2} - (h_k+h_\ell)^{1/2} + h_\ell^{1/2}\right]\end{aligned}$$

and

$$\begin{aligned}\beta_{\ell k} &= \int\limits_{\tau_\ell}\int\limits_{\tau_k} |\tau-\eta|^{3/2} \mathrm{d}\eta\,\mathrm{d}\tau = \frac{4}{35}\left[-(t_{k_2}-t_{\ell_2})^{7/2} + (t_{k_2}-t_{\ell_1})^{7/2} - (t_{\ell_2}-t_{\ell_1})^{7/2}\right] \\ &= \frac{4}{35}\left[-h_k^{7/2} + (h_k+h_\ell)^{7/2} - h_\ell^{7/2}\right].\end{aligned}$$

By using the local uniformity of the elements ($h_\ell \sim h_k$) we get

$$\alpha_{\ell k}\beta_{\ell k} \le c\, h_\ell^4$$

with some constant $c > 0$ and conclude

$$c_{\ell k} \le c \int\limits_{\tau_\ell}\int\limits_{\tau_k} \frac{[u(\tau)-u(\eta)]^2}{|\tau-\eta|^{3/2}} \mathrm{d}\eta\,\mathrm{d}\tau.$$

Altogether we have

$$|Q_I^0 u|^2_{H^{1/4}(0,T)} = \sum_{\ell=1}^N \sum_{k=1}^N c_{\ell k} \le \tilde{c} \sum_{\ell=1}^N \sum_{k=1}^N \int\limits_{\tau_\ell}\int\limits_{\tau_k} \frac{[u(t)-u(s)]^2}{|t-s|^{3/2}} \mathrm{d}s\,\mathrm{d}t = \tilde{c}|u|^2_{H^{1/4}(0,T)}$$

with some constant $\tilde{c} > 0$ and the assertion follows. $\square$

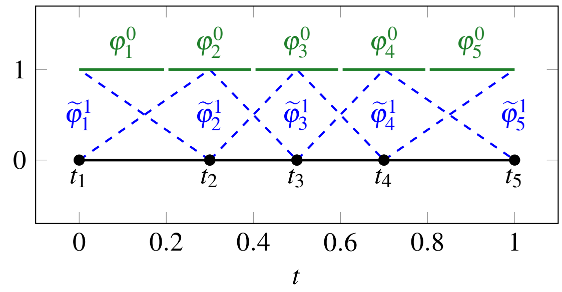


Figure 8.1: Sample dual mesh on $I = (0,T)$. The piecewise linear and globally continuous basis functions $\widetilde{\varphi}_i^1$ are used for the discretization of the hypersingular operator D, while the single layer operator V is discretized by using piecewise constant basis functions φ_i^0.

For the space–time boundary $\Sigma = \Sigma_a \cup \Sigma_b$ we get the same estimates for the L^2 projection operator $Q_\Sigma^0 : L^2(\Sigma) \to S_h^0(\Sigma_N) \subset L^2(\Sigma)$ defined by (8.7) by applying Lemma 8.4 on the boundary parts Σ_a and Σ_b separately. We therefore conclude that there exists a constant $c_S^0 > 0$ such that

$$\left\|Q_\Sigma^0 u\right\|_{H^{1/4}(\Sigma)} \le c_S^0 \left\|u\right\|_{H^{1/4}(\Sigma)} \quad \text{for all } u \in H^{1/4}(\Sigma).$$

According to Theorem 8.3 the stability estimate (8.4) holds and thus, the discretization of the hypersingular operator D with $Y_h = S_h^0(\Sigma_N)$ yields the boundedness of the condition number of the preconditioned system matrix $C_{\mathsf{V}}^{-1}\mathsf{V}_h$.

Piecewise Linear Basis Functions defined on a Dual Mesh

As a second approach we consider the space of piecewise linear and globally continuous basis functions defined with respect to a dual mesh $\widetilde{\Sigma}_{\widetilde{N}} := \{\tilde{\sigma}_\ell\}_{\ell=1}^{\widetilde{N}}$ [29] for the discretization of the hypersingular operator D. Figure 8.1 shows a sample dual mesh of one of the two boundary parts Σ_a and Σ_b and the corresponding basis functions. The stability results in this paragraph are based on [60]. Note that the proof of related stability estimates in [60] is done with respect to the Sobolev space $H^s(\Gamma)$ where Γ is an open or closed Lipschitz manifold in $\mathbb{R}^n$. However, we can transfer the results to the Sobolev space $H^s(0,T)$ if we identify the time interval $I = (0,T)$ with an open manifold in $\mathbb{R}^2$ and then use the results in [60] with $n = 2$.

Let $\{(x_k,t_k)\}_{k=1}^N$ denote the set of all vertices of the dual mesh. Note that the number of vertices of the dual mesh $\widetilde{\Sigma}_{\widetilde{N}}$ coincides with the number of boundary elements of Σ_N. We define $P(k)$ to be the index set of all elements $\tilde{\sigma}_\ell$ where $(x_k,t_k) \in \tilde{\sigma}_\ell$. Moreover, we define the nodal mesh size

$$\hat{h}_k := \frac{1}{|P(k)|} \sum_{\ell \in P(k)} h_\ell \quad \text{for } k = 1,\ldots,N$$

and assume that the dual mesh is locally quasi-uniform as well. We define $Y_h := S_h^1(\widetilde{\Sigma}_{\widetilde{N}}) = \operatorname{span}\left\{\widetilde{\varphi}_i^1\right\}_{i=1}^N$ to be the space of piecewise linear and globally continuous basis functions which is defined with respect to the dual boundary element mesh $\widetilde{\Sigma}_{\widetilde{N}}$. Let the L^2 projection $\widetilde{Q}_\Sigma^1 u \in S_h^1(\widetilde{\Sigma}_{\widetilde{N}})$ for $u \in L^2(\Sigma)$ be defined as the solution of the variational problem

$$\langle \widetilde{Q}_\Sigma^1 u, \tau_h \rangle_{L^2(\Sigma)} = \langle u, \tau_h \rangle_{L^2(\Sigma)} \quad \text{for all } \tau_h \in S_h^0(\Sigma_N).$$

This Galerkin–Petrov variational formulation is uniquely solvable, since the trial and test spaces satisfy a related stability condition [60, Lemma 3.1].

Note that in [60] the dual mesh is used for the definition of the piecewise constant basis functions, while the piecewise linear functions are defined with respect to the primal mesh. We use the reverse approach. However, in the one-dimensional case this does not affect the structure and the properties of the boundary element meshes and of the corresponding trial spaces.

Again, in order to prove the stability condition (8.4) we need to establish the $H^{1/4}(\Sigma)$-stability of the operator $\widetilde{Q}_\Sigma^1$. In order to prove the $H^{1/4}(\Sigma)$-stability we have to assume appropriate local mesh conditions: Let $\tilde{\sigma}_\ell$ be an arbitrary boundary element of the dual mesh $\widetilde{\Sigma}_{\widetilde{N}}$. We need to assume that there exists a constant $c_0 > 0$ such that

$$(\mathsf{H}_\ell \mathsf{G}_\ell H_\ell^{-1} \boldsymbol{x}_\ell, \boldsymbol{x}_\ell) \geq c_0 (\mathsf{D}_\ell \boldsymbol{x}_\ell, \boldsymbol{x}_\ell) \quad \text{for all } \boldsymbol{x}_\ell \in \mathbb{R}^{|J(\ell)|} \tag{8.9}$$

where $J(\ell)$ denotes the index set of all nodes adjacent to the element $\tilde{\sigma}_\ell$ and where the local matrices are defined as

$$\mathsf{G}_\ell[j,i] := \langle \varphi_{p(i)}^0, \widetilde{\varphi}_{p(j)}^1 \rangle_{L^2(\tilde{\sigma}_\ell)}, \quad \mathsf{D}_\ell := \operatorname{diag} \mathsf{G}_\ell, \quad \mathsf{H}_\ell := \operatorname{diag}(\hat{h}_{p(i)}^{1/4}) \quad \text{for } i,j = 1,\ldots,|J(\ell)|$$

where $p(i)$ denotes the i-th element in $J(\ell)$. Then there exists a constant $c_S^1 > 0$ such that [60, Theorem 4.2]

$$\left\| \widetilde{Q}_\Sigma^1 u \right\|_{H^{1/4}(\Sigma)} \leq c_S^1 \|u\|_{H^{1/4}(\Sigma)} \quad \text{for all } u \in H^{1/4}(\Sigma).$$

Explicit conditions for the dual boundary element mesh yielding assumption (8.9) are given in [60, Section 5].

Hence, Theorem 8.3 implies the stability condition (8.4). Consequently, the discretization of the hypersingular operator D with $Y_h = S_h^1(\widetilde{\Sigma}_{\widetilde{N}})$ yields the boundedness of the condition number of the matrix $\mathsf{C}_V^{-1}\mathsf{V}_h$ with $\mathsf{C}_V^{-1} = \mathsf{M}_h^{-1}\mathsf{D}_h\mathsf{M}_h^{-\mathsf{T}}$.

8.1.2 Two- and Three-Dimensional Problem

We consider a tensor product decomposition of Σ as described in Section 6.3 with given locally quasi-uniform spatial and temporal decompositions $\Gamma_{N_x} = \{\gamma_\ell\}_{\ell=1}^{N_x}$ and $I_{N_t} = \{\tau_i\}_{i=1}^{N_t}$, respectively. We use the space $X_h := X_{h_x,h_t}^{0,0}(\Sigma_N) = S_{h_x}^0(\Gamma_{N_x}) \otimes S_{h_t}^0(I_{N_t})$ of piecewise constant basis functions for the discretization of the weakly singular integral equation (8.3) and set $S_{h_x}^0(\Gamma_{N_x}) = \operatorname{span}\{\psi_i^0\}_{i=1}^{N_x}$ and $S_{h_t}^0(I_{N_t}) = \operatorname{span}\{\varphi_\ell^0\}_{\ell=1}^{N_t}$. Let $\{x_k\}_{k=1}^{M_x}$ denote the set of all vertices of the boundary element mesh Γ_{N_x}. We define $P(k)$ to be the index set of all elements γ_ℓ with $x_k \in \gamma_\ell$. Moreover, we define the nodal mesh size

$$\hat{h}_{k,x} := \frac{1}{|P(k)|} \sum_{\ell \in P(k)} h_{\ell,x} \quad \text{for } k = 1,\dots,M_x. \tag{8.10}$$

Since the boundary element mesh Γ_{N_x} is assumed to be locally quasi-uniform, there exists a constant $c \geq 1$ such that

$$\frac{1}{c} \leq \frac{\hat{h}_{k,x}}{h_{\ell,x}} \leq c \quad \text{for all } \ell \in P(k),\, k = 1,\dots,M_x.$$

For the given boundary element mesh Γ_{N_x} we construct a dual mesh $\widetilde{\Gamma}_{\widetilde{N}_x} := \{\tilde{\gamma}_l\}_{\ell=1}^{\widetilde{N}_x}$ according to [29, 60] and assume that the dual mesh is locally quasi-uniform as well. With $S_{h_x}^1(\widetilde{\Gamma}_{\widetilde{N}_x}) = \operatorname{span}\{\widetilde{\psi}_i^1\}_{i=1}^{N_x}$ we denote the space of piecewise linear and globally continuous basis functions defined with respect to the dual mesh $\widetilde{\Gamma}_{\widetilde{N}_x}$. Note that the number of vertices of the dual mesh $\widetilde{\Gamma}_{\widetilde{N}_x}$ coincides with the number of boundary elements of Γ_{N_x}. For the definition of suitable boundary element spaces for the discretization of the hypersingular operator D we can use the already known results from the discussion of the one-dimensional problem.

Remark 8.1. *Usually the dual mesh is used for the definition of the piecewise constant basis function, while the piecewise linear and globally continuous basis functions are defined with respect to the primal mesh . This is especially necessary for the spatially three-dimensional case, where the dual boundary element mesh is not a triangular mesh anymore. However, using piecewise constant basis functions on this non-triangular mesh is still eligible. In this case, the boundary integral equation* (8.3) *is discretized by using the dual basis functions, while the boundary element space corresponding to the primal mesh is used to compute suitable preconditioners.*

Piecewise Constant Basis Functions in Time

For the discretization of the operator D we choose

$$Y_h := S_{h_x}^1(\widetilde{\Gamma}_{\widetilde{N}_x}) \otimes S_{h_t}^0(I_{N_t}) \subset H^{1/2,1/4}(\Sigma).$$

According to Theorem 8.3 we need to establish the $H^{1/2,1/4}(\Sigma)$-stability of the L^2 projection operator $\widetilde{Q}_\Sigma^{1,0} : L^2(\Sigma) \to Y_h \subset L^2(\Sigma)$ defined by

$$\langle \widetilde{Q}_\Sigma^{1,0} u, \tau_h \rangle_{L^2(\Sigma)} = \langle u, \tau_h \rangle_{L^2(\Sigma)} \quad \text{for all } \tau_h \in X_h \tag{8.11}$$

in order to conclude the boundedness of the condition number in Theorem 8.2. Note that (8.11) is a Galerkin–Petrov variational formulation and thus, we need to prove a $L^2(\Sigma)$-stability estimate for the given trial spaces.

Lemma 8.5. *For the given boundary element spaces X_h and Y_h there holds the stability estimate*

$$c\,\|v_h\|_{L^2(\Sigma)} \le \sup_{0 \ne \tau_h \in X_h} \frac{\langle v_h, \tau_h \rangle_{L^2(\Sigma)}}{\|\tau_h\|_{L^2(\Sigma)}} \quad \textit{for all } v_h \in Y_h$$

with some constant $c > 0$.

Proof. The following proof is based on [60, Lemma 3.1]. For

$$v_h = \sum_{i=1}^{N_x} \sum_{\ell=1}^{N_t} v_{i\ell}\, \widetilde{\psi}_i^1 \varphi_\ell^0 \in Y_h, \quad \tau_h = \sum_{i=1}^{N_x} \sum_{\ell=1}^{N_t} \tau_{i\ell}\, \psi_i^0 \varphi_\ell^0 \in X_h$$

we have

$$\|v_h\|^2_{L^2(\Sigma)} \simeq \sum_{i=1}^{N_x} \sum_{\ell=1}^{N_t} v_{i\ell}^2 h_{i,x}^{n-1} h_{\ell,t}, \quad \|\tau_h\|^2_{L^2(\Sigma)} \simeq \sum_{i=1}^{N_x} \sum_{\ell=1}^{N_t} \tau_{i\ell}^2 h_{i,x}^{n-1} h_{\ell,t}.$$

For $v_h \in Y_h$ we define

$$\tau_h^\star = \sum_{i=1}^{N_x} \sum_{\ell=1}^{N_t} v_{i\ell} \psi_i^0 \varphi_\ell^0 \in X_h.$$

Then

$$\|\tau_h^*\|_{L^2(\Sigma)} \simeq \|v_h\|_{L^2(\Sigma)}, \quad |\langle v_h, \tau_h^\star \rangle_{L^2(\Sigma)}| \simeq \sum_{i=1}^{N_x} \sum_{\ell=1}^{N_t} v_{i\ell}^2 h_{i,x}^{n-1} h_{\ell,t} \simeq \|v_h\|^2_{L^2(\Sigma)}$$

and the proposed stability estimate follows. □

Hence the variational problem (8.11) is uniquely solvable. Let the L^2 projection operators $Q_\Sigma^{\cdot,0} : L^2(\Sigma) \to L^2(\Sigma)$ and $\widetilde{Q}_\Sigma^{1,\cdot} : L^2(\Sigma) \to L^2(\Sigma)$ be defined as

$$\begin{aligned} (Q_\Sigma^{\cdot,0} u)(x,t) &:= (Q_I^0 u(x,\cdot))(t), \\ (\widetilde{Q}_\Sigma^{1,\cdot} u)(x,t) &:= (\widetilde{Q}_\Gamma^1 u(\cdot,t))(x) \end{aligned} \tag{8.12}$$

where $Q_I^0 : L^2(0,T) \to S_{h_t}^0(I_{N_t}) \subset L^2(0,T)$ is given by (8.8) and the projection operator $\widetilde{Q}_\Gamma^1 : L^2(\Gamma) \to S_{h_x}^1(\widetilde{\Gamma}_{\widetilde{N}_x}) \subset L^2(\Gamma)$ is defined by

$$\langle \widetilde{Q}_\Gamma^1 u, v_h \rangle_{L^2(\Gamma)} = \langle u, v_h \rangle_{L^2(\Gamma)} \quad \text{for all } v_h \in S_{h_x}^0(\Gamma_{N_x}).$$

This Galerkin–Petrov formulation is uniquely solvable since the trial and test spaces satisfy a related stability condition [60, Lemma 3.1]. Moreover, we have the representation $\widetilde{Q}_\Sigma^{1,0} = \widetilde{Q}_\Sigma^{1,\cdot} Q_\Sigma^{\cdot,0} = Q_\Sigma^{\cdot,0} \widetilde{Q}_\Sigma^{1,\cdot}$.

Let $\tilde{\gamma}_\ell$ be an arbitrary boundary element of the dual mesh $\widetilde{\Gamma}_{\widetilde{N}_x}$. We assume that there exsists a constant $c_0 > 0$ such that

$$(\mathsf{H}_\ell \mathsf{G}_\ell \mathsf{H}_\ell^{-1} \boldsymbol{x}_\ell, \boldsymbol{x}_\ell) \geq c_0 (\mathsf{D}_\ell \boldsymbol{x}_\ell, \boldsymbol{x}_\ell) \quad \text{for all } \boldsymbol{x}_\ell \in \mathbb{R}^{|J(\ell)|} \tag{8.13}$$

where $J(\ell)$ denotes the index set of all nodes adjacent to the element $\tilde{\gamma}_\ell$ and the local matrices are defined as

$$\mathsf{G}_\ell[j,i] := \langle \psi_{p(i)}^0, \widetilde{\psi}_{p(j)}^1 \rangle_{L^2(\tilde{\gamma}_\ell)}, \quad \mathsf{D}_\ell := \operatorname{diag} \mathsf{G}_\ell, \quad \mathsf{H}_\ell := \operatorname{diag}(\hat{h}_{p(i),x}^{1/2}) \quad \text{for } i,j = 1,\dots,|J(\ell)|$$

where $p(i)$ denotes the i-th element in $J(\ell)$. Here, the nodal mesh size $\hat{h}_{i,x}$ is defined analogously to (8.10) but with respect to the dual mesh $\widetilde{\Gamma}_{\widetilde{N}_x}$. Then there exists a constant $c > 0$ such that [60, Theorem 4.2]

$$\left\| \widetilde{Q}_\Gamma^1 u \right\|_{H^{1/2}(\Gamma)} \leq c \, \|u\|_{H^{1/2}(\Gamma)} \quad \text{for all } u \in H^{1/2}(\Gamma). \tag{8.14}$$

Thus, by combining the stability estimate in Lemma 8.4 and estimate (8.14) we obtain the following stability result.

Theorem 8.6. *Let assumption* (8.13) *be satisfied. Then there exists a constant* $c > 0$ *such that*

$$\left\| \widetilde{Q}_\Sigma^{1,0} u \right\|_{H^{1/2,1/4}(\Sigma)} \leq c \, \|u\|_{H^{1/2,1/4}(\Sigma)} \quad \textit{for all } u \in H^{1/2,1/4}(\Sigma).$$

Proof. For $u \in H^{1/2,1/4}(\Sigma)$ we have

$$\left\| \widetilde{Q}_\Sigma^{1,0} u \right\|_{H^{1/2,1/4}(\Sigma)}^2 = \left\| \widetilde{Q}_\Sigma^{1,0} u \right\|_{L^2(\Sigma)}^2 + |\widetilde{Q}_\Sigma^{1,0} u|_{H^{1/4}(0,T;L^2(\Gamma))}^2 + |\widetilde{Q}_\Sigma^{1,0} u|_{L^2(0,T;H^{1/2}(\Gamma))}^2.$$

By using Lemma 8.5 and the definition of the operator $\widetilde{Q}_\Sigma^{1,0}$ we can estimate the first term by

$$\left\| \widetilde{Q}_\Sigma^{1,0} u \right\|_{L^2(\Sigma)} \leq c \sup_{0 \neq \tau_h \in X_h} \frac{\langle \widetilde{Q}_\Sigma^{1,0} u, \tau_h \rangle_{L^2(\Sigma)}}{\|\tau_h\|_{L^2(\Sigma)}} = c \sup_{0 \neq \tau_h \in X_h} \frac{\langle u, \tau_h \rangle_{L^2(\Sigma)}}{\|\tau_h\|_{L^2(\Sigma)}} \leq c \, \|u\|_{L^2(\Sigma)}.$$

An application of Lemma 8.4, the definition (8.12) of the operators $\widetilde{Q}_\Sigma^{1,\cdot}$ and $Q_\Sigma^{\cdot,0}$, and the $L^2(\Gamma)$-stability of $\widetilde{Q}_\Gamma^1$ [60] yield

$$\begin{aligned}|\widetilde{Q}_\Sigma^{1,0}u|^2_{H^{1/4}(0,T;L^2(\Gamma))} &= |\widetilde{Q}_\Sigma^{1,\cdot} Q_\Sigma^{\cdot,0}u|^2_{H^{1/4}(0,T;L^2(\Gamma))} \le |Q_\Sigma^{\cdot,0}u|^2_{H^{1/4}(0,T;L^2(\Gamma))} \\ &\le c\,\|u\|^2_{H^{1/4}(0,T;L^2(\Gamma))}.\end{aligned}$$

Similarly, by using estimate (8.14), definition (8.12) and the $L^2(0,T)$-stability of Q_I^0 we get

$$\begin{aligned}|\widetilde{Q}_\Sigma^{1,0}u|^2_{L^2(0,T;H^{1/2}(\Gamma))} &= |Q_\Sigma^{\cdot,0}\widetilde{Q}_\Sigma^{1,\cdot}u|^2_{L^2(0,T;H^{1/2}(\Gamma))} \le |\widetilde{Q}_\Sigma^{1,\cdot}u|^2_{L^2(0,T;H^{1/2}(\Gamma))} \\ &\le c\,\|u\|^2_{L^2(0,T;H^{1/2}(\Gamma))}\end{aligned}$$

and finally conclude

$$\left\|\widetilde{Q}_\Sigma^{1,0}u\right\|_{H^{1/2,1/4}(\Sigma)} \le c\,\|u\|_{H^{1/2,1/4}(\Sigma)} \quad \text{for all } u \in H^{1/2,1/4}(\Sigma).$$

□

According to Theorem 8.3 the stability estimate (8.4) holds and thus, the discretization of the hypersingular operator D with $Y_h = S^1_{h_x}(\widetilde{\Gamma}_{\widetilde{N}_x}) \otimes S^0_{h_t}(I_{N_t})$ yields the boundedness of the condition number of the preconditioned system matrix $C_{\mathsf{V}}^{-1}\mathsf{V}_h$.

Piecewise Linear Basis Functions in Time defined on a Dual Mesh

As a second approach we consider the space

$$Y_h := S^1_{h_x}(\widetilde{\Gamma}_{\widetilde{N}_x}) \otimes S^1_{h_t}(\widetilde{I}_{\widetilde{N}_t}) \subset H^{1/2,1/4}(\Sigma)$$

for the discretization of the operator D. Here, $S^1_{h_x}(\widetilde{\Gamma}_{\widetilde{N}_x})$ and $S^1_{h_t}(\widetilde{I}_{\widetilde{N}_t})$ denote the spaces of piecewise linear and globally continuous functions defined with respect to the previously introduced locally quasi-uniform dual meshes $\widetilde{\Gamma}_{\widetilde{N}_x}$ and $\widetilde{I}_{\widetilde{N}_t}$, respectively. The temporal dual mesh $\widetilde{I}_{\widetilde{N}_t}$ is defined analogously to $\widetilde{\Sigma}_{\widetilde{N}}$ for the spatially one-dimensional problem in Subsection 8.1.1. Let the L^2 projection operator $\widetilde{Q}_\Sigma^{1,1} : L^2(\Sigma) \to Y_h \subset L^2(\Sigma)$ be defined by the variational problem

$$\langle \widetilde{Q}_\Sigma^{1,1}u, \tau_h\rangle_{L^2(\Sigma)} = \langle u, \tau_h\rangle_{L^2(\Sigma)} \quad \text{for all } \tau_h \in X_h. \tag{8.15}$$

As before, (8.15) is a Galerkin–Petrov variational problem and thus, an $L^2(\Sigma)$-stability estimate for the given trial spaces is necessary in order to conclude unique solvability.

Lemma 8.7. *For the given boundary element spaces X_h and Y_h there holds the stability estimate*

$$c\,\|v_h\|_{L^2(\Sigma)} \le \sup_{0\ne\tau_h\in X_h} \frac{\langle v_h, \tau_h\rangle_{L^2(\Sigma)}}{\|\tau_h\|_{L^2(\Sigma)}} \quad \text{for all } v_h \in Y_h$$

with some positive constant $c > 0$.

Proof. Follows the proof of Lemma 8.5. □

Hence the variational problem (8.15) is uniquely solvable and it remains to establish the $H^{1/2,1/4}(\Sigma)$-stability of the operator $\widetilde{Q}_\Sigma^{1,1}$. The proof of the stability estimate is the same as in the case of $\widetilde{Q}_\Sigma^{1,0}$, i.e. we utilize the stability of the L^2 projection operators in space and time separately.

Theorem 8.8. *Let the assumptions* (8.9) *and* (8.13) *be satisfied. Then there exists a constant $c > 0$ such that*

$$\left\|\widetilde{Q}_\Sigma^{1,1} u\right\|_{H^{1/2,1/4}(\Sigma)} \le c\,\|u\|_{H^{1/2,1/4}(\Sigma)} \quad \text{for all } u \in H^{1/2,1/4}(\Sigma).$$

Proof. Follows the proof of Theorem 8.6. □

Theorem 8.3 then yields the stability estimate (8.4).

8.1.3 Numerical Results

For the following numerical experiments we consider the initial Dirichlet boundary value problem (5.6) with the heat capacity constant $\alpha = 10$ and time horizon $T = 1$. We solve the weakly singular boundary integral equation (5.7) in order to compute the unknown Neumann datum $w = \gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$. The Galerkin boundary element discretization is done by using piecewise constant basis functions defined with respect to a given space–time boundary element mesh Σ_N. The resulting system of linear equations $\mathsf{V}_h \boldsymbol{w} = \boldsymbol{f}$ is solved by using a preconditioned GMRES method with a relative accuracy of 10^{-8} as stopping criteria.

One-Dimensional Problem

We consider the spatial domain $\Omega = (0,1)$. For the discretization of the integral equation we use the space of piecewise constant basis functions $S_h^0(\Sigma_N)$. As a preconditioner we use the discretization of the hypersingular operator D with $S_h^0(\Sigma_N)$, denoted by $\mathsf{C}_{\mathsf{V},0}$, as well as the discretization with piecewise linear and globally continuous basis functions $S_h^1(\widetilde{\Sigma}_{\widetilde{N}})$ which are defined with respect to the dual mesh $\widetilde{\Sigma}_{\widetilde{N}}$, denoted by $\mathsf{C}_{\mathsf{V},1}$.

Uniform Refinement. The first example corresponds to the initial datum

$$u_0(x) = \sin(2\pi x) \quad \text{for } x \in \Omega = (0,1)$$

and a globally uniform boundary element mesh with mesh size $h = 2^{-L}$. Table 8.1 shows the $L^2(\Sigma)$-error $\|w - w_h\|_{L_2(\Sigma)}$ and the estimated order of convergence (eoc). Moreover, the iteration numbers of the non-preconditioned and preconditioned GMRES method are given, confirming the theoretical findings.

				$\mathsf{C}_\mathsf{V}^{-1} = \mathsf{I}$		$\mathsf{C}_\mathsf{V}^{-1} = \mathsf{C}_{\mathsf{V},0}^{-1}$		$\mathsf{C}_\mathsf{V}^{-1} = \mathsf{C}_{\mathsf{V},1}^{-1}$	
L	N	$\|w - w_h\|_{L_2(\Sigma)}$	eoc	κ	It.	κ	It.	κ	It.
2	8	$1.045 \cdot 10^{-0}$	1.60	3.98	4	1.49	4	19.95	4
3	16	$4.759 \cdot 10^{-1}$	1.14	6.24	8	1.60	8	19.57	7
4	32	$2.320 \cdot 10^{-1}$	1.04	9.15	16	1.65	11	19.56	8
5	64	$1.144 \cdot 10^{-1}$	1.02	13.09	26	1.66	10	19.56	7
6	128	$5.676 \cdot 10^{-2}$	1.01	18.57	33	1.66	10	19.56	7
7	256	$2.827 \cdot 10^{-2}$	1.01	26.28	39	1.66	9	19.56	6
8	512	$1.410 \cdot 10^{-2}$	1.00	37.18	46	1.66	9	19.56	6
9	1 024	$7.043 \cdot 10^{-3}$	1.00	52.59	54	1.66	8	19.56	6
10	2 048	$3.524 \cdot 10^{-3}$	1.00	74.37	63	1.66	8	19.56	5

Table 8.1: $L^2(\Sigma)$-error and convergence rate of the Galerkin approximation w_h, condition number κ of the system matrix, and iteration number of the GMRES method (It.) for different preconditioning strategies in the case of uniform refinement in 1D. The parameter N denotes the number of boundary elements on level L.

Adaptive Refinement. For the second example we consider the initial datum

$$u_0(x) = 5\exp(-10x)\sin(\pi x) \quad \text{for } x \in \Omega = (0,1)$$

which motivates the use of a locally quasi-uniform boundary element mesh resulting from some adaptive refinement strategy. The numerical results given in Table 8.2 again confirm the theoretical findings, in particular the robustness of the proposed preconditioning strategies for adaptive refined meshes which is not the case when using none or only diagonal preconditioning $\mathsf{C}_{\mathsf{V},d} = \operatorname{diag}\mathsf{V}_h$.

Two-Dimensional Problem

We consider the domain $\Omega = (0,1)^2$ and use the space $X_h = X^{0,0}_{h_x,h_t}(\Sigma_N)$ for the Galerkin discretization of the boundary integral equation. As a preconditioner we use the discretization of the hypersingular operator D with $Y_h = S^1_h(\widetilde{\Gamma}_{\widetilde{N}_x}) \otimes S^0_h(I_{N_t})$, denoted by $\mathsf{C}_{\mathsf{V},10}$.

			$\mathsf{C}_\mathsf{V}^{-1} = \mathsf{I}$		$\mathsf{C}_\mathsf{V}^{-1} = \mathsf{C}_{\mathsf{V},d}^{-1}$		$\mathsf{C}_\mathsf{V}^{-1} = \mathsf{C}_{\mathsf{V},0}^{-1}$		$\mathsf{C}_\mathsf{V}^{-1} = \mathsf{C}_{\mathsf{V},1}^{-1}$	
L	N	$\|w-w_h\|_{L_2(\Sigma)}$	κ	It.	κ	It.	κ	It.	κ	It.
6	24	$1.204 \cdot 10^{-1}$	$2.05 \cdot 10^{3}$	24	5.88	19	1.56	9	19.93	10
7	36	$7.356 \cdot 10^{-2}$	$6.16 \cdot 10^{3}$	36	7.61	23	1.60	8	20.34	12
8	55	$4.518 \cdot 10^{-2}$	$1.56 \cdot 10^{4}$	55	9.42	26	1.70	8	23.97	11
9	84	$2.840 \cdot 10^{-2}$	$3.97 \cdot 10^{4}$	83	12.38	30	1.71	8	24.60	11
10	137	$1.695 \cdot 10^{-2}$	$6.15 \cdot 10^{4}$	127	15.35	34	1.72	7	24.00	10
11	222	$1.034 \cdot 10^{-2}$	$1.46 \cdot 10^{5}$	193	20.85	38	1.78	7	19.59	8
12	332	$6.937 \cdot 10^{-3}$	$2.99 \cdot 10^{5}$	270	25.07	41	1.76	7	24.30	10
13	431	$5.429 \cdot 10^{-3}$	$8.05 \cdot 10^{5}$	354	29.24	44	1.82	7	23.98	10
14	499	$4.772 \cdot 10^{-3}$	$2.16 \cdot 10^{6}$	425	31.59	45	1.82	7	24.02	10

Table 8.2: $L^2(\Sigma)$-error of the Galerkin approximation w_h, condition number κ of the system matrix, and iteration number of the GMRES method (It.) for different preconditioning strategies in the case of adaptive refinement in 1D. The parameter N denotes the number of boundary elements on level L.

Uniform Refinement. We consider the exact solution

$$u(x,t) = \exp\left(-\frac{t}{\alpha}\right)\sin\left(x_1\cos\frac{\pi}{8} + x_2\sin\frac{\pi}{8}\right) \quad \text{for } (x,t) = (x_1,x_2,t) \in Q$$

and determine the Dirichlet datum g and the initial datum u_0 accordingly. We use a globally quasi-uniform boundary element mesh with mesh size $h = \mathcal{O}(2^{-L})$. Table 8.3 shows the $L^2(\Sigma)$-error $\|w-w_h\|_{L_2(\Sigma)}$ and the estimated order of convergence (eoc), which is linear as expected. Moreover, the iteration numbers of the non-preconditioned and preconditioned GMRES method are given, again confirming the theoretical findings. Instead of using M_h in the preconditioner one may compute a lumped mass matrix. Hence, the matrix becomes diagonal and the inverse can be applied efficiently. Due to computational costs, the condition number of the system matrix was not computed for all refinement levels.

Adaptive Refinement. For the second example in the spatially two-dimensional case we consider the initial datum

$$u_0(x_1,x_2) = 40\exp\left(-10(x_1+x_2)\right)\sin\left(\pi x_1\right)\sin\left(\pi x_2\right) \quad \text{for } (x_1,x_2) \in \Omega = (0,1)^2$$

which motivates the use of a boundary element mesh that is locally quasi-uniform in space and time, resulting from some adaptive refinement strategy. The iteration numbers in Table 8.4 confirm the robustness of the introduced space–time preconditioner for locally quasi-uniform meshes. The condition and iteration numbers when using the diagonal preconditioner $\mathsf{C}_{\mathsf{V},d} = \operatorname{diag}\mathsf{V}_h$ are also listed.

				$\mathsf{C}_\mathsf{V}^{-1} = \mathsf{I}$		$\mathsf{C}_\mathsf{V}^{-1} = \mathsf{C}_{\mathsf{V},10}^{-1}$	
L	N	$\|w - w_h\|_{L_2(\Sigma)}$	eoc	κ	It.	κ	It.
0	4	$1.364 \cdot 10^{-0}$	-	1.63	1	-	-
1	16	$1.147 \cdot 10^{-0}$	0.25	3.11	2	3.59	4
2	64	$6.018 \cdot 10^{-1}$	0.93	5.50	8	2.81	11
3	256	$3.018 \cdot 10^{-1}$	1.00	9.84	14	2.91	12
4	1 024	$1.450 \cdot 10^{-1}$	1.01	18.47	20	2.99	12
5	4 096	$7.460 \cdot 10^{-2}$	1.01	35.82	28	3.02	11
6	16 384	$4.691 \cdot 10^{-3}$	1.00	-	50	-	11
7	65 536	$2.341 \cdot 10^{-3}$	1.00	-	67	-	10

Table 8.3: $L^2(\Sigma)$-error and convergence rate of the Galerkin approximation w_h, condition number κ of the system matrix, and iteration number of the GMRES method (It.) in the case of uniform refinement in 2D. The parameter N denotes the number of boundary elements on level L.

8.2 Neumann Boundary Value Problem

In the following section we consider the initial Neumann boundary value problem (5.10) with source term $f \in [H^{1,1/2}_{;,0}(Q)]'$, Neumann datum $w \in H^{-1/2,-1/4}(\Sigma)$ and initial datum $u_0 \in L^2(\Omega)$. We use the direct formulation (5.11) in order to compute the unknown Dirichlet datum $g = \gamma_0^{\text{int}} u \in H^{1/2,1/4}(\Sigma)$ of the solution $u \in H^{1,1/2}(Q)$. Hence we have to find $g \in H^{1/2,1/4}(\Sigma)$ such that

$$\langle Dg, v\rangle_\Sigma = \langle (\frac{1}{2}I - K')w - M_1 u_0 - N_1 f, v\rangle_\Sigma \quad \text{for all } v \in H^{1/2,1/4}(\Sigma). \tag{8.16}$$

The ellipticity of the hypersingular operator $D : H^{1/2,1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma)$ ensures unique solvability of (8.16).

For the discretization of (8.16) we consider a conforming trial space $Y_h = \operatorname{span}\{\psi_\ell\}_\ell^M \subset H^{1/2,1/4}(\Sigma)$ defined with respect to an admissible boundary element mesh Σ_N as introduced in Chapter 6. The space–time discretization leads to the system of linear equations $\mathsf{D}_h \boldsymbol{g} = \boldsymbol{f}$ with

$$\mathsf{D}_h[\ell, k] := \langle D\psi_k, \psi_\ell\rangle_\Sigma, \quad \boldsymbol{f}[\ell] := \langle (\frac{1}{2}I - K')w - M_1 u_0 - N_1 f, \psi_\ell\rangle_\Sigma \quad \text{for } \ell, k = 1, \ldots, M.$$

For the computation of the matrix D_h in the spatially two- and three-dimensional case we use the alternative representations (4.13) and (4.14) of the associated bilinear form which

			$\mathsf{C}_{\mathsf{V}}^{-1} = \mathsf{I}$		$\mathsf{C}_{\mathsf{V}}^{-1} = \mathsf{C}_{\mathsf{V},d}^{-1}$		$\mathsf{C}_{\mathsf{V}}^{-1} = \mathsf{C}_{\mathsf{V},10}^{-1}$	
L	N	$\|w - w_h\|_{L_2(\Sigma)}$	κ	It.	κ	It.	κ	It.
0	16	$6.634 \cdot 10^{-1}$	$3.00 \cdot 10^{0}$	8	3.11	8	3.59	10
1	30	$6.275 \cdot 10^{-1}$	$1.50 \cdot 10^{1}$	15	4.11	10	3.51	13
2	48	$5.442 \cdot 10^{-1}$	$1.05 \cdot 10^{2}$	26	6.76	13	3.61	15
3	80	$4.190 \cdot 10^{-1}$	$8.18 \cdot 10^{2}$	50	13.14	18	4.10	15
4	156	$2.829 \cdot 10^{-1}$	$6.42 \cdot 10^{3}$	75	26.10	22	5.16	16
5	266	$1.941 \cdot 10^{-1}$	$4.77 \cdot 10^{4}$	115	46.73	25	5.88	17
6	528	$1.422 \cdot 10^{-1}$	$3.87 \cdot 10^{5}$	162	96.93	32	6.42	18
7	1 920	$8.076 \cdot 10^{-2}$	$2.81 \cdot 10^{6}$	301	185.06	49	4.58	14

Table 8.4: $L^2(\Sigma)$-error of the Galerkin approximation w_h, condition number κ of the system matrix, and iteration number of the GMRES method (It.) for different preconditioning strategies in the case of adaptive refinement in 2D. The parameter N denotes the number of boundary elements on level L.

is attained by applying integration by parts. As in the case of the previously discussed initial Dirichlet boundary value problem, we want to solve $\mathsf{D}_h \boldsymbol{g} = \boldsymbol{f}$ without an application of time-stepping schemes to make use of parallelization in time, e.g. use an operator preconditioned GMRES method. For the derivation of the theoretical basis of the operator preconditioning technique for the Neumann problem we can reuse some of the already proven stability results in Section 8.1.

The hypersingular boundary integral operator $D : H^{1/2,1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma)$ and the single layer boundary integral operator $V : H^{-1/2,-1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma)$ are both elliptic, and thus, the stability estimates (8.1) for the induced bilinear forms

$$\begin{aligned} a(u,v) &:= \langle Du, v\rangle_\Sigma \quad \text{for all } u,v \in H^{1/2,1/4}(\Sigma), \\ b(w,\tau) &:= \langle Vw, \tau\rangle_\Sigma \quad \text{for all } w,\tau \in H^{-1/2,-1/4}(\Sigma) \end{aligned} \tag{8.17}$$

are satisfied. Hence the Galerkin discretization of V allows the construction of a suitable preconditioner for D_h. While the discretization of the hypersingular operator D is done with respect to Y_h, for the Galerkin discretization of the single layer operator V we need to use a conforming trial space $X_h = \operatorname{span}\{\varphi_\ell\}_{\ell=1}^M \subset H^{-1/2,-1/4}(\Sigma)$ of the same dimension M. Similar to the Dirichlet boundary value problem, the continuous bilinear form $m(\cdot,\cdot)$ in (8.2) is chosen to be the duality product on $H^{1/2,1/4}(\Sigma) \times H^{-1/2,-1/4}(\Sigma)$ and thus, for boundary element spaces $Y_h, X_h \subset L^2(\Sigma)$ we obtain $m(v_h,\tau_h) = \langle v_h, \tau_h\rangle_{L^2(\Sigma)}$.

Theorem 8.9. *Assume that the discrete stability estimate*

$$\sup_{0 \neq \tau_h \in X_h} \frac{\langle v_h, \tau_h\rangle_{L^2(\Sigma)}}{\|\tau_h\|_{H^{-1/2,-1/4}(\Sigma)}} \geq c_1^M \|v_h\|_{H^{1/2,1/4}(\Sigma)} \quad \textit{for all } v_h \in Y_h \tag{8.18}$$

holds. Then there exists a constant $c_\kappa \geq 1$ *such that*

$$\kappa\left(\mathsf{M}_h^{-1}\mathsf{V}_h\mathsf{M}_h^{-\top}\mathsf{D}_h\right) \leq c_\kappa$$

where, for $k,\ell = 1,\ldots,M$,

$$\mathsf{D}_h[\ell,k] = \langle D\psi_k,\psi_\ell\rangle_\Sigma\ , \quad \mathsf{V}_h[\ell,k] = \langle V\varphi_k,\varphi_\ell\rangle_\Sigma\ , \quad \mathsf{M}_h[\ell,k] = \langle \psi_k,\varphi_\ell\rangle_{L^2(\Sigma)}\ .$$

Proof. Application of Theorem 8.1 with the bilinear forms (8.17) and $m(v,\tau) := \langle v,\tau\rangle_\Sigma$ for $v \in H^{1/2,1/4}(\Sigma)$ and $\tau \in H^{-1/2,-1/4}(\Sigma)$. □

Thus, $\mathsf{C}_\mathsf{D}^{-1} = \mathsf{M}_h^{-1}\mathsf{V}_h\mathsf{M}_h^{-\top}$ turns out to be a robust preconditioner for D_h. Since X_h and Y_h have the same dimension, M_h is a square matrix. It remains to define a suitable boundary element space X_h such that the mass matrix M_h is invertible and that the stability condition (8.18) is satisfied.

In order to prove the stability condition (8.18) we can reuse some of the theoretical findings in the previous section, i.e. the $H^{1/2,1/4}(\Sigma)$-stability of the operator $Q_\Sigma : L^2(\Sigma) \to Y_h$ defined by the variational problem (8.5), which we assume to be uniquely solvable, see Section 8.1 for more details.

Theorem 8.10. *Let* Y_h *and* X_h *be such that* (8.6) *is satisfied. Moreover, let the* L^2 *projection operator* Q_Σ *defined by* (8.5) *be* $H^{1/2,1/4}(\Sigma)$*-stable, i.e. there exists a constant* $c > 0$ *such that*

$$\|Q_\Sigma u\|_{H^{1/2,1/4}(\Sigma)} \leq c\,\|u\|_{H^{1/2,1/4}(\Sigma)} \quad \textit{for all } u \in H^{1/2,1/4}(\Sigma).$$

Then the stability condition (8.18) *holds.*

Proof. In order to prove the stability estimate (8.18) we introduce the projection operator $\Pi_\Sigma : H^{1/2,1/4}(\Sigma) \to X_h \subset L^2(\Sigma)$ which is defined by the variational problem

$$\langle \Pi_\Sigma u, v_h\rangle_{L^2(\Sigma)} = \langle u, v_h\rangle_{H^{1/2,1/4}(\Sigma)} \quad \text{for all } v_h \in Y_h \tag{8.19}$$

with $u \in H^{1/2,1/4}(\Sigma)$. Note that the stiffness matrix of the variational problem (8.19) is the same as for the projection operator $Q_\Sigma^* : L^2(\Sigma) \to X_h \subset L^2(\Sigma)$ defined by

$$\langle Q_\Sigma^* w, v_h\rangle_{L^2(\Sigma)} = \langle w, v_h\rangle_{L^2(\Sigma)} \quad \text{for all } v_h \in Y_h \tag{8.20}$$

with $w \in L^2(\Sigma)$. By definition we have

$$\langle Q_\Sigma^* w, v\rangle_{L^2(\Sigma)} = \langle Q_\Sigma^* w, Q_\Sigma v\rangle_{L^2(\Sigma)} = \langle w, Q_\Sigma v\rangle_{L^2(\Sigma)} \quad \text{for all } w,v \in L^2(\Sigma).$$

The stability analysis of (8.20) can be done analogously to Q_Σ by assuming a related $L^2(\Sigma)$-stability condition of the trial spaces Y_h and X_h, see Section 8.1 and [61, Section 1.4

and Chapter 2]. Thus, unique solvability of (8.20) implies unique solvability of (8.19). Let $u \in H^{1/2,1/4}(\Sigma)$. By using the $H^{1/2,1/4}(\Sigma)$-stability of the operator Q_Σ we get

$$\begin{aligned}
\|\Pi_\Sigma u\|_{H^{-1/2,-1/4}(\Sigma)} &= \sup_{0\neq v\in H^{1/2,1/4}(\Sigma)} \frac{\langle \Pi_\Sigma u, v\rangle_{L^2(\Sigma)}}{\|v\|_{H^{1/2,1/4}(\Sigma)}} = \sup_{0\neq v\in H^{1/2,1/4}(\Sigma)} \frac{\langle \Pi_\Sigma u, Q_\Sigma v\rangle_{L^2(\Sigma)}}{\|v\|_{H^{1/2,1/4}(\Sigma)}} \\
&= \sup_{0\neq v\in H^{1/2,1/4}(\Sigma)} \frac{\langle u, Q_\Sigma v\rangle_{H^{1/2,1/4}(\Sigma)}}{\|v\|_{H^{1/2,1/4}(\Sigma)}} \\
&\leq \|u\|_{H^{1/2,1/4}(\Sigma)} \sup_{0\neq v\in H^{1/2,1/4}(\Sigma)} \frac{\|Q_\Sigma v\|_{H^{1/2,1/4}(\Sigma)}}{\|v\|_{H^{1/2,1/4}(\Sigma)}} \leq c\,\|u\|_{H^{1/2,1/4}(\Sigma)}\,.
\end{aligned}$$

Hence the projection operator $\Pi_\Sigma : H^{1/2,1/4}(\Sigma) \to X_h \subset H^{-1/2,-1/4}(\Sigma)$ is bounded. For $v_h \in H^{1/2,1/4}(\Sigma)$ we then obtain

$$\sup_{0\neq \tau_h\in X_h} \frac{\langle v_h, \tau_h\rangle_{L^2(\Sigma)}}{\|\tau_h\|_{H^{-1/2,-1/4}(\Sigma)}} \geq \frac{\langle v_h, \Pi_\Sigma v_h\rangle_{L^2(\Sigma)}}{\|\Pi_\Sigma v_h\|_{H^{-1/2,-1/4}(\Sigma)}} = \frac{\|v_h\|^2_{H^{1/2,1/4}(\Sigma)}}{\|\Pi_\Sigma v_h\|_{H^{-1/2,-1/4}(\Sigma)}} \geq \frac{1}{c}\,\|v_h\|_{H^{1/2,1/4}(\Sigma)}$$

which concludes the proof. □

Hence, according to Theorem 8.9, the condition number $\kappa(\mathsf{C}_\mathsf{D}^{-1}\mathsf{D}_h)$ with the preconditioner $\mathsf{C}_\mathsf{D}^{-1} = \mathsf{M}_h^{-1}\mathsf{V}_h\mathsf{M}_h^{-\top}$ is bounded. It remains to choose, for given $Y_h \subset H^{1/2,1/4}(\Sigma)$, a suitable boundary element space $X_h \subset H^{-1/2,-1/4}(\Sigma)$ for the discretization of V.

8.2.1 One-Dimensional Problem

In the spatially one-dimensional case we use the space $S_h^p(\Sigma_N)$ for the discretization of the hypersingular integral equation (8.16) which is defined with respect to an arbitrary decomposition of the space–time boundary $\Sigma = \Sigma_a \cup \Sigma_b$, see Fig. 6.1. Here, $p \in \{0,1\}$ denotes the polynomial degree of the basis functions. We assume that the boundary element mesh is locally quasi-uniform.

Since the boundary element space $Y_h := S_h^p(\Sigma_N)$ also satisfies $Y_h \subset H^{-1/4}(\Sigma)$ we can choose $X_h := S_h^p(\Sigma_N)$ for the discretization of the single layer operator V as well. According to Theorem 8.10 we need to establish the $H^{1/4}(\Sigma)$-stability of the L^2 projection operator $Q_\Sigma^p : L^2(\Sigma) \to S_h^p(\Sigma_N) \subset L^2(\Sigma)$.

The case $p = 0$ was already examined in Subsection 8.1.1, see Lemma 8.4.

The setting $p = 1$ is analysed in [59], where the proof of the stability estimate is done with respect to the Sobolev space $H^s(\Omega)$, where Ω is an open domain in $\mathbb{R}^n$ $(n = 1,2,3)$. Hence we can transfer the results to the Sobolev space $H^s(0,T)$ if we identify the time interval $I=(0,T)$ with the domain $\Omega\subset\mathbb{R}^1$. For necessary assumptions on the mesh see [59, Section 3 and Section 4].

Hence there exist constants $\tilde{c}_S^p>0$, $p=0,1$, such that

$$\left\|Q_I^p u\right\|_{H^{1/4}(0,T)}\leq \tilde{c}_S^p\left\|u\right\|_{H^{1/4}(0,T)}\quad\text{for all } u\in H^{1/4}(0,T),\tag{8.21}$$

where $Q_I^p:L^2(0,T)\to L^2(0,T)$ is defined by the variational formulation (6.3). The stability of the projection operator Q_Σ^p then follows by applying (8.21) for each of the two boundary parts Σ_a and Σ_b. We therefore conclude that there exist constants $c_S^p>0$, $p=0,1$, such that

$$\left\|Q_\Sigma^p u\right\|_{H^{1/4}(\Sigma)}\leq c_S^p\left\|u\right\|_{H^{1/4}(\Sigma)}\quad\text{for all } u\in H^{1/4}(\Sigma).$$

According to Theorem 8.10 the stability estimate (8.18) holds and thus, the discretization of the single layer boundary integral operator V with $X_h=S_h^p(\Sigma_N)$ yields the boundedness of the condition number of the preconditioned system matrix $\mathsf{C}_\mathsf{D}^{-1}\mathsf{D}_h$.

As a second approach we could use a discretization of the operator V with the basis functions of the space $S_h^q(\widetilde{\Sigma}_{\widetilde{N}})$ which is defined with respect to a dual mesh $\widetilde{\Sigma}_{\widetilde{N}}$ as introduced in Subsection 8.1.1. Here, $q=(p+1)$ mod 2. The proof of the $H^{1/4}(\Sigma)$-stability of the related L^2 projection operator follows the same path as the proof of the $H^{1/4}(\Sigma)$-stability of $\widetilde{Q}_\Sigma^1$ in Subsection 8.1.1, see also [60, 61].

8.2.2 Two- and Three-Dimensional Problem

As in the case of the Dirichlet boundary value problem we consider a tensor product decomposition of Σ as described in Section 6.3 with given locally quasi-uniform spatial and temporal decompositions $\Gamma_{N_x}=\{\gamma_\ell\}_{\ell=1}^{N_x}$ and $I_{N_t}=\{\tau_i\}_{i=1}^{N_t}$, respectively. We use the space $Y_h:=X_{h_x,h_t}^{1,p_t}(\Sigma_N)=S_{h_x}^1(\Gamma_{N_x})\otimes S_{h_t}^{p_t}(I_{N_t})$ for the discretization of the hypersingular integral equation (8.16) and set $S_{h_x}^1(\Gamma_{N_X})=\operatorname{span}\left\{\psi_i^1\right\}_{i=1}^{M_X}$ and $S_{h_t}^{p_t}(I_{N_T})=\operatorname{span}\left\{\varphi_\ell\right\}_{\ell=1}^{M_T}$. Here, $p_t\in\{0,1\}$ denotes the polynomial degree of the basis functions in the temporal dimension.

Since $Y_h\subset H^{-1/2,-1/4}(\Sigma)$, we can choose $X_h:=Y_h$ for the discretization of the single layer operator V as well. According to Theorem 8.10 we need to establish the $H^{1/2,1/4}(\Sigma)$-stability of the L^2 projection operator $Q_\Sigma^{1,p_t}:L^2(\Sigma)\to Y_h\subset L^2(\Sigma)$ which is defined by the uniquely solvable Galerkin–Bubnov variational problem

$$\langle Q_\Sigma^{1,p_t}u,\tau_h\rangle_{L^2(\Sigma)}=\langle u,\tau_h\rangle_{L^2(\Sigma)}\quad\text{for all } \tau_h\in X_h=Y_h$$

with $u \in L^2(\Sigma)$. Let the operators $Q_\Sigma^{\cdot,p_t} : L^2(\Sigma) \to L^2(\Sigma)$ and $Q_\Sigma^{1,\cdot} : L^2(\Sigma) \to L^2(\Sigma)$ be defined as

$$\begin{aligned} (Q_\Sigma^{\cdot,p_t} u)(x,t) &:= (Q_I^{p_t} u(x,\cdot))(t), \\ (Q_\Sigma^{1,\cdot} u)(x,t) &:= (Q_\Gamma^1 u(\cdot,t))(x) \end{aligned} \tag{8.22}$$

where $Q_I^{p_t} : L^2(0,T) \to S_{h_t}^{p_t}(I_{N_t}) \subset L^2(0,T)$ is given by (6.3) and the projection operator $Q_\Gamma^1 : L^2(\Gamma) \to S_{h_x}^1(\Gamma_{N_x}) \subset L^2(\Gamma)$ is defined by the variational problem (6.5) for $p = 1$. Then we have the representation $Q_\Sigma^{1,p_t} = Q_\Sigma^{1,\cdot} Q_\Sigma^{\cdot,p_t} = Q_\Sigma^{\cdot,p_t} Q_\Sigma^{1,\cdot}$.

Let γ_ℓ be an arbitrary boundary element of the mesh Γ_{N_x}. We assume that there exsists a constant $c_0 > 0$ such that

$$(\mathsf{H}_\ell \mathsf{G}_\ell \mathsf{H}_\ell^{-1} \boldsymbol{x}_\ell, \boldsymbol{x}_\ell) \geq c_0 (\mathsf{D}_\ell \boldsymbol{x}_\ell, \boldsymbol{x}_\ell) \quad \text{for all } \boldsymbol{x}_\ell \in \mathbb{R}^{|J(\ell)|} \tag{8.23}$$

where $J(\ell)$ denotes the index set of all nodes adjacent to the element γ_ℓ and the local matrices are defined as

$$\mathsf{G}_\ell[j,i] := \langle \psi_{p(i)}, \psi_{p(j)} \rangle_{L^2(\gamma_\ell)}, \quad \mathsf{D}_\ell := \operatorname{diag} \mathsf{G}_\ell, \quad \mathsf{H}_\ell := \operatorname{diag}(\hat{h}_{p(i),x}^{1/2}) \quad \text{for } i,j = 1,\dots,|J(\ell)|$$

where $p(i)$ denotes the i-th element in $J(\ell)$. The nodal mesh size $\hat{h}_{i,x}$ is given by (8.10). Then there exists a constant $c > 0$ such that [59, Theorem 3.2]

$$\left\| Q_\Gamma^1 u \right\|_{H^{1/2}(\Gamma)} \leq c \, \|u\|_{H^{1/2}(\Gamma)} \quad \text{for all } u \in H^{1/2}(\Gamma). \tag{8.24}$$

Note that in [59] the stability analysis of related L^2 projection operators is done with respect to the Sobolev space $H^s(\Omega)$ where Ω is a bounded domain in $\mathbb{R}^n$ $(n = 1,2,3)$. However, the stability results are also applicable for Sobolev spaces defined on the boundary Γ, i.e. for $H^s(\Gamma)$ with $s \in [0,1]$. By combining (8.21) and (8.24) we obtain the following result.

Theorem 8.11. *Let assumption* (8.23) *be satisfied. Then there exists a constant* $c_S > 0$ *such that*

$$\left\| Q_\Sigma^{1,p_t} u \right\|_{H^{1/2,1/4}(\Sigma)} \leq c_S \, \|u\|_{H^{1/2,1/4}(\Sigma)} \quad \textit{for all } u \in H^{1/2,1/4}(\Sigma).$$

Proof. For $u \in H^{1/2,1/4}(\Sigma)$ we have

$$\left\| Q_\Sigma^{1,p_t} u \right\|_{H^{1/2,1/4}(\Sigma)}^2 = \left\| Q_\Sigma^{1,p_t} u \right\|_{L^2(\Sigma)}^2 + |Q_\Sigma^{1,p_t} u|_{H^{1/4}(0,T;L^2(\Gamma))}^2 + |Q_\Sigma^{1,p_t} u|_{L^2(0,T;H^{1/2}(\Gamma))}^2.$$

The first term on the right hand side can be estimated by employing the standard $L^2(\Sigma)$-stability of the projection operator Q_Σ^{1,p_t}. An application of estimate (8.21), definition (8.22) of the operators $Q_\Sigma^{1,\cdot}$ and $Q_\Sigma^{\cdot,p_t}$, and the $L^2(\Gamma)$-stability of Q_Γ^1 yield

$$\begin{aligned} |Q_\Sigma^{1,p_t} u|_{H^{1/4}(0,T;L^2(\Gamma))}^2 = |Q_\Sigma^{1,\cdot} Q_\Sigma^{\cdot,p_t} u|_{H^{1/4}(0,T;L^2(\Gamma))}^2 &\leq |Q_\Sigma^{\cdot,p_t} u|_{H^{1/4}(0,T;L^2(\Gamma))}^2 \\ &\leq c \, \|u\|_{H^{1/4}(0,T;L^2(\Gamma))}^2. \end{aligned}$$

By using estimate (8.24), definition (8.22) and the $L^2(0,T)$-stability of $Q_I^{p_t}$ we get

$$|Q_\Sigma^{1,p_t} u|^2_{L^2(0,T;H^{1/2}(\Gamma))} = |Q_\Sigma^{\cdot,p_t} Q_\Sigma^{1,\cdot} u|^2_{L^2(0,T;H^{1/2}(\Gamma))} \leq |Q_\Sigma^{1,\cdot} u|^2_{L^2(0,T;H^{1/2}(\Gamma))}$$
$$\leq c\, \|u\|^2_{L^2(0,T;H^{1/2}(\Gamma))}\,.$$

A combination of the estimates yields the desired result. □

According to Theorem 8.10 the stability estimate (8.18) holds and thus, the discretization of the single layer boundary integral operator V with $X_h = X_{h_x,h_t}^{1,p_t}(\Sigma_N)$ yields the boundedness of $\kappa(\mathsf{C}_\mathsf{D}^{-1}\mathsf{D}_h)$.

We could also discretize the single layer operator V by using tensor product spaces which are defined with respect to a suitable combination of the dual meshes $\widetilde{\Gamma}_{\widetilde{N}_x}, \widetilde{I}_{\widetilde{N}_t}$. The stability analysis then follows the same idea as described for the boundary element spaces introduced in the previous sections by employing the stability of the projections in space and time separately. E.g. for $Y_h = X_{h_x,h_t}^{1,0}(\Sigma_N)$ and $Y_h = X_{h_x,h_t}^{1,1}(\Sigma_N)$ we could use the boundary element spaces $X_h = S_{h_x}^0(\widetilde{\Gamma}_{\widetilde{N}_x}) \otimes S_{h_t}^0(I_{N_t})$ or $X_h = S_{h_x}^0(\widetilde{\Gamma}_{\widetilde{N}_x}) \otimes S_{h_t}^0(\widetilde{I}_{\widetilde{N}_t})$ for the discretization of V, respectively, i.e. piecewise constant basis functions defined with respect to a dual boundary element mesh.

8.2.3 Numerical Results

For the following numerical experiments we consider the initial Neumann boundary value problem (5.10) with the heat capacity constant $\alpha = 10$ and time horizon $T = 1$. We solve the hypersingular boundary integral equation (5.11) in order to compute the unknown Dirichlet datum $g = \gamma_0^{\text{int}} u \in H^{1/2,1/4}(\Sigma)$. The Galerkin boundary element discretization is done by using a conforming trial space $Y_h \subset H^{1/2,1/4}(\Sigma)$ defined with respect to an admissible space–time boundary element mesh Σ_N. The resulting system of linear equations $\mathsf{D}_h \boldsymbol{g} = \boldsymbol{f}$ is solved by using a preconditioned GMRES method with a relative accuracy of 10^{-8} as stopping criteria.

One-Dimensional Problem

For the simple spatially one-dimensional case we choose $\Omega = (0,1)$. We consider the exact solution

$$u(x,t) = \exp\left(-4\pi^2 \frac{t}{\alpha}\right)\cos(2\pi x) \quad \text{for } (x,t) \in Q = (0,1)^2,$$

and determine the Neumann datum w and the initial datum u_0 accordingly. We use a globally uniform boundary element mesh with mesh size $h = 2^{-L}$ and the space boundary element space $Y_h := S_h^0(\Sigma_N)$ for the approximation of g. As a preconditioner we use the discretization of the single layer operator V with $X_h := Y_h$, denoted by $\mathsf{C}_{\mathsf{D},0}$.

Table 8.5 shows the $L^2(\Sigma)$-error $\|g - g_h\|_{L_2(\Sigma)}$ and the estimated order of convergence (eoc). Moreover, the iteration numbers of the non-preconditioned and preconditioned GMRES method are given, confirming the theoretical findings, i.e. the robustness of the operator preconditioning technique for the Neumann problem.

				$\mathsf{C}_\mathsf{D}^{-1} = \mathsf{I}$		$\mathsf{C}_\mathsf{D}^{-1} = \mathsf{C}_{\mathsf{D},0}^{-1}$	
L	N	$\|g - g_h\|_{L_2(\Sigma)}$	eoc	κ	It.	κ	It.
2	8	$1.486 \cdot 10^{-1}$	0.06	5.62	4	2.22	4
3	16	$1.315 \cdot 10^{-1}$	0.18	7.92	8	2.45	8
4	32	$9.805 \cdot 10^{-2}$	0.42	12.86	16	2.17	14
5	64	$5.885 \cdot 10^{-2}$	0.74	20.40	31	2.06	14
6	128	$3.077 \cdot 10^{-2}$	0.94	29.51	44	2.06	14
7	256	$1.529 \cdot 10^{-2}$	1.01	41.88	58	2.06	14
8	512	$7.500 \cdot 10^{-3}$	1.03	59.34	75	2.06	14
9	1 024	$3.682 \cdot 10^{-3}$	1.03	84.01	95	2.07	14
10	2 048	$1.815 \cdot 10^{-3}$	1.02	118.87	120	2.07	14

Table 8.5: $L^2(\Sigma)$-error and convergence rate of the Galerkin approximation g_h, condition number κ of the system matrix, and iteration number of the GMRES method (It.) in the case of uniform refinement in 1D. The parameter N denotes the number of boundary elements on level L.

Two-Dimensional Problem

We consider the domain $\Omega = (0,1)^2$ and the exact solution

$$u(x,t) = \exp\left(-\frac{t}{\alpha}\right) \sin\left(x_1 \cos\frac{\pi}{8} + x_2 \sin\frac{\pi}{8}\right) \quad \text{for } (x,t) = (x_1,x_2,t) \in Q = (0,1)^3.$$

We determine the Neumann datum w and the initial datum u_0 accordingly. We use a globally quasi-uniform space–time tensor product boundary element mesh with mesh size $h = \mathcal{O}(2^{-L})$ and the space $Y_h := X_{h,h}^{1,0}(\Sigma_N)$ for the approximation of g. As a preconditioner we use the discretization of the single layer boundary integral operator V with $X_h := Y_h$, denoted by $\mathsf{C}_{\mathsf{D},10}$.

Table 8.6 shows the $L^2(\Sigma)$-error $\|g - g_h\|_{L_2(\Sigma)}$ and the estimated order of convergence (eoc) which is linear as expected. Moreover, the iteration numbers of the preconditioned and non-preconditioned GMRES method are given, which again confirm the robustness of the introduced preconditioning strategy.

				$\mathsf{C}_\mathsf{D}^{-1} = \mathsf{I}$		$\mathsf{C}_\mathsf{D}^{-1} = \mathsf{C}_{\mathsf{D},10}^{-1}$	
L	N	$\|g - g_h\|_{L_2(\Sigma)}$	eoc	κ	It.	κ	It.
0	4	$1.564 \cdot 10^{-1}$	-	2.40	3	1.71	3
1	16	$8.274 \cdot 10^{-2}$	0.92	4.67	11	5.31	8
2	64	$4.325 \cdot 10^{-2}$	0.94	6.66	12	6.72	9
3	256	$1.897 \cdot 10^{-2}$	1.19	8.99	14	8.87	11
4	1 024	$8.733 \cdot 10^{-3}$	1.12	15.95	22	9.30	14
5	4 096	$4.131 \cdot 10^{-3}$	1.08	30.16	36	9.32	14
6	16 384	$1.987 \cdot 10^{-3}$	1.06	-	54	-	14
7	65 536	$9.709 \cdot 10^{-4}$	1.03	-	80	-	13

Table 8.6: $L^2(\Sigma)$-error and convergence rate of the Galerkin approximation g_h, condition number κ of the system matrix, and iteration number of the GMRES method (It.) in the case of uniform refinement in 2D. The parameter N denotes the number of boundary elements on level L.

9 PARALLELIZATION

In this chapter we present a method for parallelization of space–time BEM for the heat equation based on a modification of the approach presented in [30, 37] for spatial problems. The method is based on a decomposition of the input mesh into submeshes of approximately the same size and a distribution of corresponding blocks of the system matrices among processors. To ensure proper load balancing during the assembly of the system matrices and matrix-vector multiplication and to minimize the total number of submeshes that have to be stored on each compute node, a distribution of matrix blocks based on a cyclic graph decomposition is used. We modify the original approach to support the special structure of the space–time system matrices. In particular, this includes a different mesh decomposition technique (instead of a spatial domain decomposition we split the space–time mesh into time slices), modification of the block distribution due to the lower triangular structure of the matrices, and special treatment of certain blocks in the case of an even number of processes. In contrast to [30,37] where the matrix blocks are approximated by applying the fast multipole or adaptive cross approximation methods, here we restrict ourselves to dense matrices. The presented structure of the parallel solver allows the inclusion of matrix approximation techniques to solve even larger problems. The results in this chapter are based on [11, 14].

Although the BEM matrices have a block Toeplitz structure in the case of uniform time-stepping, we do not exploit this fact as our final goal is adaptivity in space and time with non-uniform time-stepping. Moreover, the block triangular Toeplitz structure makes distributed parallelization rather complicated due to different lengths of (sub)diagonals. Some of the blocks would have to be replicated on multiple processes in order to keep the matrix-vector multiplication balanced. For a parallelization scheme exploiting the Toeplitz structure in the case of the wave equation see, e.g., [70].

Numerical or semi-analytic evaluation of the surface integrals is one of the most time-consuming parts of space–time BEM. The high computational intensity of the method makes it well suited for current multi- and many-core processors equipped with wide SIMD (Single Instruction Multiple Data) registers. Vector instruction set extensions in modern CPUs (AVX512, AVX2, SSE) support simultaneous operations with up to eight double precision operands, contributing significantly to the theoretical peak performance of a processor. While current compilers support automatic vectorization to some extent, one has to use low level approaches (assembly language, compiler intrinsic functions), external libraries (Vc [31], Intel MKL Vector Mathematical Functions [28], etc.), or OpenMP pragmas [48] to achieve a reasonable speedup. Some remarks on the implementation of vectorization in order to compute the matrix entries and related numerical experiments can be found in [14]. Besides vectorization we also utilize OpenMP for thread parallelization in shared memory.

In Section 9.1 we introduce the model problem and the setup of the system of linear equations which is obtained by a tensor product decomposition of the space–time boundary Σ as described in Section 6.3. Section 9.2 is devoted to the description of our parallel implementation of the matrix assembly and to the solution of the system of linear equations based on OpenMP and MPI. In Section 9.3 we provide scalability experiments validating the suggested approach.

9.1 Model Problem and Space–Time Discretization

As a model problem we consider the initial Dirichlet boundary value problem for the heat equation with homogeneous source term and $\Omega \subset \mathbb{R}^n$ $(n = 2,3)$, i.e.

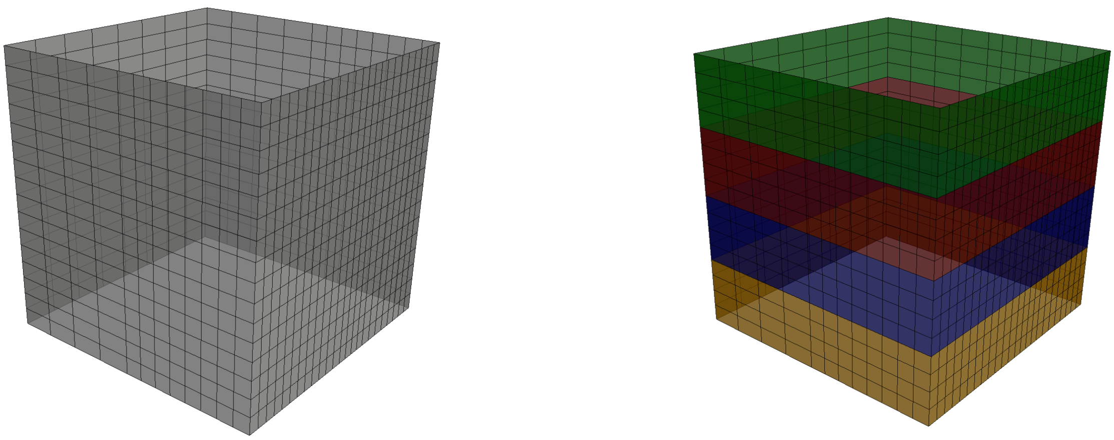
$$\begin{aligned} \alpha \partial_t u(x,t) - \Delta_x u(x,t) &= 0 && \text{for } (x,t) \in Q, \\ \gamma_0^{\text{int}} u(x,t) &= g(x,t) && \text{for } (x,t) \in \Sigma, \\ u(x,0) &= u_0(x) && \text{for } x \in \Omega \end{aligned} \tag{9.1}$$

with the heat capacity constant $\alpha > 0$, some given boundary datum $g \in H^{1/2,1/4}(\Sigma)$ and initial datum $u_0 \in L^2(\Omega)$. We determine the unknown Neumann datum $w := \gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$ by solving the variational formulation of the weakly singular boundary integral equation, i.e. we have to find $w \in H^{-1/2,-1/4}(\Sigma)$ such that

$$\langle V w, \tau \rangle_\Sigma = \langle (\frac{1}{2} I + K) g - M_0 u_0, \tau \rangle_\Sigma \quad \text{for all } \tau \in H^{-1/2,-1/4}(\Sigma), \tag{9.2}$$

which is uniquely solvable due to the ellipticity of V, see Chapter 5. In order to discretize the variational problem (9.2) we consider a space–time tensor product decomposition of Σ as introduced in Section 6.3. For given decompositions $\Gamma_{N_x} = \{\gamma_i\}_{i=1}^{N_x}$ and $I_{N_t} = \left\{\tau_j\right\}_{j=1}^{N_t}$ of the spatial boundary Γ and the time interval $(0,T)$, respectively, we define the space–time boundary element mesh Σ_N as in (6.6) with $N := N_x N_t$. A sample decomposition of the space–time boundary of $Q = (0,1)^3$, i.e. for the spatially two-dimensional heat equation, is shown in Fig. 9.1a.

For the Galerkin discretization of (9.2) we use the space $X_{h_x,h_t}^{0,0}(\Sigma_N) = \operatorname{span}\left\{\varphi_\ell^0\right\}_{\ell=1}^{N}$ of piecewise constant basis functions φ_ℓ^0, which is defined with respect to the decomposition Σ_N. For the approximation of the Dirichlet datum g we use the space $X_{h_x,h_t}^{1,0}(\Sigma_N) = \operatorname{span}\left\{\varphi_i^{10}\right\}_{i=1}^{M_\Sigma}$ of functions that are piecewise linear and globally continuous in space and piecewise constant in time, while the initial datum u_0 is discretized by using the space of piecewise linear and globally continuous functions $S_h^1(\Omega_{N_\Omega}) = \operatorname{span}\left\{\varphi_j^1\right\}_{j=1}^{M_\Omega}$, which is



(a) Tensor product decomposition.

(b) Submeshes.

Figure 9.1: Sample space–time boundary decompositions for $Q = (0,1)^3$.

defined with respect to a given admissible decomposition (triangulation) $\Omega_{N_\Omega} := \{\omega_i\}_{i=1}^{N_\Omega}$ of the domain Ω. This leads to the system of linear equations

$$\mathsf{V}_h \boldsymbol{w} = (\frac{1}{2}\mathsf{M}_h + \mathsf{K}_h)\boldsymbol{g} - \mathsf{M}_h^0 \boldsymbol{u}_0 \tag{9.3}$$

where

$$\mathsf{V}_h[\ell,k] := \frac{1}{\alpha}\int_{\sigma_\ell}\int_{\sigma_k} U^\star(x-y,t-\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t, \tag{9.4}$$

$$\mathsf{K}_h[\ell,i] := \frac{1}{\alpha}\int_{\sigma_\ell}\int_{\Sigma} \partial_{n_y} U^\star(x-y,t-\tau)\,\varphi_i^{10}(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t, \tag{9.5}$$

$$\mathsf{M}_h^0[\ell,j] := \int_{\sigma_\ell}\int_{\Omega} U^\star(x-y,t)\,\varphi_j^1(y)\,\mathrm{d}y\,\mathrm{d}s_x\,\mathrm{d}t, \tag{9.6}$$

and

$$\mathsf{M}_h[\ell,i] := \int_{\sigma_\ell}\int_{\Sigma} \varphi_i^{10}(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t.$$

The vectors $\boldsymbol{w} \in \mathbb{R}^N$, $\boldsymbol{g} \in \mathbb{R}^{M_\Sigma}$ and $\boldsymbol{u}_0 \in \mathbb{R}^{M_\Omega}$ in (9.3) represent the coefficients of the approximations w_h, g_h and u_h^0. Due to the ellipticity of the single layer operator V, the matrix V_h is positive definite and therefore (9.3) is uniquely solvable.

For the solution of (9.3) we use a preconditioned GMRES method. More precisely, we apply the operator preconditioning technique described in Section 8.1 to obtain a robust preconditioner for the system (9.3), i.e. we use a suitable discretization of the hypersingular operator $D : H^{1/2,1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma)$. Since the discretization of the weakly singular integral equation (9.2) is done with respect to $X^{0,0}_{h_x,h_t}(\Sigma_N)$, we choose

$$X^{1,0}_{h_x,h_t}(\widetilde{\Sigma}_N) := S^1_{h_x}(\widetilde{\Gamma}_{\widetilde{N}_x}) \otimes S^0_{h_t}(I_{N_t}) \subset H^{1/2,1/4}(\Sigma)$$

for the Galerkin discretization of the hypersingular operator D and thus, we obtain a robust preconditioner $\mathsf{C}_{\mathsf{V}}^{-1} = \widetilde{\mathsf{M}}_h^{-1}\mathsf{D}_h\widetilde{\mathsf{M}}_h^{-\mathrm{T}}$, see Section 8.1. Here, $\widetilde{\mathsf{M}}_h$ denotes the mass matrix defined in Theorem 8.2. Moreover, we set $X^{1,0}_{h_x,h_t}(\widetilde{\Sigma}_N) = \operatorname{span}\{\widetilde{\varphi}^{10}_\ell\}_{\ell=1}^N$. The Galerkin matrices for the preconditioner are then given by

$$\mathsf{D}_h[\ell,k] := -\frac{1}{\alpha}\int\limits_\Sigma \widetilde{\varphi}^{10}_\ell(x,t)\gamma^{\mathrm{int}}_{1,x}\int\limits_\Sigma \gamma^{\mathrm{int}}_{1,y}U^\star(x-y,t-\tau)\widetilde{\varphi}^{10}_k(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t, \tag{9.7}$$

$$\widetilde{\mathsf{M}}_h[\ell,k] := \int\limits_\Sigma\int\limits_{\sigma_k} \widetilde{\varphi}^{10}_\ell(x,t)\,\mathrm{d}s_y\,\mathrm{d}\tau\,\mathrm{d}s_x\,\mathrm{d}t.$$

We assume that the elements of I_{N_t}, referred to as time layers, are sorted from $t=0$ to $t=T$. Due to the causal behaviour of the fundamental solution (4.6) the matrices V_h, K_h and D_h are block lower triangular matrices where each block corresponds to one pair of time layers, see (9.8) in the case of V_h. The structures of K_h and D_h are identical to V_h.

$$\mathsf{V}_h = \begin{bmatrix} \mathsf{V}_{0,0} & 0 & \cdots & 0 \\ \mathsf{V}_{1,0} & \mathsf{V}_{1,1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \mathsf{V}_{N_t-1,0} & \mathsf{V}_{N_t-1,1} & \cdots & \mathsf{V}_{N_t-1,N_t-1} \end{bmatrix} \tag{9.8}$$

The structure of the initial matrix M^0_h is different. The number of its columns depends on the number of vertices of the initial mesh Ω_{N_Ω}, while the number of rows depends on the number of space–time boundary elements σ. Due to the given sorting of the elements of I_{N_t} the matrix can be decomposed into block-rows where each block-row corresponds to one time layer. For the mass matrices M_h and $\widetilde{\mathsf{M}}_h$ we obtain block-diagonal structures where each diagonal block represents the local mass matrix of one time layer.

By using the representation formula (5.1) with the computed approximations w_h, g_h and u^0_h, we can compute an approximation $\tilde{u}$ of the solution u in the space–time domain Q, i.e. for $(x,t)\in Q$ we obtain

$$\tilde{u}(x,t) = \sum_{i=1}^{M_\Omega} u^0_i(\widetilde{M}_0\varphi^1_i)(x,t) + \sum_{\ell=1}^{N} w_\ell(\widetilde{V}\varphi^0_\ell)(x,t) - \sum_{j=1}^{M_\Sigma} g_\ell(W\varphi^{10}_j)(x,t). \tag{9.9}$$

For the evaluation of the discretized representation formula (9.9) in Q we define a specific set of evaluation points. Let $\{x_\ell\}_{\ell=1}^{E_\Omega}$ be a set of nodes in the interior of the domain Ω, e.g. the nodes of the already given decomposition Ω_{N_Ω} on a specific level. Moreover, let

$\{t_k\}_{k=1}^{E_I}$ be an ordered set of time steps distributed on the interval $I = (0,T)$. The set of evaluation points is then given as

$$\{(x,t)_i\}_{i=1}^{E} = \{(x_\ell,t_k)\colon \ell = 1,...,E_\Omega; k = 1,...,E_I\} \tag{9.10}$$

with $E = E_\Omega E_I$. We have to evaluate the integrals in (9.9) for each evaluation point, i.e. we have to compute

$$\boldsymbol{u_h} = \widetilde{\mathsf{M}}_h^0 \boldsymbol{u}_0 + \widetilde{\mathsf{V}}_h \boldsymbol{w} - \mathsf{W}_h \boldsymbol{g} \tag{9.11}$$

where

$$\begin{aligned}\widetilde{\mathsf{M}}_h^0[i,j] &:= (\widetilde{M}_0 \varphi_j^1)((x,t)_i),\\ \widetilde{\mathsf{V}}_h[i,\ell] &:= (\widetilde{V} \varphi_\ell^0)((x,t)_i),\\ \mathsf{W}_h[i,k] &:= (W \varphi_k^{10})((x,t)_i).\end{aligned} \tag{9.12}$$

Note that we do not have to explicitly assemble the matrices (9.12) in order to compute $\boldsymbol{u_h}$ and that the matrix representation (9.11) is only used to write the introduced evaluation of (9.9) in multiple evaluation points in a compact form. Remarks on integration routines for a stable computation of the matrix entries and for the evaluation of the representation formula (9.9) are given in Subsection 7.1.3.

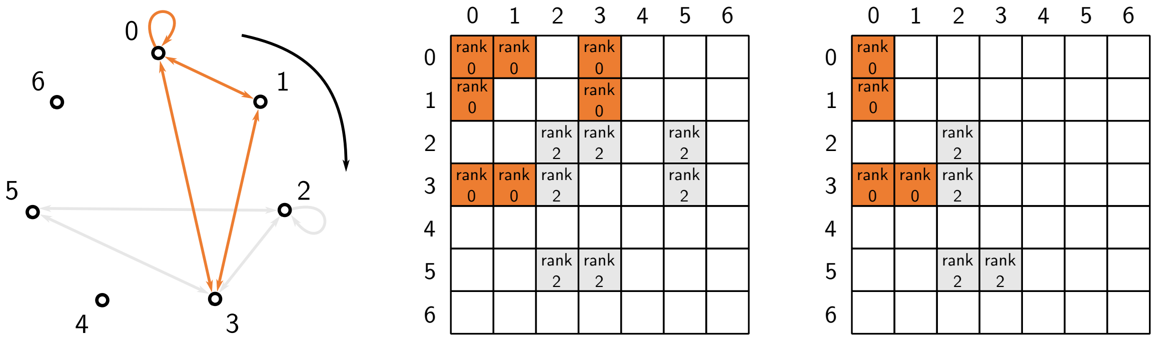
9.2 Parallel Implementation

In the following sections we focus on several levels of parallelism. In Subsection 9.2.1 we modify the method for the distribution of stationary BEM system matrices to support time-dependent problems. In Subsection 9.2.2 we describe the shared-memory parallelization of the code. OpenMP vectorization is discussed in [14]. Our aim is to fully utilize the capabilities of modern clusters equipped with multi- or many-core CPUs with wide SIMD registers in this way.

9.2.1 MPI Distribution

The original method presented in [37] for spatial problems decomposes the input surface mesh into P submeshes which splits a system matrix A (the single layer, double layer or hypersinuglar operator matrix) into $P \times P$ blocks

$$\mathsf{A} = \begin{bmatrix} \mathsf{A}_{0,0} & \mathsf{A}_{0,1} & \cdots & \mathsf{A}_{0,P-1} \\ \mathsf{A}_{1,0} & \mathsf{A}_{1,1} & \cdots & \mathsf{A}_{1,P-1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathsf{A}_{P-1,0} & \mathsf{A}_{P-1,1} & \cdots & \mathsf{A}_{P-1,P-1} \end{bmatrix}$$

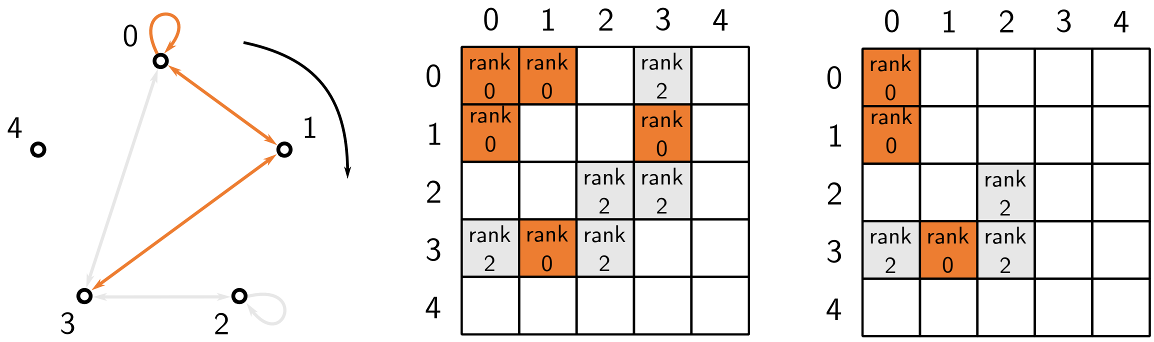


(a) Generating graph. (b) Spatial problem. (c) Space–time problem.

Figure 9.2: Distribution of the system matrix blocks among seven processes.

and distributes these blocks among P processes such that the number of shared mesh parts is minimal and each process owns a single diagonal block (since these usually include most of the singular entries). To find the optimal distribution, each matrix block $\mathsf{A}_{i,j}$ is regarded as an edge (i, j) of a directed complete graph K_P with P vertices. Finding a distribution of the matrix blocks corresponds to a decomposition of K_P into P subgraphs. First, a generator graph $G_0 \subset K_P$ is defined such that each oriented edge of G_0 corresponds to a block to be assembled by the process 0. The graphs $G_1, G_2, \ldots, G_{P-1}$ correspond to the remaining processes and are generated by a clock-wise rotation of G_0 along vertices of K_P placed on a circle, see Figures 9.2a–9.2b. The main task is to find the generating graph G_0. Optimal generating graphs with a minimal number of vertices are known for special values of P ($P = 3, 7, 13, 21, \ldots$) only and are provided in [37]. Since these numbers of processes are rather unusual in high performance computing, a heuristic algorithm for finding nearly optimal decompositions for the remaining odd and even numbers of processes P is described in [30]. Note that for odd numbers of processes the respective graph is decomposed into smaller undirected generating graphs, therefore the matrix blocks are distributed symmetrically, i.e. every process owns both blocks (i, j) and (j,i), see Figures 9.3a and 9.3b. However, when decomposing graphs for even number of processes, some edges have to be oriented and blocks are not distributed symmetrically, see Figures 9.4a–9.4b. A table with decompositions for $P = 2^k, k \in \{1, 2, \ldots, 10\}$ is presented in [30]. The described distribution aims at minimizing the number of submeshes shared among processes. This reduces memory consumption per process and global communication during the matrix-vector multiplication. To balance the load it is natural to assign each process a single diagonal block since these usually contain most of the singular entries and have to be treated with a special care.

Adapting this method for the distribution of the matrices V_h, K_h and D_h given by (9.4), (9.5) and (9.7), respectively, for the time-dependent problem (9.3) is relatively straightforward. First, instead of a spatial domain decomposition the space–time mesh is decomposed into slices in the temporal dimension, see Figure 9.1b. In contrast to spatial problems, the



(a) Generating graph. (b) Spatial problem. (c) Space–time problem.

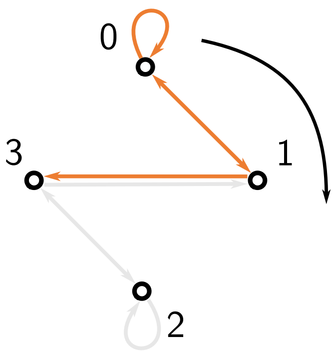
Figure 9.3: Distribution of the system matrix blocks among five processes.

system matrices are block lower triangular with lower triangular blocks on the main diagonal due to the properties of the fundamental solution and the selected discrete spaces, see (9.8). This justifies the original idea to assign a single diagonal block per process because of their different computational demands. The distribution of the remaining blocks has to be modified to take the lower triangular block structure into account . In the case of an odd number of processes, the remaining blocks below the main diagonal are distributed according to the original scheme and the distribution of the blocks above the main diagonal is ignored, see Figures 9.2c and 9.3c. In the case of an even number of processes, the original decomposition is not symmetric, therefore some blocks have to be split between two processes, see Figure 9.4c. The construction of the generating graph ensures that each process owns exactly one shared block, therefore not influencing the load balancing. All shared blocks are located on the block subdiagonal starting with a block at the position $(P/2, 0)$.

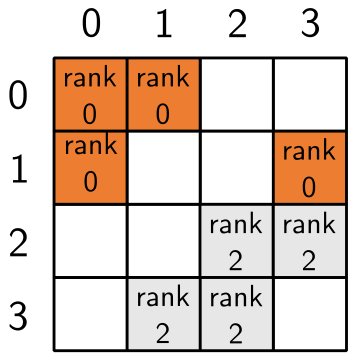
Let us note that in [30, 37] the submatrices are approximated using the fast multipole or adaptive cross approximation methods. Here we restrict to the dense format and leave the data-sparse approximation as a topic of future work.

Next we define a distribution of the initial matrix M_h^0 given by(9.6) which has a different structure compared to the matrices V_h, K_h and D_h. The number of its columns depends on the number of vertices of the initial mesh Ω_{N_Ω}, while the number of rows depends on the number of space–time elements σ_ℓ. We distribute whole block-rows of the matrix among processes, i.e. the initial mesh is not decomposed and for the space–time mesh we use the same decomposition as for the matrices V_h, K_h and D_h. In particular, each process is responsible for the block-row corresponding to its first submesh.

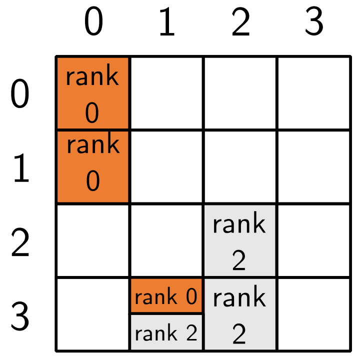
The mass matrices M_h and $\widetilde{\mathsf{M}}_h$ are block-diagonal where each diagonal block represents the local mass matrix of one of the generated submeshes. These blocks are distributed among the processes. Hence each process assembles a single diagonal block corresponding to its first submesh.



(a) Generating graph.



(b) Spatial problem.



(c) Space–time problem.

Figure 9.4: Distribution of the system matrix blocks among four processes.

It remains to establish an efficient scheme for a distributed evaluation of the discretized representation formula (9.9) in the given set of evaluation points (9.10). In order to reach a reasonable speedup we have to make the following assumption on the set of evaluations points. Recall that $\{t_k\}_{k=1}^{E_I}$ is an ordered set of time steps distributed in the interval $I = (0,T)$. We assume that each of the given time slices has the same amount of time steps E_I/P. This is necessary in order to balance the computation times between the processes.

In order to describe the parallel evaluation of (9.9) in the given set of evaluation points we consider the matrix representation (9.11). We have to distribute the matrix-vector products in an appropriate way. Therefore, we split the set of evaluation points into P subsets according to the already given time slices and we obtain similar block structures for $\widetilde{\mathsf{V}}_h$, W_h and $\widetilde{\mathsf{M}}_h^0$ as we have had for the BEM matrices V_h, K_h and M_h^0. Thus, to distribute the matrix-vector multiplication we can use exactly the same decomposition as for the system matrices. Note that, as already mentioned in Section 9.1, we do not have to explicitly assemble the matrices $\widetilde{\mathsf{V}}_h$, W_h and $\widetilde{\mathsf{M}}_h^0$.

9.2.2 OpenMP Threading

In this subsection we describe an efficient way of employing OpenMP threading in order to decrease the computation times of the assembly of the BEM matrices V_h, K_h, D_h and M_h^0, and for the evaluation of the discretized representation formula (9.9). For better readability we consider the non-distributed system of linear equations (9.3), i.e. without the MPI distribution presented in Subsection 9.2.1. The developed scheme can be transferred to the distributed matrices created by the cyclic graph decomposition.

In order to assemble the boundary element matrices V_h, K_h and D_h we use an element-based strategy, where we loop over all pairs of space–time boundary elements, assemble a local matrix and map it to the global matrix, see Listing 9.1 for V_h, K_h. For the assembly of D_h we use the same strategy as given in Listing 9.1, only with different parameters, i.e. $\widetilde{N}_x$ instead of N_x. OpenMP threading is employed for the outer loop over the elements. Recall that due to the given sorting of the elements of I_{N_t}, the matrices V_h, K_h and D_h are lower triangular block matrices, see (9.8). Hence the computational complexity is different for each iteration of the outer loop. Therefore, we apply dynamic scheduling and the outer loop starts with the elements located in the last time layer $N_t - 1$. The number of iterations of the inner loop, denoted with `N(l)` in Listing 9.1, depends on the current outer iteration variable `l` since we do not have to assemble the blocks in the upper triangular matrix. The function `N(l)` returns the number of boundary elements which are either located in the same time layer as the element σ_ℓ or in one of the time layers in the past. In this way we ensure that the length of the inner loop is decreasing. This is advantageous for the load balance.

```
int N(l) { return N_x * (1 + floor(l/N_x)); }

#pragma omp parallel for schedule(dynamic, 1)
for(int l = N-1; l >= 0; --l) {
  for(int k = 0; k < N(l); ++k) {
    getLocalMatrix(l, k, localMatrix);
    globalMatrix.add(l, k, localMatrix);
} }
```

Listing 9.1: Threaded element-based assembly of V_h and K_h.

The structure of the initial matrix M_h^0 is different, see Section 9.1. In order to assemble the matrix M_h^0 we again use the element-based strategy, where we loop over all boundary elements and elements of the initial mesh Ω_{N_Ω}, similarly as in Listing 9.1. Threading is employed for the outer loop over the boundary elements and dynamic scheduling is used again. The number of iterations of the inner loop does not depend on the index of the outer loop, since there are in general no vanishing entries compared to V_h, K_h and D_h.

Since the support of the piecewise constant test functions φ_ℓ^0 is limited to a single boundary element σ_ℓ, no thread-private operations are necessary in the `add` function for the assembly of the matrices V_h, K_h and M_h^0, whereas for the assembly of D_h an `atomic` OpenMP clause is necessary in the `add` function due to the overlap of the support of the basis functions $\widetilde{\varphi}_i^{10}$ used for the discretization of D_h, i.e. functions that are piecewise linear and globally continuous in space.

A similar strategy is used for the evaluation of the discretized representation formula (9.9). We iterate over an array of evaluation points which are sorted in the temporal direction and again use dynamic scheduling, see Listing 9.2.

```
#pragma omp parallel for schedule(dynamic, 1)
for(int i = E-1; i >= 0; --i) {
  representationFormula(i, result);
}
```

Listing 9.2: Threaded evaluation of the representation formula.

All presented threading strategies can be carried over to the assembly of the blocks generated by the cyclic graph decomposition presented in Subsection 9.2.1. The main diagonal blocks of the matrices V_h, K_h and D_h are structured as in (9.8), assuming that the time layers within the corresponding submesh are sorted appropriately. Thus, we apply the same threading strategy for the diagonal blocks as already discussed in this subsection. For the non-diagonal blocks of the matrices V_h, K_h and D_h we use dynamic scheduling as well, but the number of iterations of the inner loop does not depend on the index of the outer loop anymore, since all the elements iterated over by the inner loop are located in the past of the element σ_ℓ, and therefore each pair of elements σ_k and σ_ℓ contributes to the block.

The threaded assembly of the block-rows of the initial matrix M_h^0 and the threaded evaluation of the distributed representation formula work exactly the same way as described before.

9.3 Numerical Results

In this section we evaluate the efficiency of the proposed parallelization techniques for the spatially two-dimensional problem. The numerical experiments for testing the shared and distributed memory scalability were executed on the Salomon cluster at IT4Innovations National Supercomputing Center in Ostrava, Czech Republic. The cluster is equipped with 1008 nodes with two 12-core Intel Xeon E5-2680v3 Haswell processors and 128 GB of RAM. Nodes of the cluster are interconnected by the InfiniBand 7D enhanced hypercube network. Vectorization experiments can be found in [14].

All presented examples refer to the initial Dirichlet boundary value problem (9.1) on the space–time domain $Q := (0,1)^2 \times (0,1)$. We consider the exact solution

$$u(x,t) := \exp\left(-\frac{t}{\alpha}\right) \sin\left(x_1 \cos\frac{\pi}{8} + x_2 \sin\frac{\pi}{8}\right) \quad \text{for } (x,t) = (x_1,x_2,t) \in Q$$

and determine the Dirichlet datum g and the initial datum u_0 accordingly. The heat capacity constant is set to $\alpha = 10$. The system of linear equations (9.3) is solved by the operator preconditioned GMRES method with a relative precision of 10^{-8}. Instead of using $\widetilde{\mathsf{M}}_h$ in the preconditioner we computed a lumped mass matrix. Thus, the matrix becomes diagonal and the inverse can be applied efficiently.

L	N	$\|w-w_h\|_{L^2(\Sigma)}$	eoc	It.	It. OP
2	64	$7.55 \cdot 10^{-2}$	1.00	14	17
3	256	$3.77 \cdot 10^{-2}$	1.00	19	18
4	1 024	$1.88 \cdot 10^{-2}$	1.00	24	20
5	4 096	$9.38 \cdot 10^{-3}$	1.00	35	20
6	16 384	$4.69 \cdot 10^{-3}$	1.00	50	20
7	65 536	$2.34 \cdot 10^{-3}$	1.00	67	20
8	262 144	$1.18 \cdot 10^{-3}$	0.99	91	19
9	1 048 576	$5.94 \cdot 10^{-4}$	0.99	122	19

Table 9.1: $L^2(\Sigma)$-error of the Galerkin approximation w_h and the corresponding order of convergence. Here, N denotes the number of boundary elements of Σ_N on level L. Additionally, the iteration numbers of the non-preconditioned GMRES method (It.) and the preconditioned GMRES method (It. OP) are listed.

In order to obtain the boundary element mesh Σ_N and the finite element mesh Ω_{N_Ω}, which is used for the discretization of the initial potential and the evaluation of the representation formula, we decompose the space–time boundary Σ and the domain $\Omega = (0,1)^2$ into four space–time rectangles and four triangles, respectively, and then apply uniform refinement. The $L^2(\Sigma)$-error of the computed Galerkin approximation w_h and the estimated order of convergence are given in Table 9.1. In our computations we choose $h_x = h_t$, where h_x and h_t denote the global mesh sizes of Γ_{N_x} and I_{N_t}, respectively.

9.3.1 Scalability in Distributed Memory

In the first part of the performance experiments we focus on the parallel scalability of the proposed solver presented in Subsection 9.2.1. We tested the assembly of the BEM matrices V_h, K_h, D_h and M_h^0, the related matrix-vector multiplication, and the evaluation of the discrete representation formula (9.9). Strong scaling of the parallel solver was tested using a tensor product decomposition of the space–time boundary Σ into 65 536, 262 144, and 1 048 576 space–time surface elements and the same number of finite elements for the triangulation of the domain Ω. This corresponds to 512, 1 024, 2 048 spatial boundary elements and 128, 256, 512 time layers. In order to test the performance of the representation formula we chose 558 080 evaluation points for all three problem sizes. More precisely, we used a finite element mesh Ω_{N_Ω} of the domain Ω with 545 nodes and computed the solution in these nodes in 1 024 different time steps, uniformly distributed in the interval $[0,1]$. We used up to 256 nodes (6 144 cores) of the Salomon cluster for our computations and executed two MPI processes per node. Each MPI process used 12 OpenMP threads for the assembly of the matrix blocks, for the matrix-vector multiplication, and for the evaluation of the representation formula. Note that the number of nodes we can use for our computations is restricted by the number of time layers of our boundary element mesh, i.e. starting with one element of our temporal decomposition I_{N_t} at level $L = 0$ and using a uniform refinement strategy we end up with 2^L time layers at level L. Thus, due to the structure of the parallel solver presented in Subsection 9.2.1 we can use 2^L MPI processes and therefore 2^{L-1} nodes at most. Conversely, for fine meshes we need a certain number of nodes to store the matrices.

Note that if we follow the refinement strategy $h_t \sim h_x^2$, the number of time layers and therefore the maximum number of MPI processes at level L is 4^L.

nodes ↓	V_h assembly [s]			V_h speedup			V_h efficiency [%]		
mesh →	65k	262k	1M	65k	262k	1M	65k	262k	1M
1	138.0	—	—	1.0	—	—	100.0	—	—
2	68.4	—	—	2.0	—	—	100.9	—	—
4	33.9	—	—	4.1	—	—	101.8	—	—
8	17.7	272.0	—	7.8	1.0	—	97.5	100.0	—
16	8.6	141.1	—	16.0	1.9	—	100.3	96.4	—
32	4.5	70.0	—	30.7	3.9	—	95.8	97.1	—
64	2.3	35.0	593.1	60.8	7.8	1.0	95.0	97.1	100.0
128	—	17.7	281.7	—	15.4	2.1	—	96.0	105.3
256	—	—	145.9	—	—	4.1	—	—	101.6

Table 9.2: Assembly of V_h for 65 536, 262 144, and 1 048 576 space–time elements.

nodes ↓	K_h assembly [s]			K_h speedup			K_h efficiency [%]		
mesh →	65k	262k	1M	65k	262k	1M	65k	262k	1M
1	162.5	—	—	1.0	—	—	100.0	—	—
2	80.8	—	—	2.0	—	—	100.5	—	—
4	40.3	—	—	4.0	—	—	100.8	—	—
8	21.8	317.4	—	7.5	1.0	—	93.2	100.0	—
16	10.2	163.4	—	15.9	1.9	—	99.6	97.1	—
32	5.2	81.2	—	31.2	3.9	—	97.6	97.7	—
64	2.6	40.9	673.4	62.5	7.8	1.0	97.6	97.0	100.0
128	—	20.7	325.6	—	15.3	2.1	—	95.8	103.4
256	—	—	172.5	—	—	3.9	—	—	97.6

Table 9.3: Assembly of K_h for 65 536, 262 144, and 1 048 576 space–time elements.

In Tables 9.2–9.6 the assembly and evaluation times including the speedup and efficiency are listed. We obtain almost optimal parallel scalability of the assembly of the BEM matrices and of the evaluation of the representation formula. Scalability of the matrix-vector

nodes ↓	D_h assembly [s]			D_h speedup			D_h efficiency [%]		
mesh →	65k	262k	1M	65k	262k	1M	65k	262k	1M
1	184.1	—	—	1.0	—	—	100.0	—	—
2	92.0	—	—	2.0	—	—	100.1	—	—
4	46.8	—	—	3.9	—	—	98.4	—	—
8	23.8	373.6	—	7.7	1.0	—	96.7	100.0	—
16	11.8	186.1	—	15.6	2.0	—	97.3	100.4	—
32	5.9	91.9	—	31.0	4.1	—	96.7	101.7	—
64	3.0	47.0	747.0	60.5	7.9	1.0	94.6	99.3	100.0
128	—	24.0	376.9	—	15.6	2.0	—	97.3	99.1
256	—	—	193.5	—	—	3.9	—	—	96.5

Table 9.4: Assembly of D_h for 65 536, 262 144, and 1 048 576 space–time elements.

nodes ↓	M_h^0 assembly [s]			M_h^0 speedup			M_h^0 efficiency [%]		
mesh →	65k	262k	1M	65k	262k	1M	65k	262k	1M
1	163.7	—	—	1.0	—	—	100.0	—	—
2	82.8	—	—	2.0	—	—	98.9	—	—
4	41.0	—	—	4.0	—	—	99.8	—	—
8	20.8	332.0	—	7.9	1.0	—	98.4	100.0	—
16	10.4	167.3	—	15.7	2.0	—	98.4	99.2	—
32	5.3	83.4	—	30.9	4.0	—	96.5	99.5	—
64	2.7	42.5	687.3	60.6	7.8	1.0	94.7	97.6	100.0
128	—	21.5	343.8	—	15.4	2.0	—	96.5	100.0
256	—	—	181.4	—	—	3.8	—	—	94.7

Table 9.5: Assembly of M_h^0 for 65 536, 262 144, and 1 048 576 space–time elements and the same number of triangles in Ω_{N_Ω}.

multiplication is evaluated in Table 9.7. Since the matrix blocks are distributed, each process only multiplies with blocks it is responsible for and exchanges the result with the remaining processes. For sufficiently large problems the scalability is optimal. In the case of smaller problems, the efficiency decreases with the increasing number of compute nodes as the communication starts to dominate over the computation. Nevertheless the efficiency is still good. The presented times apply to dense matrix-vector products. The efficiency is expected to decrease to some extent when using matrix approximation methods without further optimizations.

nodes ↓	$\tilde{u}$ evaluation [s]			$\tilde{u}$ speedup			$\tilde{u}$ efficiency [%]		
mesh →	65k	262k	1M	65k	262k	1M	65k	262k	1M
1	420.3	—	—	1.0	—	—	100.0	—	—
2	211.2	—	—	2.0	—	—	99.5	—	—
4	110.7	—	—	3.8	—	—	94.9	—	—
8	55.6	219.0	—	7.6	1.0	—	94.5	100.0	—
16	27.6	110.2	—	15.2	2.0	—	95.2	99.4	—
32	13.6	55.1	—	30.9	4.0	—	96.6	99.4	—
64	7.0	28.5	112.9	60.0	7.7	1.0	93.8	96.1	100.0
128	—	14.0	56.0	—	15.6	2.0	—	97.6	100.8
256	—	—	30.0	—	—	4.0	—	—	100.4

Table 9.6: Evaluation of the representation formula $\tilde{u}$ for 65 536, 262 144, and 1 048 576 space–time elements in 558 080 evaluation points.

nodes ↓	$\mathsf{V}_h\boldsymbol{f}$ time [s]			$\mathsf{V}_h\boldsymbol{f}$ speedup			$\mathsf{V}_h\boldsymbol{f}$ efficiency [%]		
mesh →	65k	262k	1M	65k	262k	1M	65k	262k	1M
1	41.9	—	—	1.0	—	—	100.0	—	—
2	22.4	—	—	1.9	—	—	93.5	—	—
4	11.3	—	—	3.7	—	—	92.7	—	—
8	5.6	89.8	—	7.5	1.0	—	93.5	100.0	—
16	2.8	45.8	—	15.0	2.0	—	93.5	98.0	—
32	1.5	22.5	—	28.1	4.0	—	87.9	99.9	—
64	0.9	11.5	182.2	46.6	7.8	1.0	72.7	97.6	100.0
128	—	6.5	96.8	—	13.8	1.9	—	86.0	94.1
256	—	—	46.0	—	—	4.0	—	—	99.0

Table 9.7: 250 matrix-vector products $\mathsf{V}_h\boldsymbol{f}$ for 65 536, 262 144, and 1 048 576 space–time elements.

9.3.2 Scalability in Shared Memory

In the second part we examine the parallel scalability in shared memory, i.e. we test the performance of the OpenMP threading introduced in Subsection 9.2.2. As before, we consider both the assembly of the BEM matrices V_h, K_h, D_h and M_h^0 as well as the evaluation of the representation formula $\tilde{u}$. The presented computation times refer to a space–time boundary element mesh Σ_N with 16 384 elements and a triangulation Ω_{N_Ω} consisting of 16 384 finite elements. For testing the efficiency of the parallel evaluation of $\tilde{u}$ we used a finite element mesh of Ω with 545 nodes and computed the solution in these nodes at 30 different times, i.e. in 16 350 points in total. We execute a single process and

	# threads	1	2	4	6	8	10	12
V_h	time $[s]$	190.9	94.8	51.6	33.2	25.6	20.0	16.9
	speedup	1.0	2.0	3.7	5.8	7.5	9.5	11.3
K_h	time $[s]$	222.2	116.6	56.1	30.0	30.7	23.2	20.4
	speedup	1.0	1.9	4.0	7.4	7.2	9.6	10.9
D_h	time $[s]$	232.7	127.3	60.3	42.3	32.7	26.5	23.2
	speedup	1.0	1.8	3.9	5.5	7.1	8.8	10.0
M_h^0	time $[s]$	236.5	121.0	59.4	39.9	30.2	24.1	20.3
	speedup	1	2.0	4.0	5.9	7.8	9.8	11.7
$\tilde{u}$	time $[s]$	81.1	44.5	20.4	14.6	10.2	8.2	7.5
	speedup	1.0	1.8	4.0	5.6	8.0	9.9	10.8

Table 9.8: Assembly and representation formula evaluation times for different numbers of OpenMP threads and a problem with 16 384 space–time surface elements, 16 384 triangles in Ω_{N_Ω}, and 16 350 evaluation points.

vary the number of OpenMP threads. In Table 9.8 we provide the assembly and evaluation times for different numbers of threads. We limit the maximal number of threads to 12 since this is the number of physical cores on a single socket and in the MPI distributed version we assign a single process to a socket. On the multi-core Xeon processors of the Salomon cluster we obtain the almost optimal speedup of 11.3 (10.9, 10.0, 11.7) for the assembly of the BEM matrices and the speedup of 10.8 for the evaluation of the representation formula.

10 FEM–BEM COUPLING

In this chapter we present a non-symmetric FEM–BEM coupling method for the discretization of parabolic transmission problems. As in the case of stationary transmission problems, see, e.g., [46,47], we can derive boundary integral equations for the exterior problem, see Section 5.4, and use a coupling method to solve the integral equations in combination with a finite element discretization of the interior problem [65]. Transmission problems for the heat equation were also analyzed in, e.g., [54], where the problem is discretized by applying a boundary element method in the interior and exterior domain, and where the corresponding boundary element discretizations are based on a Galerkin method in space and convolution quadrature in time. However, for more general parabolic problems in the interior domain a boundary element discretization is not applicable anymore.

We consider a non-symmetric FEM–BEM coupling method. In addition to the derivation of the variational formulation for the coupled problem, we present a space–time Galerkin method in order to discretize the problem and compute an approximation of the overall solution. However, the numerical analysis of the method is not part of this work.

10.1 Transmission Problem

Let $Q^{\mathrm{ext}} := \Omega^{\mathrm{ext}} \times (0,T)$ with $\Omega^{\mathrm{ext}} := \mathbb{R}^n \setminus \overline{\Omega}$. We consider the transmission problem for the heat equation

$$\begin{aligned} \alpha\partial_t u_i(x,t) - \operatorname{div}_x [A(x,t)\nabla_x u_i(x,t)] &= f(x,t) && \text{for } (x,t) \in Q, \\ \alpha\partial_t u_e(x,t) - \Delta_x u_e(x,t) &= 0 && \text{for } (x,t) \in Q^{\mathrm{ext}}, \\ u_i(x,0) &= 0 && \text{for } x \in \Omega, \\ u_e(x,0) &= 0 && \text{for } x \in \Omega^{\mathrm{ext}} \end{aligned} \tag{10.1}$$

with given source term $f \in [H^{1,1/2}_{;,0}(Q)]'$ and transmission conditions

$$u_i(x,t) = u_e(x,t), \quad n_x \cdot [A(x,t)\nabla_x u_i(x,t)] = \partial_{n_x} u_e(x,t) =: w_e(x,t) \quad \text{for } (x,t) \in \Sigma. \tag{10.2}$$

We assume that the coefficient matrix $A(x,t) \in \mathbb{R}^{n\times n}$ is symmetric and uniform positive definite, i.e. there exists $\theta > 0$ such that

$$\theta|\xi|^2 \le [A(x,t)\,\xi]\cdot\xi$$

for all $(x,t) \in Q$ and all $\xi \in \mathbb{R}^n$. The solution u_e of the exterior problem satisfies an appropriate radiation condition for $t \in (0,T)$ and $|x| \to \infty$. Moreover, u_e is given by the representation formula (5.15), i.e. have

$$u_e(\widetilde{x},t) = -(\widetilde{V}\gamma_1^{\mathrm{ext}} u_e)(\widetilde{x},t) + (W\gamma_0^{\mathrm{ext}} u_e)(\widetilde{x},t) \quad \text{for } (\widetilde{x},t) \in Q^{\mathrm{ext}}.$$

By applying the Dirichlet trace operator we get the weakly singular boundary integral equation for the exterior problem, see Section 5.4, i.e.

$$\gamma_0^{\text{ext}} u_e = -V \gamma_1^{\text{ext}} u_e + (\frac{1}{2} I + K) \gamma_0^{\text{ext}} u_e \quad \text{on } \Sigma. \tag{10.3}$$

10.2 Non-Symmetric Coupling

We start with the derivation of the domain variational formulation of (10.1) in Q, i.e. we consider the initial boundary value problem

$$\begin{aligned} \alpha \partial_t u_i(x,t) - \operatorname{div}_x [A(x,t) \nabla_x u_i(x,t)] &= f(x,t) \quad \text{for } (x,t) \in Q, \\ u_i(x,0) &= 0 \qquad\quad \text{for } x \in \Omega \end{aligned} \tag{10.4}$$

with $f \in [H^{1,1/2}_{;,0}(Q)]'$ and the Neumann boundary condition

$$n_x \cdot [A(x,t) \nabla_x u_i(x,t)] = w_i(x,t) \quad \text{for } (x,t) \in \Sigma.$$

Due to the uniform positivity of the coefficient matrix $A(x,t) \in \mathbb{R}^{n \times n}$ we can define an equivalent norm in $L^2(0,T;H^1_0(\Omega))$ given by

$$\|u\|^2_{L^2(0,T;H^1_0(\Omega))} := \langle A \nabla_x u, \nabla_x u \rangle_{L^2(Q)}.$$

The analysis of (10.1) then follows the same path as described in [65] where the coefficient matrix A is the identity on $\mathbb{R}^n$, see also [63]. The variational formulation of (10.4) is to find $u_i \in H^{1,1/2}_{;0,}(Q)$ such that

$$a(u_i, v) = \langle f, v \rangle_Q + \langle w_i, \gamma_0^{\text{int}} v \rangle_\Sigma \quad \text{for all } v \in H^{1,1/2}_{;,0}(Q)$$

with the continuous bilinear form $a(\cdot,\cdot)$ given by

$$a(u,v) := \alpha \langle \partial_t u_i, v \rangle_Q + \langle A \nabla_x u_i, \nabla_x v \rangle_{L^2(Q)}$$

for $u \in H^{1,1/2}_{;0,}(Q)$ und $v \in H^{1,1/2}_{;,0}(Q)$. All the terms on the right hand side are well defined for the given trial and test spaces, see Section 3.1. The variational formulation of the boundary integral equation (10.3) is to find $w_e = \gamma_1^{\text{ext}} u_e \in H^{-1/2,-1/4}(\Sigma)$ such that

$$\langle V w_e, \tau \rangle_\Sigma + \langle (\frac{1}{2} I - K) \gamma_0^{\text{ext}} u_e, \tau \rangle_\Sigma = 0 \quad \text{for all } \tau \in H^{-1/2,-1/4}(\Sigma).$$

Together with the transmission conditions (10.2), i.e. $\gamma_0^{\text{int}} u_i = \gamma_0^{\text{ext}} u_e$ and $w_i = w_e$, we get the variational formulation of the coupled problem. We have to find $u_i \in H^{1,1/2}_{;0,}(Q)$ and $w_e \in H^{-1/2,-1/4}(\Sigma)$ such that

$$a(u_i, v) - \langle w_e, \gamma_0^{\text{int}} v\rangle_\Sigma = \langle f, v\rangle_Q,$$
$$\langle V w_e, \tau\rangle_\Sigma + \langle (\frac{1}{2} I - K)\gamma_0^{\text{int}} u_i, \tau\rangle_\Sigma = 0$$

for all $v \in H^{1,1/2}_{;,0}(Q)$ and $\tau \in H^{-1/2,-1/4}(\Sigma)$. By using the transformation operator $\mathcal{H}_T$ introduced in Section 3.2 we obtain an equivalent Galerkin–Bubnov variational formulation: Find $u_i \in H^{1,1/2}_{;0,}(Q)$ and $w_e \in H^{-1/2,-1/4}(\Sigma)$ such that

$$\begin{aligned} a(u_i, \mathcal{H}_T v) - \langle w_e, \gamma_0^{\text{int}} \mathcal{H}_T v\rangle_\Sigma &= \langle f, \mathcal{H}_T v\rangle_Q, \\ \langle V w_e, \tau\rangle_\Sigma + \langle (\frac{1}{2} I - K)\gamma_0^{\text{int}} u_i, \tau\rangle_\Sigma &= 0 \end{aligned} \tag{10.5}$$

for all $v \in H^{1,1/2}_{;0,}(Q)$ and $\tau \in H^{-1/2,-1/4}(\Sigma)$. The reformulation with the transformation operator $\mathcal{H}_T$ is crucial for the stability of related FEM discretizations in Q [65].

10.3 Space–Time Discretization

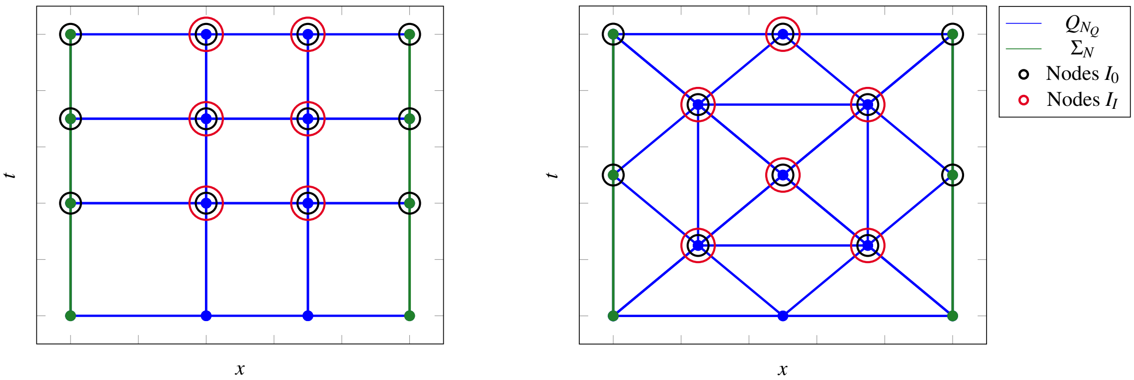
For the Galerkin discretization of the variational formulation (10.5) we consider a decomposition $Q_{N_Q} = \{q_\ell\}_{\ell=1}^{N_Q}$ of the space–time domain Q into finite elements q_ℓ [63, 65]. This could either be a tensor product decomposition or an abitrary triangulation.

Let $\{(x_k, t_k)\}_{k=1}^{M_Q}$ be the set of nodes of the finite element mesh. We define I_0 to be the index set of nodes which do not belong to $\overline{\Omega} \times \{0\}$, and we set $M_0 := |I_0|$. Moreover, I_I is the index set of nodes which do not belong to $\overline{\Sigma} \cup (\overline{\Omega} \times \{0\})$, and we set $M_I := |I_I|$. The nodes are assumed to be sorted in a suitable way. More precisely, we have $I_0 \subset \{1, ..., M_0\}$ and $I_I \subset \{1, ..., M_I\}$. The space–time boundary elements $\Sigma_N = \{\sigma_\ell\}_{\ell=1}^N$ of the induced decomposition of Σ are given by

$$\Sigma_N := \left\{\sigma \subset \overline{\Sigma} : \exists\, q \in Q_{N_Q} : \sigma = \partial q \cap \overline{\Sigma}\right\}.$$

Figure 10.1 shows sample decompositions for the spatially one-dimensional problem.

Let $X_h = \operatorname{span}\left\{\varphi_k^0\right\}_{k=1}^N \subset H^{-1/2,-1/4}(\Sigma)$ be the space of piecewise constant basis functions and $Y_h = \operatorname{span}\left\{\varphi_i^1\right\}_{i=1}^{M_Q} \subset H^{1,1/2}(Q)$ be the space of functions that are piecewise linear and globally continuous, defined with respect to the decompositions Σ_N and Q_{N_Q}, respectively. Moreover, we define $Y_{h,0} = Y_h \cap H^{1,1/2}_{;0,}(Q)$ to be the space of functions in Y_h



(a) Tensor product decomposition. (b) Triangulation.

Figure 10.1: Sample space–time decompositions of the domain Q and the boundary Σ in the spatially one-dimensional case.

vanishing on $\overline{\Omega} \times \{0\}$. Due to the sorting of the nodes we have $Y_{h,0} = \operatorname{span}\left\{\varphi_i^1\right\}_{i=1}^{M_0}$. We approximate w_e and u_i by

$$w_{e,h} = \sum_{k=1}^{N} w^k \varphi_k^0 \in X_h, \quad u_{i,h} = \sum_{j=1}^{M_0} u^j \varphi_j^1 \in Y_{h,0}.$$

Hence it remains to compute the unknown coefficients w^k and u^j. The discretized Galerkin–Bubnov variational formulation of (10.5) is to find $u_{i,h} \in Y_{h,0}$ and $w_{e,h} \in X_h$ such that

$$\begin{aligned} &a(u_{i,h}, \mathcal{H}_T v_h) - \langle w_{e,h}, \gamma_0^{\text{int}} \mathcal{H}_T v_h \rangle_\Sigma = \langle f, \mathcal{H}_T v_h \rangle_Q, \\ &\langle V w_{e,h}, \tau_h \rangle_\Sigma + \langle (\frac{1}{2} I - K) u_{i,h}, \tau_h \rangle_\Sigma = 0 \end{aligned}$$

for all $v \in Y_{h,0}$ and $\tau_h \in X_h$. This formulation is equivalent to the system of linear equations

$$\begin{pmatrix} \mathsf{A}_{QQ} & \mathsf{A}_{Q\Sigma} & \\ \mathsf{A}_{\Sigma Q} & \mathsf{A}_{\Sigma\Sigma} & -\widetilde{\mathsf{M}}_h^{\mathrm{T}} \\ & \frac{1}{2}\mathsf{M}_h - \mathsf{K}_h & \mathsf{V}_h \end{pmatrix} \begin{pmatrix} \boldsymbol{u}^Q \\ \boldsymbol{u}^\Sigma \\ \boldsymbol{w} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}^Q \\ \boldsymbol{f}^\Sigma \\ \boldsymbol{0} \end{pmatrix} \tag{10.6}$$

with

$$\mathsf{A}[j,i] = a(\varphi_i^1, \mathcal{H}_T \varphi_j^1), \quad \boldsymbol{f}[j] = \langle f, \mathcal{H}_T \varphi_j^1 \rangle_Q$$

for $i, j = 1, \ldots, M_0$, and

$$\begin{aligned} \mathsf{M}_h[\ell, i] &= \langle \varphi_{M_I+i}^1, \varphi_\ell^0 \rangle_\Sigma, \quad \mathsf{K}_h[\ell, i] = \langle K \varphi_{M_I+i}^1, \varphi_\ell^0 \rangle_\Sigma, \\ \mathsf{V}_h[\ell, k] &= \langle V \varphi_k^0, \varphi_\ell^0 \rangle_\Sigma, \quad \widetilde{\mathsf{M}}_h[\ell, i] = \langle \mathcal{H}_T \varphi_{M_I+i}^1, \varphi_\ell^0 \rangle_\Sigma \end{aligned}$$

for $i = 1, \ldots, M_0 - M_I$ and $k, \ell = 1, \ldots, N$.

Consequently, we can compute the unkown coefficients w^k and u^j and thus, the corresponding approximations $w_{e,h}$ and $u_{i,h}$. An approximation $u_{e,h}$ of the exterior problem can be determined by using the representation formula

$$u_{e,h}(\widetilde{x},t) := -(\widetilde{V} w_{e,h})(\widetilde{x},t) + (W \gamma_0^{\mathrm{int}} u_{i,h})(\widetilde{x},t) \quad \text{for } (\widetilde{x},t) \in Q^{\mathrm{ext}}.$$

10.4 Numerical Results

We consider the transmission problem (10.1) with given source term $f \in [H^{1,1/2}_{;,0}(Q)]'$ and time horizon $T = 1$. The coefficient matrix A is chosen to be the identity on $\mathbb{R}^n$. The heat capacity constant is set to $\alpha = 1$. We present a numerical experiment for the spatially one-dimensional problem and use a tensor product decomposition of the space–time domain Q [65] in order to discretize the variational formulation (10.5). The example refers to a globally quasi-uniform and shape regular finite element mesh with mesh size $h = \mathcal{O}(2^{-L})$, L denoting the refinement level. The system of linear equations (10.6) is solved by using the GMRES method with a relative accuracy of 10^{-8} as stopping criteria.

In order to describe a reference solution of the transmission problem we choose some function $u_i \in H^{1,1/2}_{;0,}(Q)$ and determine the source term f accordingly. Then

$$u_e(\widetilde{x},t) = -(\widetilde{V} \gamma_1^{\mathrm{int}} u_i)(\widetilde{x},t) + (W \gamma_0^{\mathrm{int}} u_i)(\widetilde{x},t) \quad \text{for } (\widetilde{x},t) \in Q^{\mathrm{ext}}$$

defines a solution of the exterior problem satisfying the transmission conditions

$$\gamma_0^{\mathrm{int}} u_i = \gamma_0^{\mathrm{ext}} u_e, \quad \gamma_1^{\mathrm{int}} u_i = \gamma_1^{\mathrm{ext}} u_e \quad \text{on } \Sigma.$$

Thus, the function u defined as $u_{|Q} := u_i$ and $u_{|Q^{\mathrm{ext}}} := u_e$ is a solution of the transmission problem (10.1).

We choose $\Omega = (0,1)$, i.e. $Q = (0,1)^2$, and consider the exact solution $u_i(x,t) = t \sin(\pi x)$ for $(x,t) \in Q$ of the interior problem. Thus, the source term is given by

$$f(x,t) = (\mathcal{L} u_i)(x,t) = \sin(\pi x) \left(\alpha + \pi^2 t\right) \quad \text{for } (x,t) \in Q.$$

Table 10.1 shows the errors $\left\|u_i - u_{i,h}\right\|_{L^2(Q)}$ and $\left\|w_e - w_{e,h}\right\|_{L^2(\Sigma)}$ of the Galerkin approximations $u_{i,h}$ and $w_{e,h}$, respectively, and the corresponding convergence rates (eoc). We obtain quadratic convergence of the finite element solution $u_{i,h}$, which is in line with the theoretical findings of the finite element method presented in [65]. For the Galerkin approximation $w_{e,h}$ of the Neumann datum $w_e = \gamma_1^{\mathrm{ext}} u_e$ we observe linear convergence, which is what we expected in view of the proven a priori error estimates for the initial Dirichlet boundary value problem in Section 7.1.

L	M_Q	N	$\left\|u_i - u_{i,h}\right\|_{L_2(Q)}$	eoc	$\left\|w_e - w_{e,h}\right\|_{L^2(\Sigma)}$	eoc
0	4	2	$4.082 \cdot 10^{-1}$	-	$9.162 \cdot 10^{-1}$	-
1	9	4	$1.333 \cdot 10^{-1}$	1.61	$5.157 \cdot 10^{-1}$	0.83
2	25	8	$3.824 \cdot 10^{-2}$	1.80	$2.737 \cdot 10^{-1}$	0.91
3	81	16	$9.887 \cdot 10^{-3}$	1.95	$1.468 \cdot 10^{-1}$	0.90
4	289	32	$2.492 \cdot 10^{-3}$	1.99	$7.712 \cdot 10^{-2}$	0.93
5	1 089	64	$6.244 \cdot 10^{-4}$	2.00	$3.752 \cdot 10^{-2}$	1.04
6	4 225	128	$1.562 \cdot 10^{-4}$	2.00	$1.915 \cdot 10^{-2}$	0.97

Table 10.1: Error and convergence rates of the Galerkin approximations $u_{i,h}$ and $w_{e,h}$ in the case of uniform refinement for a tensor product decomposition of Q in 1D. M_Q denotes the number of nodes of the finite element mesh, while N is the number of boundary elements on level L.

11 CONCLUSION

In this work we have described space–time boundary element discretizations for initial boundary value problems for the heat equation. After the derivation of the representation formula for the solution of the model problem (1.1) we have analyzed the heat potentials and the resulting boundary integral operators as well as the unique solvability of related boundary integral equations in the setting of anisotropic Sobolev spaces. The unknown Cauchy data can be determined by solving boundary integral equations. The ellipticity of the single layer boundary integral operator and the hypersingular operator ensure unique solvability of various boundary value problems. We have compared two different space–time discretization techniques in order to compute an approximation of the unknown Cauchy data, namely a tensor product decomposition and an arbitrary triangulation of the space–time boundary Σ. Both methods allow us to parallelize the computation of the global solution of the whole space–time system, which leads to improved parallel scalability in distributed memory systems in contrast to, e.g., time-stepping schemes. One possible drawback of the tensor product approach is that we can only apply adaptive refinement in space and time separately. This can be resolved, e.g., by allowing hanging nodes in the mesh, which is reasonable if the discretization of the integral equation is done by using piecewise constant basis functions. However, an arbitrary triangulation of the space–time boundary Σ allows for adaptive refinement in space and time simultaneously while maintaining the admissibility of the mesh. We have derived a priori error estimates for both discretization techniques, and we have provided numerical experiments in order to evaluate the theoretical findings.

In the numerical experiments we have used the exact solution in order to compute the errors of the Galerkin approximations and for the application of adaptive refinement. Of course, in general we do not know the exact solution. Thus, we have to establish a posteriori error estimators for space–time boundary element methods in order to define suitable adaptive refinement strategies. One possible approach is the method described in [55] in the case of the Laplace equation, which is based on an approximation of a second kind Fredholm integral equation by a Neumann series in order to compute the error. However, this method utilizes the contraction property of the double layer potential, which is, in the case of the heat equation, not yet proven for a general Lipschitz domain Ω. The development of a posteriori error estimators for space–time boundary element methods for the heat equation is left for future work.

As already mentioned before, one big advantage of space–time discretization methods is the ability to use parallel iterative solution strategies for time-dependent problems. In Chapter 9 we have introduced a parallel space–time boundary element solver for the heat equation. The solver utilizes MPI for distributed memory parallelization, while OpenMP is used for shared memory parallelization and vectorization. The distribution of the system matrices among computational nodes is based on the method presented in [30, 37] for spatial problems. We have successfully adapted the method to support the time-dependent problem for the heat equation. A space–time computational mesh is decomposed into slices which inherently define blocks in the system matrices. These blocks are distributed among MPI processes by using the graph-decomposition-based scheme. The numerical experiments show optimal scalability of the global system matrix assembly in distributed memory and almost optimal scalability of the individual block assembly in shared memory. An additional performance gain can be obtained by using SIMD vectorization [14]. We have also demonstrated distributed-memory scalability of the matrix-vector multiplication and the evaluation of the representation formula.

The presented parallel solver provides opportunities for further research and development of numerical methods. While in [30, 37] the individual matrix blocks are approximated using either the adaptive cross approximation or the fast multipole method, we limited ourselves to classical BEM, leading to dense system matrices. Their data-sparse approximation is a topic of future work. Together with data-sparse methods, the developed technology will serve as a base for the development of a parallel fast three-dimensional solver. The same parallelization techniques in distributed and shared memory can be applied for solving initial Neumann boundary value problems where the unknown Dirichlet datum $g \in H^{1/2,1/4}(\Sigma)$ can be determined by solving the hypersingular boundary integral equation (5.2). We obtain the same matrix structures as described in Section 9.1. The extension of the parallel solver to an arbitrary triangulation of the space–time boundary, especially with application of adaptive refinement, is still open. However, for a globally uniform triangular boundary element mesh the structure of the system matrices is similar as in the case of a tensor product decomposition and we can utilize the ideas from the presented approach in order to extend the parallel solver to discretizations based on a triangular boundary element mesh.

In order to get a competitive space–time solver an efficient iterative solution technique for the global space–time system is necessary, i.e. the solution requires an application of space–time preconditioners. A popular preconditioning strategy in boundary element methods is operator preconditioning [23,64] which is based on boundary integral operators of opposite order, such as the single layer operator V and the hypersingular operator D, but which requires a related stability condition for the boundary element spaces used for the discretization to be satisfied. We have analyzed this robust preconditioning strategy for the time-dependent heat equation, and we have discussed suitable choices of boundary element spaces. Moreover, we have extended the parallel solver introduced in Chapter 9 to the preconditioned space–time system. For the spatially two- and three-dimensional problem we have restricted ourselves to a tensor product decomposition of Σ. Again, the establishment of related stability conditions for a triangulation of the space–time boundary is left for future work. One may use the space $S_h^1(\Sigma_N)$ of piecewise linear and globally continuous basis functions for the discretization of V and D, respectively. However, due to the approximation properties of $S_h^1(\Sigma_N)$ such an approach for solving initial Dirichlet boundary value problems is restricted to spatial domains Ω with smooth boundary where the unknown flux is continuous.

The matrices related to the discretized space–time integral equations are dense and thus, fast methods are necessary in order to tackle large scale problems, especially for space–time systems. Fast methods for solving boundary integral equations for the heat equations were introduced in [66, 68]. The parabolic fast multipole method applied to a space–time Galerkin discretization is discussed in [40] where the discretization is done with respect to a tensor product decomposition of the space–time boundary. The extension of fast methods, e.g., adaptive cross approximation or the parabolic fast multipole method, to an arbitrary triangulation of Σ is still an open problem.

As already mentioned before, one advantage of boundary element methods is the natural handling of problems in exterior, unbounded domains. The introduced domain variational formulation (3.11) in the setting of anisotropic Sobolev spaces allows us to establish symmetric and non-symmetric FEM–BEM coupling methods in an appropriate functional framework, as we have shown in Chapter 10.

REFERENCES

[1] R. Andreev. Stability of sparse space–time finite element discretizations of linear parabolic evolution equations. *IMA J. Numer. Anal.*, 33(1):242–260, 2012.

[2] W. Arendt and K. Urban. *Partielle Differenzialgleichungen*. Springer Spektrum, Heidelberg, 2010.

[3] D. N. Arnold and P. J. Noon. Boundary integral equations of the first kind for the heat equation. In *Boundary elements IX, Vol. 3 (Stuttgart, 1987)*, pages 213–229. Comput. Mech., Southampton, 1987.

[4] D. N. Arnold and P. J. Noon. Coercivity of the single layer heat potential. *J. Comput. Math.*, 7(2):100–104, 1989.

[5] M. Behr. Simplex space–time meshes in finite element simulations. *Int. J. Numer. Meth. Fluids*, 57:1412–1434, 2008.

[6] J. Bergh and J. Lofstrom. *Interpolation Spaces, An Introduction*. Springer, Berlin-Heidelberg, 1976.

[7] R. Chapko and R. Kress. Rothe's method for the heat equation and boundary integral equations. *J. Integral Equations Appl.*, 9(1):47–69, 1997.

[8] X. Claeys and R. Hiptmair. Electromagnetic scattering at composite objects : a novel multi-trace boundary integral formulation. *ESAIM Math. Model. Numer. Anal.*, 46(6):1421–1445, 2012.

[9] X. Claeys and R. Hiptmair. Multi-Trace Boundary Integral Formulation for Acoustic Scattering by Composite Structures. *Comm. Pure Appl. Math.*, 66(8):1163–1201, 2013.

[10] M. Costabel. Boundary integral operators for the heat equation. *Integral Equations Operator Theory*, 13:498–552, 1990.

[11] S. Dohr, M. Merta, G. Of, O. Steinbach, and J. Zapletal. A parallel solver for a preconditioned space–time boundary element method for the heat equation. Submitted (2018).

[12] S. Dohr, K. Niino, and O. Steinbach. Space–time boundary element methods for the heat equation. In U. Langer and O. Steinbach, editors, *Space–Time Methods: Applications to Partial Differential Equations*, Radon Ser. Comput. Appl. Math. De Gruyter, Berlin, 2019.

[13] S. Dohr and O. Steinbach. Preconditioned space–time boundary element methods for the one-dimensional heat equation. In *Domain Decomposition Methods in Science and Engineering XXIV*, volume 125 of *Lect. Notes Comput. Sci. Eng.* Springer International Publishing, 2018.

[14] S. Dohr, J. Zapletal, G. Of, M. Merta, and M. Kravcenko. A parallel space–time boundary element method for the heat equation. *Comput. Math. Appl.*, 2019.

[15] J. Dongarra et al. The International Exascale Software Project roadmap. *Int. J. High Perform. Comput. Appl.*, 25(1):3–60, 2011.

[16] J. Dongarra et al. Applied Mathematics Research for Exascale Computing. Technical report, U.S. Department of Energy, 2014.

[17] A. Ern and J.L. Guermond. *Theory and Practice of Finite Elements*. Appl. Math. Sci. Springer, New York, 2004.

[18] L. C. Evans. Partial Differential Equations. *Grad. Stud. Math.*, 19, 1997.

[19] M. Fontes. Initial-Boundary Value Problems for Parabolic Equations. *Ann. Acad. Sci. Fenn. Math.*, 34:583–605, 2009.

[20] M. J. Gander and M. Neumüller. Analysis of a new space–time parallel multigrid algorithm for parabolic problems. *SIAM J. Sci. Comput.*, 38(4):A2173–A2208, 2016.

[21] M. Hamina. Some boundary element methods for heat conduction problems. PhD thesis, University of Oulu, 2000.

[22] H. Harbrecht and J. Tausch. A fast sparse grid based space–time boundary element method for the nonstationary heat equation. *Numer. Math.*, 140(1):239–264, 2018.

[23] R. Hiptmair. Operator Preconditioning. *Comput. Math. Appl.*, 52:699–706, 2006.

[24] R. Hiptmair and C. Jerez-Hanckes. Multiple traces boundary integral formulation for Helmholtz transmission problems. *Adv. Comput. Math.*, 37(1):39–91, 2012.

[25] G. C. Hsiao, P. Kopp, and W. L. Wendland. A Galerkin collocation method for some integral equations of the first kind. *Computing*, 25(2):89–130, 1980.

[26] G. C. Hsiao and J. Saranen. Boundary integral solution of the two-dimensional heat equation. *Math. Methods Appl. Sci.*, 16(2):87–114, 1993.

[27] G.C. Hsiao and W.L. Wendland. *Boundary Integral Equations*. Appl. Math. Sci. Springer Berlin-Heidelberg, 2008.

[28] Intel Corporation. Vector Mathematical Functions, 2018. [Online; accessed 29-August-2018].

[29] R. Hiptmair, C. Jerez-Hanckes and C. Urzúa-Torres. Mesh-Independent Operator Preconditioning for Boundary Elements on Open Curves. *SIAM J. Numer. Anal.*, 52:2295–2314, 2014.

[30] M. Kravcenko, M. Merta, and J. Zapletal. Distributed fast boundary element methods for Helmholtz problems. Submitted (2018).

[31] M. Kretz and V. Lindenstruth. Vc: A C++ library for explicit vectorization. *Software: Practice and Experience*, 42(11):1409–1430, 2012.

[32] S. Larsson and C. Schwab. Compressive Space–Time Galerkin Discretizations of Parabolic Partial Differential Equations. 2015. arXiv:1501.04514.

[33] J. Lions, Y. Maday, and G. Turinici. Résolution d'EDP par un schéma en temps « pararéel ». *C. R. Acad. Sci. - Series I - Mathematics*, 332(7):661–668, 2001.

[34] J. L. Lions and E. Magenes. *Non-Homogeneous Boundary Value Problems and Applications. Volume I.* Springer, Berlin-Heidelberg-New York, 1972.

[35] J. L. Lions and E. Magenes. *Non-Homogeneous Boundary Value Problems and Applications. Volume II.* Springer, Berlin-Heidelberg-New York, 1972.

[36] C. Lubich and R. Schneider. Time discretization of parabolic boundary integral equations. *Numer. Math.*, 63(4):455–481, 1992.

[37] D. Lukas, P. Kovar, T. Kovarova, and M. Merta. A parallel fast boundary element method using cyclic graph decompositions. *Numer. Algorithms*, 70(4):807–824, 2015.

[38] W. McLean. *Strongly Elliptic Systems and Boundary Integral Equations*. Cambridge University Press, 2000.

[39] M. Messner. A Fast Multipole Galerkin Boundary Element Method for the Transient Heat Equation. *Monographic Series TU Graz: Computation in Engineering and Science*, 23, 2014.

[40] M. Messner, M. Schanz, and J. Tausch. A fast Galerkin method for parabolic space–time boundary integral equations. *J. Comput. Phys.*, 258:15–30, 2014.

[41] M. Messner, M. Schanz, and J. Tausch. An efficient Galerkin boundary element method for the transient heat equation. *SIAM J. Sci. Comput.*, 37(3):A1554–A1576, 2015.

[42] C. Mollet. Stability of Petrov–Galerkin Discretizations: Application to the Space–Time Weak Formulation for Parabolic Evolution Problems. *Comput. Meth. Appl. Math.*, 14(2):231–255, 2014.

[43] M. Neumüller. Space–Time Methods. *Monographic Series TU Graz: Computation in Engineering and Science*, 20, 2013.

[44] M. Neumüller and O. Steinbach. Refinement of Flexible Space–Time Finite Element Meshes and Discontinuous Galerkin Methods. *Comput. Vis. Sci.*, 14(5):189–205, 2011.

[45] P. J. Noon. The Single Layer Heat Potential and Galerkin Boundary Element Methods for the Heat Equation. PhD thesis, University of Maryland, 1988.

[46] G. Of, G. Rodin, O. Steinbach, and M. Taus. Coupling of Discontinuous Galerkin Finite Element and Boundary Element Methods. *SIAM J. Sci. Comput.*, 34(3):A1659–A1677, 2012.

[47] G. Of and O. Steinbach. Is the one-equation coupling of finite and boundary element methods always stable? *ZAMM Z. Angew. Math. Mech.*, 93:476–484, 2013.

[48] OpenMP Application Programming Interface, 2015. [Online; accessed 29-August-2018].

[49] T. X. Phan. Boundary Element Methods for Boundary Control Problems. *Monographic Series TU Graz: Computation in Engineering and Science*, 9, 2011.

[50] A. Piriou. Une classe d'opérateurs pseudo-différentiels du type de Volterra. *Ann. Inst. Fourier*, 20(1):77–94, 1970.

[51] A. Piriou. Problèmes aux limites généraux pour des opérateurs différentiels paraboliques dans un domaine borné. *Ann. Inst. Fourier*, 21(1):59–78, 1971.

[52] J. Radon. Zur mechanischen Kubatur. *Monatsh. Math.*, 52(4):286–300, 1948.

[53] S. Sauter and C. Schwab. *Boundary Element Methods*. Springer, Berlin-Heidelberg, 2011.

[54] F. Sayas, A. Rieder, S. Zhang, and T. Qiu. Time-domain boundary integral equation modeling of heat transmission problems. 2017. arXiv:1711.02375.

[55] H. Schulz and O. Steinbach. A new a posteriori error estimator in adaptive direct boundary element methods: the Dirichlet problem. *Calcolo*, 37:79–96, 2000.

[56] C. Schwab and R. Stevenson. Space–Time Adaptive Wavelet Methods for Parabolic Evolution Problems. *Math. Comput.*, 78(267):1293–1318, 2009.

[57] F. Sgallari. A weak formulation of boundary integral equations for time dependent parabolic problems. *Appl. Math. Model.*, 9(4):295–301, 1985.

[58] R. Speck, D. Ruprecht, M. Emmett, M. Minion, M. Bolten, and R. Krause. A space–time parallel solver for the three-dimensional heat equation. In *Parallel Computing: Accelerating Computational Science and Engineering (CSE)*, volume 25 of *Advances in Parallel Computing*, pages 263–272. IOS Press, 2014.

[59] O. Steinbach. On the stability of the L_2 projection in fractional Sobolev spaces. *Numer. Math.*, 88:367–379, 2001.

[60] O. Steinbach. On a generalized L_2 projection and some related stability estimates in Sobolev spaces. *Numer. Math.*, 90:775–786, 2002.

[61] O. Steinbach. *Stability Estimates for Hybrid Coupled Domain Decomposition Methods*. Springer, Berlin-Heidelberg-New York, 2003.

[62] O. Steinbach. *Numerical Approximation Methods for Elliptic Boundary Value Problems*. Springer, New York, 2008.

[63] O. Steinbach. Space–Time Finite Element Methods for Parabolic Problems. *Comput. Methods Appl. Sci.*, 15:551–566, 2015.

[64] O. Steinbach and W. L. Wendland. The construction of some efficient preconditioners in the boundary element method. *Adv. Comput. Math.*, 9:191–216, 1998.

[65] O. Steinbach and M. Zank. Coercive space–time finite element methods for initial boundary value problems. Submitted (2018).

[66] J. Tausch. A fast method for solving the heat equation by layer potentials. *J. Comput. Phys.*, 224:956–969, 2007.

[67] J. Tausch. Nyström discretization of parabolic boundary integral equations. *Appl. Numer. Math.*, 59(11):2843–2856, 2009.

[68] J. Tausch. Fast Nyström Methods for Parabolic Boundary Integral Equations. In *Fast Boundary Element Methods in Engineering and Industrial Applications*, pages 185–219. Springer, Berlin-Heidelberg, 2012.

[69] V. Thomée. *Galerkin Finite Element Methods for Parabolic Problems*. Springer, Berlin-Heidelberg, 2006.

[70] A. Veit, M. Merta, J. Zapletal, and D. Lukáš. Efficient solution of time-domain boundary integral equations arising in sound-hard scattering. *Internat. J. Numer. Methods Eng.*, 107(5):430–449, 2016.

[71] M. Zank. Inf-Sup Stable Space–Time Methods for Time-Dependent Partial Differential Equations . PhD thesis, Graz University of Technology, 2019.

[72] E. Zeidler. *Nonlinear Functional Analysis and its Applications II/ A: Linear Monotone Operators*. Springer, New York, 1990.