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Stefan Dohr, Kazuki Niino and Olaf Steinbach

Abstract. In this note we describe a space-time boundary element method for the numerical solution of the time-dependent heat equation. As model problem we consider the initial Dirichlet boundary value problem where the solution can be expressed in terms of given Dirchlet and initial data, and the unknown Neumann datum which is determined by the solution of an appropriate boundary integral equation. For its numerical approximation we consider a discretization which is done with respect to a space-time decomposition of the boundary of the space-time domain. This space-time discretization technique allows us to parallelize the computation of the global solution of the whole space-time system. 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 the initial Dirichlet boundary value problem we state a priori error estimates of the approximations. Moreover we present numerical experiments to confirm the theoretical findings.

Keywords. Space-time boundary element methods, heat equation, a priori error estimates.

AMS classification. 65M38, 65R20, 65M50, 65M12.

1 Introduction

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

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

with given source term f, Dirichlet datum g and initial datum u_0. Unique solvability of problem (1.1) in the setting of anisotropic Sobolev spaces [22] was shown in, e.g., [5, 13, 36]. An explicit formula describing the solution of problem (1.1) is given by the

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so-called representation formula for the heat equation, see, e.g., [2], i.e. for $(x,t) \in Q$ we have

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

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 [12]. Due to this representation of the solution it suffices to determine the Neumann datum $\partial_n u_{|\Sigma}$ in order to compute the solution u of problem (1.1). Hence the problem is reduced to the lateral boundary Σ of the space-time domain Q. We can determine the unknown Neumann datum $\partial_n u_{|\Sigma}$ by applying the Dirichlet trace operator to the representation formula (1.2) and solving the resulting space-time boundary integral equation. 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., [34, 36].

Boundary integral equations and corresponding boundary element methods for the approximation of the solution of the initial Dirichlet boundary value problem for the heat equation (1.1) have been studied for a long time [2, 3, 5, 18]. Besides well known time-stepping methods [4], the convolution quadrature method [23] or the Nyström method [38, 39], one can use the Galerkin approach [5, 16, 25, 26, 27, 29] for the discretization of the global space-time integral equation. Space-time discretization methods in general are gaining in popularity due to their ability to drive adaptivity in space and time simultaneously, and to use parallel iterative solution strategies for time-dependent problems [6, 14, 28]. 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 limited to the spatial dimension. 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. In [6, 8, 9] a robust preconditioning strategy for space-time integral equations for the heat equation based on boundary integral operators of opposite order [17, 35] is discussed. A parallel solver for space-time boundary element methods for the heat equation was introduced in [10] and extended to the preconditioned system in [7].

In this paper we analyze the heat potentials in (1.2) and the arising boundary integral operators as well as the solvability of the space-time boundary integral equations. The analysis of the boundary integral operators and equations is mainly based on [2, 3, 5]. We start with a discussion of the domain variational formulation of (1.1), see [36], and derive the mapping properties of the related boundary integral operators as well as the ellipticity of the single layer and hypersingular boundary integral operators. Moreover we discuss two different space-time discretization methods in order to compute an approximation of the unknown Neumann datum $\partial_n u_{|\Sigma}$. The first one is the so-called tensor product approach [26, 29], 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 equation. The second approach 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. This approach additionally allows us to apply 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.

The structure of the paper is as follows. In Section 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 [21, 22]. In Section 3 we recall existence and uniqueness results [13, 20, 36] for the domain variational formulation of (1.1). This domain variational formulation is later on used to prove the ellipicity of the single layer and hypersingular boundary integral operators. Sections 4 and 5 are devoted to the analysis of the arising boundary integral operators and boundary integral equations. In Section 6 we introduce the already mentioned space-time discretization 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 the boundary integral equations in Section 7, where we also derive a priori error estimates for the Galerkin approximation of the unknown Neumann datum. In Section 8 we provide results of numerical experiments validating the introduced discretization techniques and we conclude with a brief outlook in Section 9.

2 Functional framework

The analysis of problem (1.1) is done in anisotropic Sobolev spaces, which are introduced and discussed in this section. Under certain conditions we can define trace operators acting on those spaces and therefore provide conditions for the given Dirichlet datum g and the unknown Neumann datum $\partial_n u_{|\Sigma}$ of the solution, resulting in existence and uniqueness theorems for solutions of the model problem (1.1). The definitions and results in this section are mainly based on [21, 22, 36]. We start with the definition of anisotropic Sobolev spaces on the space-time domain Q in Section 2.1, and extend this to the space-time boundary Σ in Sections 2.2 and 2.3.

2.1 Anisotropic Sobolev spaces on Q

The anisotropic Sobolev space $H^{1,1/2}(Q)$ is defined as

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

The norm of a function $u \in H^{1,1/2}(Q)$ is given by

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

with

$$|u|^2_{H^{1/2}(0,T;L^2(\Omega))} := \int_0^T \int_0^T \frac{\|u(\cdot,t) - u(\cdot,\tau)\|^2_{L^2(\Omega)}}{|t-\tau|^2}\, \mathrm{d}\tau\, \mathrm{d}t.$$

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

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

where

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

with

$$|u|^2_{H^{1/2}_{0,}(0,T;L^2(\Omega))} := \int_0^T \frac{\|u(\cdot,t)\|^2_{L^2(\Omega)}}{t}\, \mathrm{d}t, \tag{2.1}$$

and write $H^{1,1/2}_{;0,}(Q) = L^2(0,T;H^1(\Omega)) \cap H^{1/2}_{0,}(0,T;L^2(\Omega))$. The space of functions in $H^{1,1/2}_{;0,}(Q)$ having zero 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 final time 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

$$|u|^2_{H^{1/2}_{,0}(0,T;L^2(\Omega))} := \int_0^T \frac{\|u(\cdot,t)\|^2_{L^2(\Omega)}}{T-t}\, \mathrm{d}t. \tag{2.2}$$

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.

2.2 Anisotropic Sobolev spaces on Σ

The spaces $H^{r,s}(\Sigma)$ for $r,s \geq 0$ are defined in a similar way. We set

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

For a smooth spatial boundary Γ these spaces are defined for arbitrary $r,s \geq 0$. However, for a general Lipschitz boundary Γ the spaces $H^{r,s}(\Sigma)$ are only defined for $0 \leq r \leq 1$ and $s \geq 0$. 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

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

and

$$|u|^2_{H^s(0,T;L^2(\Gamma))} := \int_0^T \int_0^T \frac{\|u(\cdot,t) - u(\cdot,\tau)\|^2_{L^2(\Gamma)}}{|t-\tau|^{1+2s}} \,\mathrm{d}\tau \,\mathrm{d}t.$$

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 only, 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., [24, 33], to obtain the convergence results in anisotropic spaces.

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

$$H^{\max(r,s)}(\Sigma) \hookrightarrow H^{r,s}(\Sigma) \hookrightarrow H^{\min(r,s)}(\Sigma) \tag{2.3}$$

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 $H^r(\Gamma) \hookrightarrow H^m(\Gamma)$ [19, Theorem 4.2.2] and $H^s((0,T)) \hookrightarrow H^m((0,T))$ we have

$$\begin{aligned} \|u\|^2_{H^{m,m}(\Sigma)} \cong \|u\|^2_{H^{m,0}(\Sigma)} + \|u\|^2_{H^{0,m}(\Sigma)} \quad &\le c \left(\|u\|^2_{H^{r,0}(\Sigma)} + \|u\|^2_{H^{0,s}(\Sigma)} \right) \\ \le c\, \|u\|^2_{H^{r,s}(\Sigma)}\,, \end{aligned} \tag{2.4}$$

and therefore $H^{r,s}(\Sigma) \hookrightarrow H^{m,m}(\Sigma)$. According to [24, Theorem B.11 ff.] and [21, 22] and since $H^1(\Sigma) \cong H^{1,1}(\Sigma)$ we have

$$H^{m,m}(\Sigma) = \left[L^2(\Sigma); H^{1,1}(\Sigma)\right]_m \cong \left[L^2(\Sigma); H^1(\Sigma)\right]_m = H^m(\Sigma). \tag{2.5}$$

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 (2.5) follows the same path as described in [22, 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 (2.4) and relation (2.5) 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 $H^M(\Sigma) \hookrightarrow H^{r,s}(\Sigma)$. □

Let us now introduce the subspace

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

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

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

Remark 2.2. For $r \ge 0$ and $0 \le s < \frac{1}{2}$ we have $H^{r,s}_{;0,0}(\Sigma) = H^{r,s}(\Sigma)$ and therefore $H^{-r,-s}(\Sigma) = \widetilde{H}^{-r,-s}(\Sigma)$.

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

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

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 2.3 (Trace Theorem, [22, Theorem 2.1]). *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

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

Lemma 2.4 ([5, 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 2.5 (Inverse Trace Theorem). *The interior Dirichlet trace operator γ_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 $v \in H^{1/2,1/4}(\Sigma)$ as well as

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

Proof. The proof is similar to [13, Theorem 4.9]. See also [5]. □

2.3 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 $j = 1, ..., J$. We then have $\overline{\Sigma} = \bigcup_{j=1}^J \overline{\Sigma}_j$. For $r \geq 0$ and $s \geq 0$ 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

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

with norm

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

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

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

with norm

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

Lemma 2.6. *For $r, s < 0$ and $w \in H_{pw}^{r,s}(\Sigma)$ there holds*

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

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

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

□

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

3 Domain variational formulation

In this section we introduce and analyze the domain variational formulation of problem (1.1) in the setting of anisotropic Sobolev spaces. We derive Greens's formulae for the heat equation in Subsection 3.1. In Subsection 3.2 we recall existence and uniqueness results for the solution of the variational formulation of the model problem with zero initial conditions. The unique solvability of problem (1.1) with a non-homogeneous initial datum is discussed in Subsection 3.3. The presented results are based on [5, 13, 36, 40]. In Subsection 3.4 we analyze the Neumann trace of solutions of the model problem (1.1).

3.1 Green's formulae

This subsection is devoted to the derivation of Green's first and second formula for the heat equation with respect to the previously introduced setting of anisotropic Sobolev spaces. These formulae are later on used to derive the representation formula for the heat equation and for the analysis of related boundary integral operators, see Section 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 3.1 ([1, 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 3.1 we get

$$\begin{aligned}\int_0^T \int_\Omega \Big[\alpha\partial_t u(x,t) - \Delta_x u(x,t)\Big] v(x,t)\,\mathrm{d}x\,\mathrm{d}t \\ = \int_0^T \int_\Omega \Big[\alpha\,\partial_t u(x,t)v(x,t) + \nabla_x u(x,t)\cdot\nabla_x v(x,t)\Big]\,\mathrm{d}x\,\mathrm{d}t \\ - \int_0^T \int_\Gamma \partial_{n_x} u(x,t)v(x,t)\,\mathrm{d}s_x\,\mathrm{d}t\,.\end{aligned} \tag{3.1}$$

This equation is the so-called Green's first formula for the heat equation. Using integration by parts on the first term of 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 3.1 we get

$$\begin{aligned}
\alpha \int_\Omega u(x,T)v(x,T)\,\mathrm{d}x &= \alpha \int_\Omega u(x,0)v(x,0)\,\mathrm{d}y \qquad (3.2)\\
&+ \int_0^T \int_\Omega \Big[\alpha\partial_t u(x,t) - \Delta_x u(x,t)\Big] v(x,t)\,\mathrm{d}x\,\mathrm{d}t\\
&- \int_0^T \int_\Omega \Big[-\alpha\partial_t v(x,t) - \Delta_x v(x,t)\Big] u(x,t)\,\mathrm{d}x\,\mathrm{d}t\\
&+ \int_0^T \int_\Gamma \partial_{n_x} u(x,t)v(x,t)\,\mathrm{d}s_x\,\mathrm{d}t - \int_0^T \int_\Gamma \partial_{n_x} v(x,t)u(x,t)\,\mathrm{d}s_x\,\mathrm{d}t.
\end{aligned}$$

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

Lemma 3.2 ([5, Lemma 2.22]). *Let $C_0^\infty(\overline{\Omega}\times(0,T])$ be the space of restrictions to $\overline{Q}$ of functions in $C_0^\infty(\mathbb{R}^n\times(0,\infty))$. Then $C_0^\infty(\overline{\Omega}\times(0,T])$ is dense in $H^{1,1/2}_{;0,}(Q,\mathcal{L})$.*

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

Corollary 3.3. *The space $C_0^\infty(\overline{\Omega}\times[0,T))$ is dense in $H^{1,1/2}_{;,0}(Q,\mathcal{L}')$.*

Before we introduce Green's formulae for functions in anisotropic Sobolev spaces, we have to ensure, that the bilinear form $\langle\partial_t u, v\rangle_Q$ is well defined. In [36] it was shown, that the bilinear form $\langle\partial_t u, v\rangle_Q$ can be extended to functions $u \in H^{1,1/2}_{;0,}(Q)$, $v \in H^{1,1/2}_{;,0}(Q)$ and that there exists a constant $c>0$, such that

$$\langle\partial_t u, v\rangle_Q \le c\,\|u\|_{H^{1,1/2}_{;0,}(Q)}\,\|v\|_{H^{1,1/2}_{;,0}(Q)} \qquad (3.3)$$

for all $u \in H^{1,1/2}_{;0,}(Q)$ and $v \in H^{1,1/2}_{;,0}(Q)$. Here and in the following, $\langle\cdot,\cdot\rangle_Q$ denotes the duality pairing as extension of the inner product in $L^2(Q)$.

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 conormal derivative of u, i.e. we have $\gamma_1^{\mathrm{int}} u = \partial_{n_x} u_{|\Sigma}$. The definition of the Neumann trace operator γ_1^{int} can be extended to the anisotropic Sobolev space space $H^{1,1/2}(Q,\mathcal{L})$.

Lemma 3.4. *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

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

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

Proof. Follows the lines of [5, Proposition 2.18]. □

Theorem 3.5 (Green's first formula). *For* $u \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ *and* $v \in H^{1,1/2}_{;,0}(Q)$ *there holds*

$$\alpha\langle \partial_t u, v\rangle_Q + \langle \nabla_x u, \nabla_x v\rangle_{L^2(Q)} = \langle \gamma_1^{int} u, \gamma_0^{int} v\rangle_\Sigma + \langle \mathcal{L}u, v\rangle_Q \tag{3.4}$$

where $\langle \cdot,\cdot\rangle_\Sigma$ *denotes the duality pairing on* $H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$.

Proof. Let $u \in C_0^\infty(\overline{\Omega} \times (0,T])$. According to (3.1) there holds

$$\langle \mathcal{L}u, v\rangle_{L^2(Q)} = \alpha\langle \partial_t u, v\rangle_{L^2(Q)} + \langle \nabla_x u, \nabla_x v\rangle_{L^2(Q)} - \langle \partial_{n_x} u, v\rangle_{L^2(\Sigma)} \tag{3.5}$$

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 (3.5) by continuity to $v \in H^{1,1/2}_{;,0}(Q)$. Whereas for fixed $v \in H^{1,1/2}_{;,0}(Q)$ all the terms are continuous with respect to u in the $H^{1,1/2}_{;0,}(Q,\mathcal{L})$ norm. Hence by applying Lemma 3.2 we can extend (3.5) to $u \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ which concludes the proof. □

Theorem 3.6 (Green's second formula). *For* $u \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ *and* $v \in H^{1,1/2}_{;,0}(Q,\mathcal{L}')$ *there holds*

$$\langle \mathcal{L}u, v\rangle_Q - \langle u, \mathcal{L}'v\rangle_Q = -\langle \gamma_1^{int} u, \gamma_0^{int} v\rangle_\Sigma + \langle \gamma_0^{int} u, \gamma_1^{int} v\rangle_\Sigma. \tag{3.6}$$

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

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

Similar as in the proof of Theorem 3.5 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 3.2 and Corollary 3.3. □

3.2 Homogeneous initial datum

In the following subsection we discuss, based on [36], the unique solvability of problem (1.1) with zero initial conditions. 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

$$\begin{aligned} \alpha\partial_t u(x,t) - \Delta_x u(x,t) &= f(x,t) && \text{for } (x,t) \in Q, \\ u(x,t) &= g(x,t) && \text{for } (x,t) \in \Sigma, \\ u(x,0) &= 0 && \text{for } x \in \Omega. \end{aligned} \tag{3.7}$$

The variational formulation of problem (3.7) is to find $u \in H^{1,1/2}_{;0,}(Q)$ such that

$$a(u,v) = \langle f, v\rangle_Q \quad \text{for all } v \in H^{1,1/2}_{0;,0}(Q) \tag{3.8}$$

with the bilinear form

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

for $u \in H^{1,1/2}_{;0,}(Q)$ and $v \in H^{1,1/2}_{;,0}(Q)$. The bilinear form

$$a(\cdot,\cdot) : H^{1,1/2}_{;0,}(Q) \times H^{1,1/2}_{;,0}(Q) \to \mathbb{R}$$

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

$$|a(u,v)| \le c_2^A \, \|u\|_{H^{1,1/2}_{;0,}(Q)} \, \|v\|_{H^{1,1/2}_{;,0}(Q)}$$

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 g to the space-time domain Q satisfying $\gamma_0^{\text{int}} \tilde{u}_g = g$. The boundedness of the inverse trace operator $\mathcal{E}_0 : H^{1/2,1/4}(\Sigma) \to H^{1,1/2}_{;0,}(Q)$ then implies

$$\|\tilde{u}_g\|_{H^{1,1/2}_{;0,}(Q)} \le c_{IT} \, \|g\|_{H^{1/2,1/4}(\Sigma)} \, . \tag{3.9}$$

Hence the variational formulation (3.8) changes to: Find $\bar{u} \in H^{1,1/2}_{0;0,}(Q)$ such that

$$a(\bar{u},v) = \langle f, v\rangle_Q - a(\tilde{u}_g, v) \quad \text{for all } v \in H^{1,1/2}_{0;,0}(Q). \tag{3.10}$$

Theorem 3.7 (Existence and uniqueness [36]). *The variational formulation* (3.10) *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 (3.10) is uniquely solvable and therefore $u = \bar{u} + \tilde{u}_g$ is the unique solution of the variational problem (3.8). A direct consequence of Theorem 3.7 is the stability estimate

$$\frac{1}{2} \, \|\bar{u}\|_{H^{1,1/2}_{0;0,}(Q)} \le \sup_{0 \ne v \in H^{1,1/2}_{0;,0}(Q)} \frac{a(\bar{u},v)}{\|v\|_{H^{1,1/2}_{0;,0}(Q)}} \quad \text{for all } \bar{u} \in H^{1,1/2}_{0;0,}(Q). \tag{3.11}$$

Theorem 3.8. *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* (3.8) *satisfying*

$$\|u\|_{H^{1,1/2}_{;0,}(Q)} \leq c_R \|f\|_{[H^{1,1/2}_{0;,0}(Q)]'} + c_B \|g\|_{H^{1/2,1/4}(\Sigma)} . \tag{3.12}$$

Proof. Unique solvability is a result of Theorem 3.7. The stability condition (3.11) and the boundedness of the bilinear form $a(\cdot,\cdot)$ imply

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

The assertion follows by using the triangle inequality for $u = \bar{u} + \tilde{u}_g$, the Poincaré inequality, and the stability (3.9) of the inverse trace operator. □

3.3 Non-homogeneous initial datum

The following analysis in the case of a given initial datum and zero boundary conditions is mainly based on [40, Chapter 23] and [34]. In this subsection we only recall the main results. Let $u_0 \in L^2(\Omega)$ be given. We consider the initial Dirichlet boundary value problem

$$\begin{aligned} \alpha\partial_t u(x,t) - \Delta_x u(x,t) &= 0 && \text{for } (x,t)\in Q,\\ u(x,t) &= 0 && \text{for } (x,t)\in\Sigma,\\ u(x,0) &= u_0(x) && \text{for } x\in\Omega. \end{aligned} \tag{3.13}$$

The space carrying the initial datum u_0 is defined as

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

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

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

where

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

and

$$\|\alpha\partial_t u\|_{L^2(0,T;H^{-1}(\Omega))} := \sup_{0\neq v\in L^2(0,T;H^1_0(\Omega))} \frac{\langle \alpha\partial_t u, v\rangle_Q}{\|v\|_{L^2(0,T;H^1_0(\Omega))}}.$$

Analogously we define the space $\mathcal{V}(Q)$ of functions with non-homogeneous 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 3.9 ([40, Theorem 23.A]). *For $u_0 \in L^2(\Omega)$ there exists a unique solution $u \in \mathcal{V}_0(Q)$ of problem* (3.13) *satisfying the stability estimate*

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

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 [5, 21]. Moreover the following norm equivalence holds.

Lemma 3.10. *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*

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

Proof. Follows the lines of [5, 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

$$\|u\|_{\mathcal{V}_0(Q)} \leq \tilde{c}_1 \, \|u\|_{H^{1,1/2}_{0;,}(Q)} \leq \tilde{c}_2 \, \|u\|_{\mathcal{V}_0(Q)}\,. \tag{3.14}$$

This follows by using the Poincaré inequality and Lemma 3.10.

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

$$u \in C([0,T]; L^2(\Omega)). \tag{3.15}$$

Hence the initial trace $\tau_0 u := u_{|t=0} \in L^2(\Omega)$ of the solution u of problem (3.13) is well defined.

The unique solution $u \in H^{1,1/2}(Q)$ of the fully non-homogeneous initial Dirichlet boundary value problem 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 (3.7) with zero initial conditions, and $\bar{u}_0 \in \mathcal{V}_0(Q)$ is the unique solution of problem (3.13). By applying the stability estimate of Theorem 3.8, the Poincaré inequality, estimate (3.14) and Theorem 3.9 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) is well defined due to $u = \bar{u}_g + \bar{u}_0$ 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 (3.15).

3.4 Neumann trace operator

For the solution $u \in H^{1,1/2}_{;0,}(Q,\mathcal{L})$ of (3.7) with $f \in L^2(Q)$ we can determine the associated conormal derivative $\gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$ as the unique solution of the variational problem

$$\langle \gamma_1^{\text{int}} u, z\rangle_\Sigma = a(u,\mathcal{E}_T z) - \langle f, \mathcal{E}_T z\rangle_Q \quad \text{for all } z \in H^{1/2,1/4}(\Sigma) \tag{3.16}$$

where $\mathcal{E}_T := \mathcal{H}_T\mathcal{E}_0 : H^{1/2,1/4}(\Sigma) \to H^{1,1/2}_{;,0}(Q)$. The operator $\mathcal{H}_T : L^2(Q) \to L^2(Q)$ is defined as follows. For $u \in L^2(Q)$ we consider the series representation

$$u(x,t) = \sum_{i=1}^{\infty} U_i(t)\phi_i(x), \quad U_i(t) = \sum_{k=0}^{\infty} u_{i,k} v_k(t) \quad \text{for } (x,t) \in Q \tag{3.17}$$

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

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

and $v_k \in H^1_{0,}(0,T)$ are given by

$$v_k(t) = \sin\left(\left(\frac{\pi}{2} + k\pi\right)\frac{t}{T}\right), \quad k \in \mathbb{N}. \tag{3.18}$$

The coefficients $u_{i,k}$ in (3.17) are given by

$$u_{i,k} = \frac{2}{T}\int_0^T \int_\Omega u(x,t) v_k(t)\phi_i(x)\,\mathrm{d}x\,\mathrm{d}t. \tag{3.19}$$

Then $\mathcal{H}_T u$ is defined as

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

where

$$(\mathcal{H}_T U_i)(t) := \sum_{k=0}^{\infty} u_{i,k} \cos\left(\left(\frac{\pi}{2} + k\pi\right)\frac{t}{T}\right).$$

The 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

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

A detailed analysis of the transformation operator $\mathcal{H}_T$ is given in [36].

We now get the following stability estimate for the Neumann trace of solutions u of problem (3.7).

Theorem 3.11. *Let* $u \in H^{1,1/2}_{;0,}(Q)$ *be the unique solution of problem* (3.7) *with* $f \in L^2(Q)$ *and* $g \in H^{1/2,1/4}(\Sigma)$*. Then the Neumann trace* $\gamma_1^{int} u \in H^{-1/2,-1/4}(\Sigma)$ *satisfies the stability estimate*

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

Proof. Using (3.16), the boundedness of the bilinear form $a(\cdot,\cdot)$ and of the operator $\mathcal{E}_T$ yields

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

□

In particular for the solution u of the initial Dirichlet boundary value problem (1.1) with homogeneous right hand side and initial datum, i.e. $f \equiv 0$ and $u_0 \equiv 0$, we get

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

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

Lemma 3.12 ([5, 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 3.13. Lemma 3.12 is also valid if we replace the space $C_0^\infty(\overline{\Omega} \times (0,T])$ by $C_0^\infty(\overline{\Omega} \times [0,T))$.

4 Boundary integral operators

In order to express the solution of the initial Dirichlet boundary value problem (1.1) by means of heat potentials as in (1.2) the existence of a fundamental solution is essential. In Subsection 4.1 we derive the fundamental solution of the heat equation and the related representation formula. In Subsections 4.2 - 4.7 we introduce and analyze the heat potentials as well as the resulting boundary integral operators.

4.1 Representation formula for the heat equation

In this subsection we derive the representation formula (1.2) for the heat equation. Therefore we consider Green's second formula (3.2) for $u \in C^2(\overline{Q})$. We want the third integral of 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. $U(y-x,\theta) = \widetilde{U}(r,\theta)$ where $r = |y-x|$. 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 using separation of variables we get

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

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 $n = 1$. When inserting (4.3) into (4.2) for general n we get

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

Thus, (4.3) is also a solution in the two- and three dimensional case if $\gamma = -\frac{n}{2}$. Recalling the definition of the functions U and $\widetilde{U}$ we therefore have

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

Due to the singularity of the function U at $(x,t)=(y,\tau)$ we consider the space-time-cylinder $Q_{t-\varepsilon}:=\Omega\times(0,t-\varepsilon)$ where $0<\varepsilon<t$. Analogously to (3.2) we get

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

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 are going to show the convergence of the first integral of 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

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

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

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

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

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

and we finally obtain

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

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

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

The integral over $\Omega \setminus B_R(x)$ converges to 0, since $\frac{\alpha}{\varepsilon} \exp\left(-\frac{\alpha|y-x|^2}{4\varepsilon}\right) \to 0$ for $y \neq x$ as $\varepsilon \to 0$. By using polar coordinates we get

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

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

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

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

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

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

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

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

$$\begin{aligned} u(x,t) = &\int_\Omega u(y,0) U^\star(x-y,t) \, \mathrm{d}y + \frac{1}{\alpha} \int_Q \mathcal{L}u(y,\tau) U^\star(x-y,t-\tau) \, \mathrm{d}y \, \mathrm{d}\tau \\ &+ \frac{1}{\alpha} \int_\Sigma \partial_{n_y} u(y,\tau) U^\star(x-y,t-\tau) \, \mathrm{d}s_y \, \mathrm{d}\tau \\ &- \frac{1}{\alpha} \int_\Sigma u(y,\tau) \partial_{n_y} U^\star(x-y,t-\tau) \, \mathrm{d}s_y \, \mathrm{d}\tau \end{aligned} \tag{4.6}$$

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

$$U^\star(x,t) = \begin{cases} \left(\frac{\alpha}{4\pi t}\right)^{n/2} \exp\left(\frac{-\alpha|x|^2}{4t}\right), & (x,t) \in \mathbb{R}^n \times (0,\infty), \\ 0\,, & \text{else}, \end{cases} \tag{4.7}$$

is called the fundamental solution of the heat equation and due to construction, $U^\star$ is a solution of the homogeneous heat equation on $\mathbb{R}^n \times (0,\infty)$, see, e.g., [12], i.e.

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

Additionally the fundamental solution has the following properties.

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

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

Proof. Let $t > 0$. We have

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

□

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

$$\lim_{t\to 0} \int_\Omega U^\star(x-y,t)u(y)\,\mathrm{d}y = u(x). \tag{4.8}$$

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

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

Since u ist continuous on Ω and $x \in \Omega$, 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, due to $u \in L^\infty(\Omega)$,

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

The substitution $z = x - y$ yields

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

and by using polar coordinates we get

$$\begin{aligned}\int\limits_{\mathbb{R}^n\backslash B_\delta(x)} U^\star(x-y,t)\,\mathrm{d}y &\le Ct^{-n/2}\int\limits_{\delta}^{\infty} r^{n-1}\exp\left(\frac{-r^2\alpha}{4t}\right)\mathrm{d}r \\ &= C'\int\limits_{a\,t^{-1/2}}^{\infty} \rho^{n-1}\exp\left(-\rho^2\right)\mathrm{d}\rho\end{aligned}$$

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

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

Altogether we obtain

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

for t small enough which concludes the proof. □

One can show that for sufficient regular input data f, g and u_0 the solution of the initial Dirichlet boundary value problem (1.1) is given by the representation formula, i.e. for $(x,t) \in Q$ we have

$$\begin{aligned}u(x,t) = &\int_\Omega U^\star(x-y,t)u_0(y)\,\mathrm{d}y + \frac{1}{\alpha}\int_Q U^\star(x-y,t-\tau)f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau \\ &+ \frac{1}{\alpha}\int_\Sigma U^\star(x-y,t-\tau)\partial_{n_y}u(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau \\ &- \frac{1}{\alpha}\int_\Sigma \partial_{n_y}U^\star(x-y,t-\tau)g(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau.\end{aligned} \tag{4.9}$$

Due to the given representation (4.9) for the solution of problem (1.1) it suffices to determine the yet unknown Cauchy datum $\partial_n u_{|\Sigma}$ to compute the solution in the space-time domain Q. This can be done by applying the Dirichlet trace operator to (4.9) and solving the resulting boundary integral equation on the space-time boundary Σ. The following subsections are devoted to the analysis of the heat potentials in (4.9) and the resulting boundary integral operators.

4.2 Initial potential

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

$$(\widetilde{M}_0 u_0)(x,t) := \int_\Omega U^\star(x-y,t) u_0(y)\,\mathrm{d}y \quad \text{for } (x,t) \in \mathbb{R}^n \times (0,T) \tag{4.10}$$

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.*

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

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

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

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*

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

Proof. Follows the lines of the proof of [29, 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 3.10 we conclude that there exists a constant $c_2^M > 0$ such that

$$\left\| \widetilde{M}_0 u_0 \right\|_{H^{1,1/2}(Q)} \leq c_2^M \left\| u_0 \right\|_{L^2(\Omega)} \quad \text{for all } u_0 \in L^2(\Omega). \tag{4.11}$$

An important property of the initial potential is the continuity in time, i.e. due to (3.15) 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 Dirichlet and Neumann trace operators we finally conclude that the integral operators

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

are linear and bounded.

4.3 Newton potential

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

$$(\widetilde{N}_0 f)(x,t) := \frac{1}{\alpha} \int_0^t \int_\Omega U^\star(x-y, t-\tau) f(y,\tau) \, \mathrm{d}y \, \mathrm{d}\tau. \tag{4.12}$$

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

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

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

$$\begin{aligned} &\left[\alpha \partial_t - \Delta_x\right] (\widetilde{N}_0 f)(x,t) \\ &\qquad = \left[\alpha \partial_t - \Delta_x\right] \left(\lim_{\varepsilon \to 0} \frac{1}{\alpha} \int_0^{t-\varepsilon} \int_\Omega U^\star(x-y, t-\tau) f(y,\tau) \, \mathrm{d}y \, \mathrm{d}\tau \right). \end{aligned}$$

Applying the Leibniz integral rule yields

$$\begin{aligned}
&\big[\alpha\partial_t - \Delta_x\big]\frac{1}{\alpha}\int_0^{t-\varepsilon}\int_\Omega U^\star(x-y,t-\tau)f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau \\
&= \int_0^{t-\varepsilon}\int_\Omega \partial_t U^\star(x-y,t-\tau)f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau + \int_\Omega U^\star(x-y,\varepsilon)f(y,t-\varepsilon)\,\mathrm{d}y \\
&\qquad - \frac{1}{\alpha}\int_0^{t-\varepsilon}\int_\Omega \Delta_x U^\star(x-y,t-\tau)f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau \\
&= \frac{1}{\alpha}\int_0^{t-\varepsilon}\int_\Omega \Big[\alpha\partial_t - \Delta_x\Big]U^\star(x-y,t-\tau)f(y,\tau)\,\mathrm{d}y\,\mathrm{d}\tau \\
&\qquad + \int_\Omega U^\star(x-y,\varepsilon)f(y,t-\varepsilon)\,\mathrm{d}y.
\end{aligned}$$

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

$$\int_\Omega U^\star(x-y,\varepsilon)f(y,t-\varepsilon)\,\mathrm{d}y \xrightarrow{\varepsilon\to 0} f(x,t) \quad \text{for } x \in \Omega.$$

Note that $[\alpha\partial_t - \Delta_x]u(x,t) = 0$ for $x \in \Omega^c$ 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 Subsections 4.4 and 4.6. The theorem provides the mapping properties of the convolution with the fundamental solution of the heat equation, see [5, Section 3] and [30, 31].

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

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

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 [5]. 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, the application of the Neumann trace operator yields the bounded operator

$$N_1 := \gamma_1^{\text{int}} \widetilde{N}_0 : L^2(Q) \to H^{-1/2,-1/4}(\Sigma),$$

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

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

Here, we have to restrict the domain to the space $L^2(Q)$ due to the definition of the Neumann trace operator γ_1^{int}.

4.4 Single layer potential

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

$$(\widetilde{V} w)(x,t) := \frac{1}{\alpha} \int_0^t \int_\Gamma U^\star(x-y, t-\tau) w(y,\tau) \, \mathrm{d}s_y \, \mathrm{d}\tau \quad \text{for } (x,t) \in \mathcal{D}_\Gamma \tag{4.13}$$

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 hence 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. For $(x,t) \in \mathcal{D}_\Gamma$ there exists a compact neighbourhood O of (x,t) such that $O \subset \mathcal{D}_\Gamma$, and hence 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 (4.13) 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 $\gamma_0' : H^{-1/2,-1/4}(\Sigma) \to \widetilde{H}^{-1,-1/2}_{\text{comp}}(\mathbb{R}^n \times (0,T))$ by

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

The single layer potential is then given by

$$\widetilde{V} := A\gamma_0' : H^{-1/2,-1/4}(\Sigma) \to \widetilde{H}^{1,1/2}_{\text{loc}}(\mathbb{R}^n \times (0,T)). \tag{4.14}$$

Due to the boundedness of the operators A and γ_0', the 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 positive constant $c_2^{\widetilde{V}} > 0$ such that

$$\left\|\widetilde{V}w\right\|_{H^{1,1/2}_{;0,}(Q)} \le c_2^{\widetilde{V}}\,\|w\|_{H^{-1/2,-1/4}(\Sigma)} \quad \text{for all } w \in H^{-1/2,-1/4}(\Sigma). \tag{4.15}$$

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

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

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

$$\begin{aligned} [\gamma_0 u] &:= \gamma_0^{\text{ext}} u - \gamma_0^{\text{int}} u, \\ [\gamma_1 u] &:= \gamma_1^{\text{ext}} u - \gamma_1^{\text{int}} u. \end{aligned} \tag{4.16}$$

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 $w \in H^{-1/2,-1/4}(\Sigma)$ 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 $[\alpha\partial_t - \Delta_x]u = 0$ on $Q \cup Q^c$. By using Green's second formula (3.6) 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

$$-\langle u, [-\alpha\partial_t - \Delta_x]\varphi\rangle_{L^2(B_R\times(0,T))} = \langle [\gamma_1 u], \gamma_0^{\text{int}}\varphi\rangle_\Sigma. \tag{4.17}$$

From the representation (4.14) of the single layer potential $\widetilde{V}$ follows that

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

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

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

Combined with (4.17) 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

$$V := \gamma_0^{\text{int}} \widetilde{V} : H^{-1/2,-1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma) \tag{4.18}$$

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

$$\|Vw\|_{H^{1/2,1/4}(\Sigma)} \le c_2^V \, \|w\|_{H^{-1/2,-1/4}(\Sigma)} \quad \text{for all } w \in H^{-1/2,-1/4}(\Sigma). \tag{4.19}$$

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. For w regular enough 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

$$(Wv)(x,t) := \frac{1}{\alpha} \int_0^t \int_\Gamma \partial_{n_y} U^\star(x-y, t-\tau) v(y,\tau) \, \mathrm{d}s_y \, \mathrm{d}\tau \quad \text{for } (x,t) \in \mathcal{D}_\Gamma. \tag{4.20}$$

The fundamental solution $U^\star(x - \cdot, t - \cdot)$ is smooth on Σ for $(x,t) \in \mathcal{D}_\Gamma$ and hence 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. For $(x,t) \in \mathcal{D}_\Gamma$ there exists a compact neighbourhood O of (x,t) such that $O \subset \mathcal{D}_\Gamma$ and hence $\operatorname{dist}(O, \Sigma) > 0$. 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 get

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

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

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

□

As in the case of the single layer potential $\widetilde{V}$ the representation (4.20) 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 convolution operator A. 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 [5, Proposition 3.3]. We conclude, that there exists a positive 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 on $\mathcal{D}_\Gamma$, i.e. we have

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

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 $v \in H^{1/2,1/4}(\Sigma)$ we define $u := Wv \in H^{1,1/2}_{;0,}(B_R \times (0,T))$, hence $[\alpha\partial_t - \Delta_x]u = 0$ on $Q \cup Q^c$. By using Green's second formula (3.6) with $\varphi \in C_0^\infty(B_R \times [0,T))$ 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

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

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

$$\langle[\gamma_1 Wv], \gamma_0^{\text{int}}\varphi\rangle_\Sigma = \langle[\gamma_0 Wv] - v, \gamma_1^{\text{int}}\varphi\rangle_\Sigma. \tag{4.21}$$

Remark 3.13 then implies, that each side in (4.21) 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

$$Kv := \frac{1}{2}\left(\gamma_0^{\text{int}}Wv + \gamma_0^{\text{ext}}Wv\right). \tag{4.22}$$

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 positive constant $c_2^K > 0$ such that

$$\|Kv\|_{H^{1/2,1/4}(\Sigma)} \le c_2^K \|v\|_{H^{1/2,1/4}(\Sigma)} \quad \text{for all } v \in H^{1/2,1/4}(\Sigma). \tag{4.23}$$

4.7 Hypersingular 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

$$\|Dv\|_{H^{-1/2,-1/4}(\Sigma)} \le c_2^D \|v\|_{H^{1/2,1/4}(\Sigma)} \quad \text{for all } v \in H^{1/2,1/4}(\Sigma) \tag{4.24}$$

with some positive constant $c_2^D > 0$. If the density v is smooth enough, we have the representation

$$(Dv)(x,t) = -\frac{1}{\alpha}\gamma_{1,x}^{\text{int}}\int_0^t\int_\Gamma \gamma_{1,y}^{\text{int}}U^\star(x-y,t-\tau)v(y,\tau)\,\mathrm{d}s_y\,\mathrm{d}\tau$$

for $(x,t) \in \Sigma$. When assuming 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.

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

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. [5, Theorem 6.1], we obtain

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

where

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

Whereas for $n = 3$ we have the representation [27, Theorem 2.1]

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

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

5 Boundary integral equations

In the following section we introduce the Calderón projection operator and deduce related properties of the boundary integral operators, including the definition of the Steklov-Poincaré operator in Subsection 5.1. In Subsection 5.2 we discuss the unique solvability of the model problem (1.1) by means of analyzing related boundary integral equations.

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 $f \in L^2(Q)$ is given by the representation formula

$$u = (\widetilde{V}\gamma_1^{\text{int}}u) - (W\gamma_0^{\text{int}}u) + (\widetilde{M_0}u_0) + (\widetilde{N}_0 f) \quad \text{in } Q. \tag{5.1}$$

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

$$\gamma_0^{\text{int}}u = (V\gamma_1^{\text{int}}u) + \frac{1}{2}\gamma_0^{\text{int}}u - (K\gamma_0^{\text{int}}u) + (M_0u_0) + (N_0 f) \quad \text{on } \Sigma. \tag{5.2}$$

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

$$\gamma_1^{\text{int}} u = \frac{1}{2}\gamma_1^{\text{int}} u + (K'\gamma_1^{\text{int}} u) + (D\gamma_0^{\text{int}} u) + (M_1 u_0) + (N_1 f) \quad \text{on } \Sigma. \tag{5.3}$$

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

$$\begin{pmatrix} \gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{1}{2}I - K & V \\ D & \frac{1}{2}I + K' \end{pmatrix}}_{=:\,\mathcal{C}} \begin{pmatrix} \gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u \end{pmatrix} + \begin{pmatrix} M_0 u_0 \\ M_1 u_0 \end{pmatrix} + \begin{pmatrix} N_0 f \\ N_1 f \end{pmatrix}. \tag{5.4}$$

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

$$\begin{aligned} \gamma_0^{\text{int}} u &= V\psi + \left(\frac{1}{2}I - K\right)\varphi, \\ \gamma_1^{\text{int}} u &= \left(\frac{1}{2}I + K'\right)\psi + D\varphi. \end{aligned} \tag{5.5}$$

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 $u_0 = 0$, 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 (5.5) 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 $\mathcal{C} = \mathcal{C}^2$. $\square$

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 section.

Theorem 5.3. *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 $(\psi, \varphi) \in H^{-1/2,-1/4}(\Sigma) \times H^{1/2,1/4}(\Sigma)$.

Proof. Follows the lines of [5, Corollary 3.10, Theorem 3.11]. □

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 positive constant* $c_1^V > 0$ *such that*

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

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

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

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

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

5.1 Steklov-Poincaré operator

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

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

Using the first integral equation we can define the Dirichlet to Neumann map

$$\gamma_1^{\text{int}} u = V^{-1} \left(\frac{1}{2} I + K \right) \gamma_0^{\text{int}} u. \tag{5.6}$$

The operator

$$S := V^{-1} \left(\frac{1}{2} I + K \right) : H^{1/2,1/4}(\Sigma) \to H^{-1/2,-1/4}(\Sigma) \tag{5.7}$$

is called Steklov-Poincaré operator for the heat equation. When inserting (5.6) into the second boundary integral equation we obtain

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

Hence we get a *symmetric* representation of the Steklov-Poincaré operator,

$$S = D + \left(\frac{1}{2} I + K' \right) V^{-1} \left(\frac{1}{2} I + K \right). \tag{5.8}$$

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 positive constant $c_1^S > 0$ such that*

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

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

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

The assertion now follows with Theorem 5.3. □

5.2 Initial Dirichlet boundary value problem

We consider the initial Dirichlet boundary value problem (1.1) with source term $f \in L^2(Q)$, boundary datum $g \in H^{1/2,1/4}(\Sigma)$, and initial datum $u_0 \in L^2(\Omega)$. The solution is given by the representation formula

$$u = (\widetilde{V}\gamma_1^{\text{int}} u) - (Wg) + (\widetilde{M_0}u_0) + (\widetilde{N}_0 f) \quad \text{in } Q.$$

It remains to determine the unknown conormal derivative $\gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$. This can be done, e.g., by using the first boundary integral equation in (5.4). We have to find $\gamma_1^{\text{int}} u \in H^{-1/2,-1/4}(\Sigma)$ such that

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

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

$$\left\langle V\gamma_1^{\text{int}} u, \tau \right\rangle_\Sigma = \left\langle \left(\frac{1}{2}I + K\right) g - M_0 u_0 - N_0 f, \tau \right\rangle_\Sigma \tag{5.9}$$

for all $\tau \in H^{-1/2,-1/4}(\Sigma)$. 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 Lemma of Lax-Milgram. The solution $\gamma_1^{\text{int}} u$ then satisfies

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

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

$$u = (\widetilde{V}w) + (\widetilde{M_0}u_0) + (\widetilde{N}_0 f) \quad \text{in } Q \tag{5.10}$$

with an unknown density $w \in H^{-1/2,-1/4}(\Sigma)$ to be determined. By applying the Dirichlet trace operator to (5.10) we obtain

$$g = (Vw) + (M_0 u_0) + (N_0 f) \quad \text{on } \Sigma. \tag{5.11}$$

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

$$\langle Vw, \tau\rangle_\Sigma = \langle g - M_0 u_0 - N_0 f, \tau\rangle_\Sigma \quad \text{for all } \tau \in H^{-1/2,-1/4}(\Sigma). \tag{5.12}$$

As in the case of the direct formulation with the first boundary integral equation the unique solvability follows with the Lemma of Lax-Milgram.

In this paper we only consider the Dirichlet boundary value problem. The analysis of the Neumann boundary value problem will be addressed in future work, see, e.g., [6]. In this case one can, e.g., use the second boundary integral equation in (5.4) to obtain the unknown Dirichlet trace $\gamma_0^{\text{int}} u$ of the solution u. Due to the ellipticity of the hypersingular operator D, the second boundary integral equation is uniquely solvable as well. Another approach would be an indirect formulation with the double layer potential W.

6 Space-time discretization

In this section we discuss two different space-time discretization techniques in order to compute an approximation of the unknown Neumann datum $\partial_n u_{|\Sigma}$ and derive related approximation properties. The first one is the so-called tensor product approach, where we consider separate decompositions of the spatial boundary Γ and the time interval $(0,T)$ and use space-time tensor product spaces to compute an approximation of $\partial_n u_{|\Sigma}$. 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, thus $\overline{\Gamma} = \bigcup_{j=1}^J \overline{\Gamma}_j$. With $\Sigma_j := \Gamma_j \times (0,T)$, $j = 1,...,J$, we then obtain $\overline{\Sigma} = \bigcup_{j=1}^J \overline{\Sigma}_j$. For the Galerkin boundary element discretization of the variational formulations (5.9) or (5.12), 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

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

6.1 One-dimensional problem

In the spatially one-dimensional case we have $\Gamma = \{a,b\}$ assuming $\Omega = (a,b)$, 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 1.

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 $H^s(\Sigma)$.

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

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

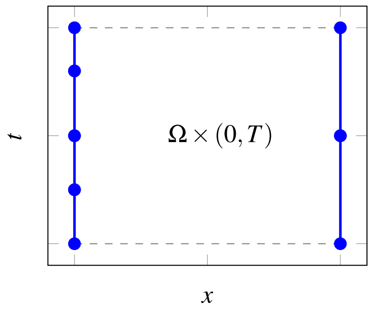


Figure 1: Sample BE mesh. We consider an arbitrary decomposition of the space–time boundary Σ. Note that there is no time-stepping scheme involved.

For the approximation of the unknown Neumann datum $w = \gamma_1^{\text{int}} u \in H^{-1/4}(\Sigma)$ we consider the space $S_h^0(\Sigma) := \operatorname{span}\{\varphi_\ell^0\}_{\ell=1}^N$ of piecewise constant basis functions φ_ℓ^0, which is defined with respect to the decomposition Σ_N. According to Remark 6.1 we can identify $H^{r,s}(\Sigma)$ with $H^s(\Sigma)$ and hence we have the same approximation properties as in the case of standard Sobolev spaces $H^s(\Sigma)$, see, e.g., [33].

Approximation properties. The L^2 projection $Q_h^0 u \in S_h^0(\Sigma)$ of $u \in L^2(\Sigma)$ is defined as the unique solution of the variational problem

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

The operator $Q_h^0 : L^2(\Sigma) \to L^2(\Sigma)$ satisfies the trivial stability estimate

$$\left\| Q_h^0 u \right\|_{L^2(\Sigma)} \leq \|u\|_{L^2(\Sigma)} \quad \text{for all } u \in L^2(\Sigma).$$

Next we summarize some error estimates for the L^2 projection $Q_h^0 u$.

Theorem 6.2 ([33, Theorem 10.2]). *Let $u \in H^s(\Sigma)$ with $s \in [0,1]$ and $Q_h^0 u \in S_h^0(\Sigma)$ be the L^2 projection of u. Then there holds the error estimate*

$$\left\| u - Q_h^0 u \right\|_{L^2(\Sigma)} \leq c\, h^s |u|_{H^s(\Sigma)}.$$

Lemma 6.3 ([33, Corollary 10.3]). *Let $u \in H^s(\Sigma)$ with $s \in [0,1]$. For $\sigma \in [-1,0]$ there holds the error estimate*

$$\left\|u - Q_h^0 u\right\|_{\widetilde{H}^\sigma(\Sigma)} \leq c\, h^{s-\sigma} |u|_{H^s(\Sigma)}.$$

Lemma 6.4 ([33, Lemma 10.10]). *Assume that the boundary decomposition Σ_N is globally quasi-uniform. For $\sigma \in [-1,0]$ there holds the inverse inequality*

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

6.2 Two- and three-dimensional problems

We consider two different decomposition approaches. The first one is a separate decomposition of the spatial boundary $\Gamma = \partial\Omega$ and the time interval $(0,T)$, also discussed in, e.g., [15, 25, 29]. In this case we use space-time tensor product spaces to discretize the variational formulations (5.9) or (5.12). We derive error estimates simply by combining approximation properties of the spatial and temporal discretizations. 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 decompositions

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

$$\overline{\Gamma} = \bigcup_{\ell=1}^{N_x} \overline{\gamma}_\ell. \tag{6.2}$$

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

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

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

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

Moreover we consider a family $\{I_{N_t}\}_{N_t\in\mathbb{N}}$ 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

$$\overline{I} = [0,T] = \bigcup_{k=1}^{N_t} \overline{\tau}_k. \tag{6.3}$$

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 $h_t := \max_{k=1,...,N_t} h_{k,t}$. Again, 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

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

The set $\mathcal{B}_N := \{\sigma_\ell\}_{l=1}^{N}$ of the boundary elements σ_ℓ in (6.1) is then given by

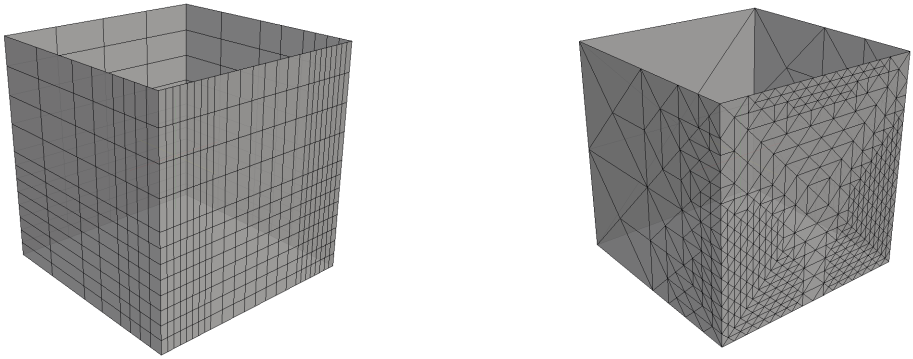
$$\mathcal{B}_N := \{\sigma = \gamma_i \times \tau_j, i \in \{1,...,N_x\}, j \in \{1,...,N_t\}\}.$$

These 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 2 (a).

Since the normal derivative of u on Σ could be discontinuous depending on the spatial boundary Γ it is reasonable to approximate the conormal derivative $w = \gamma_1^{\text{int}} u$ by discontinuous functions. Thus, we use the space of piecewise constant basis functions for the approximation of w. Let $S_h^0(I) := \operatorname{span}\{\varphi_\ell^0\}_{l=1}^{N_t}$ be the space of piecewise constant basis functions on $(0,T)$ corresponding to the temporal decomposition I_{N_t}, and let $S_h^0(\Gamma) := \operatorname{span}\{\psi_i^0\}_{i=1}^{N_x}$ be the space of piecewise constant basis functions on Γ, which is defined with respect to the spatial decomposition Γ_{N_x}. The boundary element space is then given as

$$S_{h_x,h_t}^{0,0}(\Sigma) := S_{h_x}^0(\Gamma) \otimes S_{h_t}^0(I). \tag{6.4}$$

Due to the structure of the decomposition we can combine the approximation properties in spatial and temporal dimension in order to derive the approximation properties of the boundary element space $S_{h_x,h_t}^{0,0}(\Sigma)$.



(a) Tensor product decomposition (b) Triangulation

Figure 2: Sample space-time boundary decompositions of $Q = (0,1)^3$.

Approximation properties. The L^2 projection $Q_{h_x}u \in S^0_{h_x}(\Gamma)$ of $u \in L^2(\Gamma)$ is defined as the unique solution of the variational problem

$$\langle Q_{h_x}u, v_h\rangle_{L^2(\Gamma)} = \langle u, v_h\rangle_{L^2(\Gamma)} \quad \text{for all } v_h \in S^0_{h_x}(\Gamma). \tag{6.5}$$

Analogously the L^2 projection $Q_{h_t}u \in S^0_{h_t}(I)$ of $u \in L^2(0,T)$ is defined as the unique solution of the variational problem

$$\langle Q_{h_t}u, v_h\rangle_{L^2(I)} = \langle u, v_h\rangle_{L^2(I)} \quad \text{for all } v_h \in S^0_{h_t}(I). \tag{6.6}$$

The L^2 projection operator $Q_{h_x,h_t} : L^2(\Sigma) \to S^{0,0}_{h_x,h_t}(\Sigma)$ with $Q_{h_x,h_t}u \in S^{0,0}_{h_x,h_t}(\Sigma)$ defined as the unique solution of the variational problem

$$\langle Q_{h_x,h_t}u, v_h\rangle_{L^2(\Sigma)} = \langle u, v_h\rangle_{L^2(\Sigma)} \quad \text{for all } v_h \in S^{0,0}_{h_x,h_t}(\Sigma), \tag{6.7}$$

has the representation $Q_{h_x,h_t} = Q^\Sigma_{h_x} Q^\Sigma_{h_t}$, where for $u \in L^2(\Sigma)$

$$(Q^\Sigma_{h_x}u)(x,t) := (Q_{h_x}u(\cdot,t))(x),$$
$$(Q^\Sigma_{h_t}u)(x,t) := (Q_{h_t}u(x,\cdot))(t).$$

Hence we can use the well known approximation properties of the operators Q_{h_x} and Q_{h_t} to derive estimates for the L^2 projection $Q_{h_x,h_t}u$, see, e.g. [5, 29].

Theorem 6.5. *Let $u \in H^{r,s}(\Sigma)$ for some $r, s \in [0,1]$ and let $Q_{h_x,h_t}u \in S^{0,0}_{h_x,h_t}(\Sigma)$ be the L^2 projection of u. Then there hold the error estimates*

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

Lemma 6.6. *Let $u \in H^{r,s}(\Sigma)$ for some $r, s \in [0,1]$. For $\sigma, \mu \in [0,1]$ there holds the error estimate*

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

Lemma 6.7 (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*

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

Proof. Let $\tau_h \in S^{0,0}_{h_x,h_t}(\Sigma)$ and $0 \leq r < \frac{1}{2}$. By applying the inverse inequality in spatial and temporal direction we get

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

Applying this estimate yields

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

and we conclude

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

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

$$\|\tau_h\|_{L^2(\Sigma)} \leq c\left(h_x^{-r/2} + h_t^{-r/4}\right)\|\tau_h\|_{\widetilde{H}^{-r/2,-r/4}(\Sigma)}\,. \tag{6.8}$$

By using interpolation results, see, e.g., [21, 22], we get

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

and together with (6.8) we conclude

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

□

For a shape regular boundary element mesh, i.e. $h_{k,x} \sim h_{k,t}$, the global mesh size is given by $h := \max_{\ell=1,\ldots,N} h_\ell$ where $h_\ell := |\sigma_\ell|^{1/n}$ is the local mesh size. We define $Q_h^{0,0} := Q_{h,h}^{0,0}$ and $S_h^{0,0}(\Sigma) := S_{h,h}^{0,0}(\Sigma)$ and we obtain the following estimates.

Corollary 6.8. *Assume that Σ_N is a shape regular boundary element mesh, and let $u \in H^{r,s}(\Sigma)$ for some $r, s \in [0,1]$. For $\sigma, \mu \in [0,1]$ there holds the error estimate*

$$\left\| u - Q_h^{0,0} u \right\|_{\widetilde{H}^{-\sigma,-\mu}(\Sigma)} \leq c\, h^{\min(r,s)+\min(\sigma,\mu)} \, \|u\|_{H^{r,s}(\Sigma)} .$$

Proof. Follows by applying Lemma 6.6 with $h_x \sim h_t$. □

Corollary 6.9. *Assume that Σ_N is a shape regular and globally quasi-uniform boundary element mesh. For $r \in [0,1)$ there holds the inverse inequality*

$$\|\tau_h\|_{L^2(\Sigma)} \leq c\, h^{-r} \, \|\tau_h\|_{\widetilde{H}^{-r,-r/2}(\Sigma)} \quad \textit{for all } \tau_h \in S_h^{0,0}(\Sigma).$$

Proof. Follows by applying Lemma 6.7 with $h_x \sim h_t$. □

Triangulation of Σ

Let $\{\Sigma_N\}_{N\in\mathbb{N}}$ be a family of admissible triangulations of 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 space-time 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 then given by $h := \max_{\ell=1,\ldots,N} h_\ell$. The family $\{\Sigma_N\}_{N\in\mathbb{N}}$ of decompositions is said to be globally quasi-uniform, if there exists a constant $c_G \geq 1$ independent of Σ_N such that

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

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

$$d_\ell \leq c_B h_\ell \quad \text{for } \ell = 1, \ldots, N \tag{6.9}$$

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 2 (b).

For the approximation of the conormal derivative $w = \gamma_1^{\text{int}} u$ we consider the space of piecewise constant basis functions $S_h^0(\Sigma) := \text{span}\left\{\varphi_\ell^0\right\}_{\ell=1}^N$, which is defined with respect to the decomposition Σ_N.

Approximation properties. The L^2 projection $Q_h u \in S_h^0(\Sigma)$ of $u \in L^2(\Sigma)$ is defined as the unique solution of the variational problem

$$\langle Q_h u, v_h \rangle_{L^2(\Sigma)} = \langle u, v_h \rangle_{L^2(\Sigma)} \quad \text{for all } v_h \in S_h^0(\Sigma). \tag{6.10}$$

By using Lemma 2.1 and the well known approximation properties in standard Sobolev spaces, e.g., [33], we immediately obtain the following results.

Theorem 6.10. *Let $u \in H^{r,s}(\Sigma)$ for some $r, s \in [0,1]$, and let $Q_h u \in S_h^0(\Sigma)$ be the L^2 projection of u. Then there hold the error estimates*

$$\begin{aligned} \|u - Q_h u\|_{L^2(\Sigma)} &\leq \|u\|_{L^2(\Sigma)}, \\ \|u - Q_h u\|_{L^2(\Sigma)} &\leq c\, h^{\min(r,s)} \|u\|_{H^{r,s}(\Sigma)}. \end{aligned}$$

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

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

we obtain

$$\begin{aligned} \|u - Q_h u\|_{L^2(\Sigma)}^2 &= \langle u - Q_h u, u - Q_h u \rangle_{L^2(\Sigma)} = \langle u - Q_h u, u \rangle_{L^2(\Sigma)} \\ &\leq \|u - Q_h u\|_{L^2(\Sigma)} \|u\|_{L^2(\Sigma)} \end{aligned}$$

and we conclude the first error estimate. For $u \in H^{r,s}(\Sigma)$ for some $r, s \in [0,1]$ and $m := \min(r,s)$ we argue as follows. Analogously to [33, Theorem 10.2] we get

$$\|u - Q_h u\|_{L^2(\Sigma)} \leq c\, h^m \|u\|_{H^m(\Sigma)}.$$

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

$$\|u - Q_h u\|_{L^2(\Sigma)} \leq c\, h^m \|u\|_{H^{r,s}(\Sigma)}.$$

□

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

$$\|u - Q_h u\|_{\widetilde{H}^{-\sigma,-\mu}(\Sigma)} \leq c\, h^{\min(r,s)+\min(\sigma,\mu)} \|u\|_{H^{r,s}(\Sigma)}.$$

Proof. Let $u \in H^{r,s}(\Sigma)$. Using (6.10) this yields

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

By applying the Cauchy-Schwarz inequality and Theorem 6.10 we obtain

$$\|u - Q_h u\|_{\widetilde{H}^{-\sigma,-\mu}(\Sigma)} \leq \|u - Q_h u\|_{L^2(\Sigma)} \sup_{0 \neq v \in H^{\sigma,\mu}(\Sigma)} \frac{\|v - Q_h v\|_{L^2(\Sigma)}}{\|v\|_{H^{\sigma,\mu}(\Sigma)}} \leq c\, h^{\min(r,s)} h^{\min(\sigma,\mu)} \|u\|_{H^{r,s}(\Sigma)}.$$

□

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

Lemma 6.12 (Global inverse inequality). *For a globally quasi-uniform boundary decomposition Σ_N and for $\sigma, \mu \in [0,1]$ there holds*

$$\|\tau_h\|_{L^2(\Sigma)} \leq c\, h^{-\max(\sigma,\mu)} \|\tau_h\|_{\widetilde{H}^{-\sigma,-\mu}(\Sigma)} \quad \textit{for all } \tau_h \in S_h^0(\Sigma). \tag{6.11}$$

Proof. Let $\tau_h \in S_h^0(\Sigma)$ and $\sigma, \mu \in [0,1]$. Application of the standard inverse inequality, see, e.g., [33, Section 10.2], yields

$$\|\tau_h\|_{L^2(\Sigma)} \leq c\, h^{-\max(\sigma,\mu)} \|\tau_h\|_{\widetilde{H}^{-\max(\sigma,\mu)}(\Sigma)}. \tag{6.12}$$

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

$$\|\tau_h\|_{\widetilde{H}^{-\max(\sigma,\mu)}(\Sigma)} = \sup_{0 \neq v \in H^{\max(\sigma,\mu)}(\Sigma)} \frac{\langle \tau_h, v\rangle_\Sigma}{\|v\|_{H^{\max(\sigma,\mu)}(\Sigma)}} \leq c \sup_{0 \neq v \in H^{\sigma,\mu}(\Sigma)} \frac{\langle \tau_h, v\rangle_\Sigma}{\|v\|_{H^{\sigma,\mu}(\Sigma)}} = c\, \|\tau_h\|_{\widetilde{H}^{-\sigma,-\mu}(\Sigma)}, \tag{6.13}$$

and the assertion follows from combining (6.12) and (6.13). □

Remark 6.13. For $r = 1/2$ and $s = 1/4$ we have $\widetilde{H}^{-1/2,-1/4}(\Sigma) = H^{-1/2,-1/4}(\Sigma)$ and therefore we obtain

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

7 Boundary element methods

In this section we discretize the variational formulation (5.9) by using the previously introduced boundary element spaces and we derive a priori error estimates for the Galerkin approximation of the Neumann datum $w = \gamma_1^{\text{int}} u$, see Subsection 7.1. The numerical analyis of the discretized indirect formulation (5.12) follows exactly the same path. In Subsection 7.2 we prove error estimates for the related approximation of the solution u in the space-time domain Q.

For the discretization of the variational formulation (5.9) we consider the space of piecewise constant basis functions $X_h \in \left\{ S_h^{0,0}(\Sigma), S_h^0(\Sigma) \right\}$ defined with respect to a shape regular boundary element mesh Σ_N. The Galerkin-Bubnov variational formulation of (5.9) 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.

Note that 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. Hence, for the tensor product approach we choose $h_t \sim h_x$. A priori error estimates and numerical experiments for a different refinement strategy, e.g. $h_t \sim h_x^2$, can be found in [5, 29].

7.1 Error estimates

Since the operator V is elliptic and bounded we can apply Cea's lemma to conclude quasi-optimality of the Galerkin approximation $w_h \in X_h$, i.e. we have

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

where $w \in H^{-1/2,-1/4}(\Sigma)$ is the unique solution of the variational problem (5.9). 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 $\Sigma_j = \Gamma_j \times (0,T)$. Due to the local definition of the trial space X_h and by applying Lemma 2.6 we obtain

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

Note that all the approximation properties shown in the previous section 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 $H^{r,s}_{\text{pw}}(\Sigma)$ and we still get the same error estimates in the appropriate norms.

One-dimensional problem

Recall that in the one-dimensional case we can identify the Sobolev spaces $H^{r,s}(\Sigma)$ with $H^s(\Sigma)$.

Theorem 7.1. *Let $w_h \in S_h^0(\Sigma)$ 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 6.3 in (7.2). □

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 $w_h \in S_h^0(\Sigma)$ 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. The assertion follows by using the triangle inequality

$$\|w - w_h\|_{L^2(\Sigma)} \leq \left\|w - Q_h^0 w\right\|_{L^2(\Sigma)]} + \left\|Q_h^0 w - w_h\right\|_{L^2(\Sigma)},$$

and by applying Lemma 6.2, Lemma 6.4 and Theorem 7.1. □

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 $w \in H^{r,s}_{pw}(\Sigma)$ for some $r, s \in [0,1]$ 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 Corollary 6.8 if $X_h = S_h^{0,0}(\Sigma)$, and Lemma 6.11 if $X_h = S_h^0(\Sigma)$ 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 $w \in H^{r,s}_{pw}(\Sigma)$ for some $r, s \in [1/4, 1]$ 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 6.5, and Corollary 6.9 for $X_h = S_h^{0,0}(\Sigma)$, and Theorem 6.10 and Remark 6.13 for $X_h = S_h^0(\Sigma)$ respectively. In both cases we get

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

Here Q_h is either the L^2 projection onto $S_h^{0,0}(\Sigma)$, or onto $S_h^0(\Sigma)$. The assertion follows with

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

Theorem 7.3, Corollary 6.8 for $X_h = S_h^{0,0}(\Sigma)$ and Lemma 6.11 for $X_h = S_h^0(\Sigma)$, respectively. □

Hence we can prove the same convergence rates for $X_h = S_h^{0,0}(\Sigma)$ and $X_h = S_h^0(\Sigma)$ 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 Section 8 show that the $L^2(\Sigma)$-error estimate is not optimal.

7.2 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 (1.1) in Q by using the representation formula (5.1) with the approximation w_h, i.e for $(x,t) \in Q$ we have

$$\tilde{u}(x,t) = (\widetilde{V} w_h)(x,t) - (W g)(x,t) + (\widetilde{M}_0 u_0)(x,t) + (\widetilde{N}_0 f)(x,t). \tag{7.3}$$

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

$$|u(x,t) - \tilde{u}(x,t)| \le \frac{1}{\alpha}\, \|U^\star(x-\cdot, t-\cdot)\|_{H^{-\sigma,-\sigma/2}(\Sigma)}\, \|w - w_h\|_{\widetilde{H}^{\sigma,\sigma/2}(\Sigma)}\,. \tag{7.4}$$

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, $Q_h : L^2 \to X_h$ denotes the L^2 projection onto the space X_h.

Theorem 7.5 (Aubin-Nitsche Trick). *Let* $w \in H^{r,s}_{pw}(\Sigma)$ *for some* $r \in [-1/2, 1]$ *and* $s \in [-1/4, 1]$ *be the unique solution of* (5.9)*, 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 $-2 \le \sigma \le -1/2$ *and* $\mu = \sigma/2$*. Then there holds the error estimate*

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

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

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

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 $z \in H^{-1-\sigma,-1/2-\mu}(\Sigma)$ 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

$$\begin{aligned} \|w - w_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} &= \sup_{0 \ne z \in H^{-1-\sigma,-1/2-\mu}(\Sigma)} \frac{\langle w - w_h, V^*z\rangle_\Sigma}{\|V^*z\|_{H^{-\sigma,-\mu}(\Sigma)}} \\ &= \sup_{0 \ne z \in H^{-1-\sigma,-1/2-\mu}(\Sigma)} \frac{\langle V(w - w_h), z - Q_h z\rangle_\Sigma}{\|V^*z\|_{H^{-\sigma,-\mu}(\Sigma)}}. \end{aligned}$$

Since V^* is bijective, there exists a constant $c > 0$, such that [11, Lemma A.40]

$$\|V^*z\|_{H^{-\sigma,-\mu}(\Sigma)} \ge c\,\|z\|_{H^{-1-\sigma,-1/2-\mu}(\Sigma)} \quad \text{for all } z \in H^{-1-\sigma,-1/2-\mu}(\Sigma).$$

Thus, by using the boundedness of the operator $V : H^{-1/2,-1/4}(\Sigma) \to H^{1/2,1/4}(\Sigma)$ we conclude

$$\begin{aligned} &\|w - w_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \\ &\qquad \le \tilde{c}\,\|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)} \sup_{0 \ne z \in H^{-1-\sigma,-1/2-\mu}(\Sigma)} \frac{\|z - Q_h z\|_{H^{-1/2,-1/4}(\Sigma)}}{\|z\|_{H^{-1-\sigma,-1/2-\mu}(\Sigma)}}. \end{aligned}$$

When considering $-1-\sigma \le 1$, i.e. $\sigma \ge -2$, we obtain from the approximation properties of the operator Q_h the error estimate

$$\|w - w_h\|_{\widetilde{H}^{\sigma,\mu}(\Sigma)} \le \hat{c}\, h^{\min(-1-\sigma,-1/2-\mu)+1/4}\, \|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)}\,,$$

and the assertion follows by applying the error estimate for the Galerkin approximation w_h in the energy norm. □

Now assume, that the solution w of the variational formulation (5.9) is sufficiently smooth, i.e. $w \in H^{1,1}_{\text{pw}}(\Sigma)$. From estimate (7.4) and by choosing $\sigma = -2$ in Theorem (7.5) we get, for $(x,t) \in Q$, the pointwise error estimate

$$\begin{aligned} |u(x,t) - \tilde{u}(x,t)| &\leq \tilde{c}\, \|U^\star(x-\cdot, t-\cdot)\|_{H^{2,1}(\Sigma)} \|w - w_h\|_{\widetilde{H}^{-2,-1}(\Sigma)} \\ &\leq c\, h^2\, \|U^\star(x-\cdot, t-\cdot)\|_{H^{2,1}(\Sigma)} \|w\|_{H^{1,1}_{\text{pw}}(\Sigma)} . \end{aligned} \tag{7.5}$$

Let us now consider problem (3.7) with source term $f = 0$. To estimate the global error $\|u - \tilde{u}\|_{H^{1,1/2}(Q)}$ we proceed as follows. We first consider the Dirichlet trace of the discretized representation formula (7.3), i.e. we have

$$\hat{g} := V w_h + \frac{1}{2} g - K g.$$

Moreover, the first boundary integral equation in (5.4) gives

$$g = V w + \frac{1}{2} g - K g,$$

and we therefore conclude the relation

$$g - \hat{g} = V(w - w_h). \tag{7.6}$$

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* (3.7) *with source term* $f = 0$*, and let* $\tilde{u} \in H^{1,1/2}_{;0,}(Q)$ *be the corresponding approximation given by* (7.3)*, where* $f = 0$ *and* $u_0 = 0$*. Then there holds the error estimate*

$$\|u - \tilde{u}\|_{H^{1,1/2}_{;0,}(Q)} \leq c\, \|w - w_h\|_{H^{-1/2,-1/4}(\Sigma)} .$$

Proof. The solution $u = \bar{u} + \mathcal{E}_0 g \in H^{1,1/2}_{;0,}(Q)$ of problem (3.7) with source term $f = 0$ 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 (3.11) to get

$$\frac{1}{2}\,\|\bar{u}-\hat{u}\|_{H^{1,1/2}_{0;0,}(Q)} \leq \sup_{0\neq v\in H^{1,1/2}_{0;,0}(Q)} \frac{a(\bar{u}-\hat{u},v)}{\|v\|_{H^{1,1/2}_{0;,0}(Q)}}$$

$$= \sup_{0\neq v\in H^{1,1/2}_{0;,0}(Q)} \frac{a(\mathcal{E}_0(\hat{g}-g),v)}{\|v\|_{H^{1,1/2}_{0;,0}(Q)}} \leq c\,\|\mathcal{E}_0(\hat{g}-g)\|_{H^{1,1/2}_{;0,}(Q)}\,.$$

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 (7.6). □

Note, that for $w \in H^{1,1}_{\text{pw}}(\Sigma)$ we finally conclude the error estimate

$$\|u-\tilde{u}\|_{H^{1,1/2}_{;0,}(Q)} \leq c\,h^{5/4}\,\|w\|_{H^{1,1}_{\text{pw}}(\Sigma)}\,.$$

8 Numerical results

We consider the model problem (1.1) with source term $f = 0$, final time $T = 1$, and with the heat capacity constant $\alpha = 10$. We present examples for the 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. The Galerkin boundary element discretization of the variational formulation (5.9) is done by using piecewise constant basis functions $X_h = \text{span}\,\{\varphi_\ell\}_{\ell=1}^N$. The resulting system of linear equations $V_h\underline{w} = \underline{f}$ with

$$V_h[\ell,k] := \langle V\varphi_k,\varphi_\ell\rangle_\Sigma, \quad f[\ell] = \langle(\frac{1}{2}I+K)g - M_0u_0,\varphi_\ell\rangle_\Sigma \quad \text{for } \ell,k = 1,...,N,$$

is solved by using the GMRES method with a relative accuracy of 10^{-8} as stopping criteria.

8.1 One-dimensional problem

Let us start with the simple one-dimensional problem. We consider the spatial domain $\Omega = (0,1)$ and homogeneous Dirichlet conditions $g = 0$. 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 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. Moreover, the iteration numbers of the GMRES method are given.

L	N	$\|w - w_h\|_{L_2(\Sigma)}$	eoc	It.
5	64	$7.950 \cdot 10^{-2}$	1.01	31
6	128	$3.959 \cdot 10^{-2}$	1.01	41
7	256	$1.976 \cdot 10^{-2}$	1.00	50
8	512	$9.872 \cdot 10^{-3}$	1.00	59
9	1 024	$4.929 \cdot 10^{-3}$	1.00	70
10	2 048	$2.468 \cdot 10^{-3}$	1.00	82
11	4 096	$1.233 \cdot 10^{-3}$	1.00	96

Table 1: $L^2(\Sigma)$-error and convergence rate of the Galerkin approximation w_h, and iteration numbers of the GMRES method in the case of uniform refinement.

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 3. In Figure 4 the convergence history of the approximation for uniform and adaptive refinement is given.

8.2 Two-dimensional problem

For the following numerical examples we choose $\Omega = (0,1)^2$, i.e. $Q = (0,1)^3$.

Uniform refinement. We consider the exact solution

$$u(x,t) = \exp\left(-\frac{t}{\alpha}\right)\sin\left(x_1\cos\frac{\pi}{8} + x_2\sin\frac{\pi}{8}\right) \quad \text{for } (x,t) = (x_1,x_2,t) \in Q,$$

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

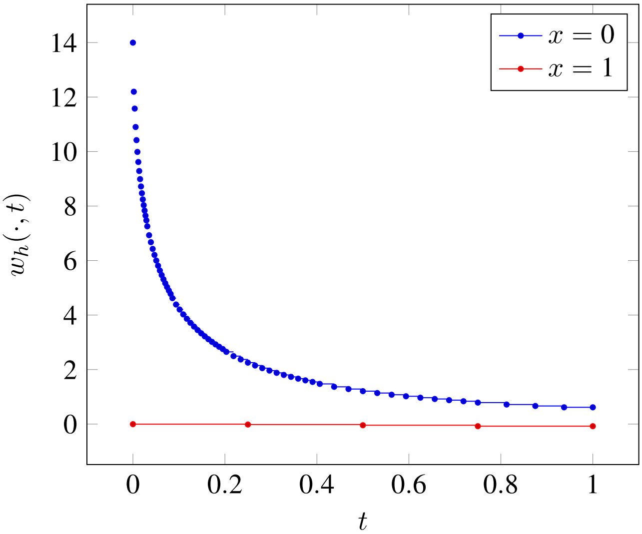


Figure 3: Galerkin approximation w_h in the case of adaptive refinement in 1D.

the tensor product approach as well as for a triangulation of the space-time boundary Σ. Table 2 and Table 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 (7.5), 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.

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 [5, 29], we get linear convergence of the approximation in the $L^2(\Sigma)$-norm in our experiments. Note that numerical results in [5, 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 5, 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 strategy. In Figure 7 the convergence history of the approximation for uniform and adaptive refinement is given, while the resulting boundary element mesh is shown in Figure 6.

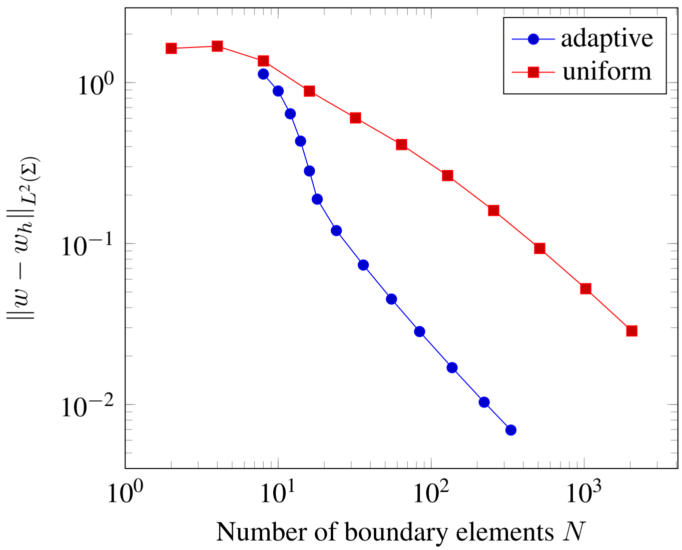


Figure 4: Convergence of the Galerkin approximation w_h for uniform and adaptive refinement in 1D.

9 Conclusion and outlook

In this work we have described space-time boundary element discretizations for the initial Dirichlet boundary value problem for the heat equation. After the derivation of the representation formula for the solution of the model problem (1.1) we summarised the mapping properties of the heat potentials and of the resulting boundary integral operators as well as we discussed the unique solvability of related boundary integral equations in the setting of anisotropic Sobolev spaces. The unknown Neumann datum $\partial_n u_{|\Sigma}$ can be determined by solving a weakly singular boundary integral equation. The ellipticity of the single layer operator ensures unique solvability of the problem. We compared two different space-time discretization techniques in order to compute an approximation of the Neumann datum $\partial_n u_{|\Sigma}$, 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. A parallel solver for space-time boundary element methods for the heat equation was introduced in [10]. 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, as we did. However, an arbitrary triangulation of the space-time boundary Σ allows for adaptive refinement in space and time

L	N	$\|w - w_h\|_{L_2(\Sigma)}$	eoc	$\|(u - \tilde{u})(x,t)\|$	eoc	It.
0	4	$2.795 \cdot 10^{-1}$	-	$2.5967 \cdot 10^{-2}$	-	2
1	16	$1.413 \cdot 10^{-1}$	0.98	$5.544 \cdot 10^{-3}$	2.23	9
2	64	$6.882 \cdot 10^{-2}$	1.04	$9.146 \cdot 10^{-4}$	2.60	14
3	256	$3.353 \cdot 10^{-2}$	1.04	$2.485 \cdot 10^{-4}$	1.88	18
4	1 024	$1.650 \cdot 10^{-2}$	1.02	$6.315 \cdot 10^{-5}$	1.98	24
5	4 096	$8.172 \cdot 10^{-3}$	1.01	$1.563 \cdot 10^{-5}$	2.01	35
6	16 384	$4.066 \cdot 10^{-3}$	1.01	$3.748 \cdot 10^{-6}$	2.06	50
7	65 536	$2.030 \cdot 10^{-3}$	1.00	$8.468 \cdot 10^{-7}$	2.15	67

Table 2: Error and convergence rates of the Galerkin approximation w_h and the approximated solution $\tilde{u}$ in the interior, and iteration numbers of the GMRES method in the case of uniform refinement for a tensor product decomposition of Σ.

L	N	$\|w - w_h\|_{L_2(\Sigma)}$	eoc	$\|(u - \widetilde{u})(x,t)\|$	eoc	It.
0	16	$1.588 \cdot 10^{-1}$	-	$2.046 \cdot 10^{-2}$	-	9
1	64	$6.326 \cdot 10^{-2}$	1.33	$5.395 \cdot 10^{-3}$	1.92	16
2	256	$2.502 \cdot 10^{-2}$	1.34	$1.337 \cdot 10^{-3}$	2.01	23
3	1 024	$1.084 \cdot 10^{-2}$	1.21	$3.336 \cdot 10^{-4}$	2.00	32
4	4 096	$5.040 \cdot 10^{-3}$	1.11	$8.348 \cdot 10^{-5}$	2.00	44
5	16 384	$2.447 \cdot 10^{-3}$	1.04	$2.093 \cdot 10^{-5}$	2.00	62
6	65 536	$1.233 \cdot 10^{-3}$	0.99	$5.265 \cdot 10^{-6}$	1.99	85

Table 3: Error and convergence rates of the Galerkin approximation w_h and the approximated solution $\tilde{u}$ in the interior, and iteration numbers of the GMRES method in the case of uniform refinement for a triangulation of Σ.

simultaneously while maintaining the admissibility of the mesh. We derived a priori error estimates for both discretization techniques and provided numerical experiments in order to confirm the theoretical findings.

In the numerical experiments we used the exact solution in order to compute the errors of the Galerkin approximation 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 [32] in 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.

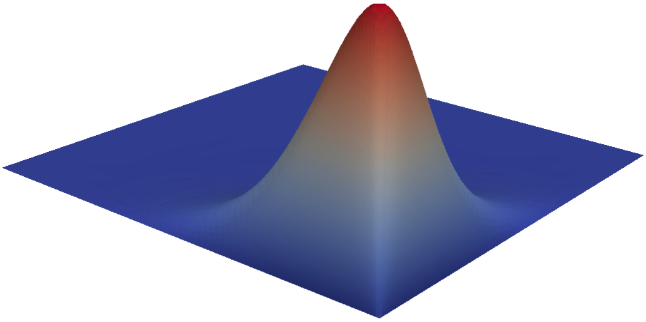


Figure 5: Initial datum u_0 for the 2D problem.

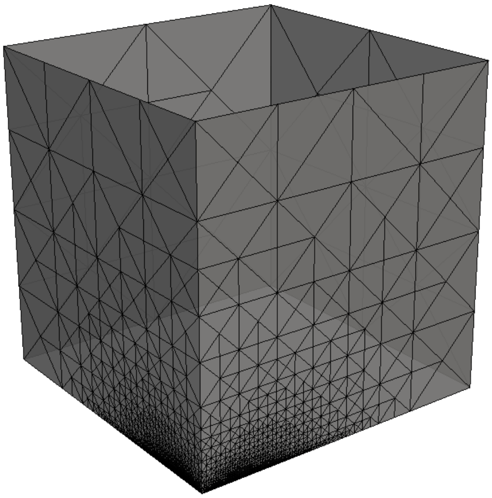


Figure 6: Triangular boundary element mesh in the case of adaptive refinement in 2D.

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 advantage of space-time discretization methods is the ability to use parallel iterative solution strategies for time-dependent problems. But 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

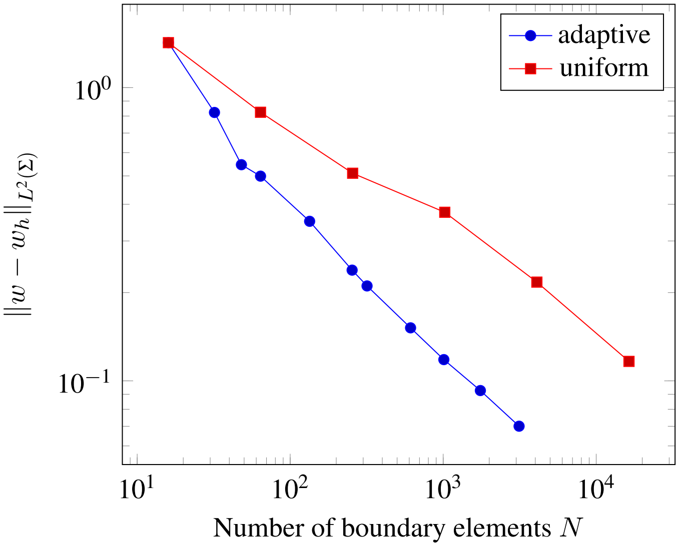


Figure 7: Convergence of the Galerkin approximation w_h for uniform and adaptive refinement in 2D.

element methods is operator preconditioning [17, 35], 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. In [8] we analyzed this robust preconditioning strategy for space-time boundary element methods for the heat equation and discussed suitable choices of boundary element spaces. The parallel solver introduced in [10] is also applicable to the preconditioned space-time system, see [7].

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 [37, 39]. The parabolic fast multipole method applied to a space-time Galerkin discretization is discussed in [26], 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 and the parabolic fast multipole method, to an arbitrary triangulation of Σ is still open and left for future work.

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 (3.10) in the setting of anisotropic Sobolev spaces allows us to establish symmetric and non-symmetric FEM-BEM coupling methods in an appropriate functional framework.

Bibliography

[1] W. Arendt and K. Urban, *Partielle Differenzialgleichungen*, Springer Spektrum, Heidelberg, 2010.

[2] D. N. Arnold and P. J. Noon, *Boundary integral equations of the first kind for the heat equation*, Boundary elements IX, Vol. 3 (Stuttgart, 1987), Comput. Mech., Southampton, 1987, pp. 213–229.

[3] ______, Coercivity of the single layer heat potential, *J. Comput. Math.* 7 (1989), 100–104.

[4] R. Chapko and R. Kress, Rothe's method for the heat equation and boundary integral equations, *J. Integral Equations Appl.* 9 (1997), 47–69.

[5] M. Costabel, Boundary integral operators for the heat equation, *Integral Equations Operator Theory* 13 (1990), 498–552.

[6] S. Dohr, *Space-time boundary element methods for the heat equation*, PhD Thesis, Graz University of Technology, to be submitted, 2019.

[7] 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).

[8] S. Dohr, K. Niino and O. Steinbach, Preconditioned space–time boundary element methods for the heat equation, *in preparation*.

[9] 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.*, Lect. Notes Comput. Sci. Eng. 125, Springer International Publishing, 2018.

[10] S. Dohr, J. Zapletal, G. Of, M. Merta and M. Kravcenko, A parallel space-time boundary element method for the heat equation, *submitted* (2018).

[11] A. Ern and J.L. Guermond, *Theory and Practice of Finite Elements*, Appl. Math. Sci., Springer New York, 2004.

[12] L. C. Evans, Partial Differential Equations, *Grad. Stud. Math.* 19 (1997).

[13] M. Fontes, Initial-Boundary Value Problems for Parabolic Equations, (2008).

[14] M.J. Gander and M. Neumüller, Analysis of a new space-time parallel multigrid algorithm for parabolic problems, *SIAM J. Sci. Comput.* 38 (2016), A2173–A2208.

[15] M. Hamina, *Some boundary element methods for heat conduction problems*, Thesis, University of Oulu, 2000.

[16] H. Harbrecht and J. Tausch, A fast sparse grid based space–time boundary element method for the nonstationary heat equation, *Numer. Math.* 140 (2018), 239–264.

[17] R. Hiptmair, Operator Preconditioning, *Comput. Math. Appl.* 52 (2006), 699–706.

[18] G. C. Hsiao and J. Saranen, Boundary integral solution of the two-dimensional heat equation, *Math. Methods Appl. Sci.* 16 (1993), 87–114.

[19] G.C. Hsiao and W.L. Wendland, *Boundary Integral Equations*, Appl. Math. Sci., Springer Berlin Heidelberg, 2008.

[20] S. Larsson and C. Schwab, Compressive Space-Time Galerkin Discretizations of Parabolic Partial Differential Equations, (2015).

[21] J. L. Lions and E. Magenes, *Non-Homogeneous Boundary Value Problems and Applications. Volume I*, Springer, Berlin-Heidelberg-New York, 1972.

[22] ______, *Non-Homogeneous Boundary Value Problems and Applications. Volume II*, Springer, Berlin-Heidelberg-New York, 1972.

[23] Ch. Lubich and R. Schneider, Time discretization of parabolic boundary integral equations, *Numer. Math.* 63 (1992), 455–481.

[24] W. McLean, *Strongly Elliptic Systems and Boundary Integral Equations*, Cambridge University Press, 2000.

[25] 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).

[26] M. Messner, M. Schanz and J. Tausch, A fast Galerkin method for parabolic space–time boundary integral equations, *J. Comput. Phys.* 258 (2014), 15–30.

[27] ______, An efficient Galerkin boundary element method for the transient heat equation, *SIAM J. Sci. Comput.* 37 (2015), A1554–A1576.

[28] M. Neumüller, Space-Time Methods, *Monographic Series TU Graz: Computation in Engineering and Science* 20 (2013).

[29] P.J. Noon, *The Single Layer Heat Potential and Galerkin Boundary Element Methods for the Heat Equation*, Thesis, University of Maryland, 1988.

[30] A. Piriou, Une classe d'opérateurs pseudo-différentiels du type de Volterra, *Ann. Inst. Fourier* 20 (1970), 77–94 (fr).

[31] ______, Problèmes aux limites généraux pour des opérateurs différentiels paraboliques dans un domaine borné, *Ann. Inst. Fourier* 21 (1971), 59–78 (fr).

[32] H. Schulz and O. Steinbach, A new a posteriori error estimator in adaptive direct boundary element methods: the Dirichlet problem, *Calcolo* 37 (2000), 79–96.

[33] O. Steinbach, *Numerical Approximation Methods for Elliptic Boundary Value Problems*, Springer, New York, 2008.

[34] ______, Space-Time Finite Element Methods for Parabolic Problems, *Comput. Methods Appl. Sci.* 15 (2015), 551–566.

[35] O. Steinbach and W. L. Wendland, The construction of some efficient preconditioners in the boundary element method, *Adv. Comput. Math.* 9 (1998), 191–216.

[36] O. Steinbach and M. Zank, Coercive space-time finite element methods for initial boundary value problems, *submitted* (2018).

[37] J. Tausch, A fast method for solving the heat equation by layer potentials, *J. Comput. Phys.* 224 (2007), 956–969.

[38] ______, Nyström discretization of parabolic boundary integral equations, *Appl. Numer. Math.* 59 (2009), 2843–2856.

[39] ———, Fast Nyström Methods for Parabolic Boundary Integral Equations, in: *Fast Boundary Element Methods in Engineering and Industrial Applications*, pp. 185–219, Springer Berlin Heidelberg, Berlin, Heidelberg, 2012.

[40] E. Zeidler, *Nonlinear Functional Analysis and its Applications II/ A: Linear Monotone Operators*, Springer, New York, 1990.

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