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Preprint Nr. 2005-08

Preprint-Serie des
Instituts für Numerische und Angewandte Mathematik
Lotzestr. 16-18
D - 37083 Göttingen

Numerische Mathematik manuscript No.
(will be inserted by the editor)

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the date of receipt and acceptance should be inserted later

Abstract This paper is concerned with a heat diffusion problem in a half-space which is motivated by the detection of material defects using thermal measurements. This problem is solved by inverting the Laplace transform with respect to time on a contour in the complex plane using an exponentially convergent quadrature rule. This leads to a finite number of time-independent problems, which can be solved in parallel using boundary integral equation methods. We provide a full numerical analysis of this scheme on compact time intervals. Our results are formulated in a way that they can easily be used for other diffusion problems in exterior or interior domains.

Keywords boundary element method, inverse Laplace transform, transmission problem, heat equation

Mathematics Subject Classification (2000) 65N38, 65M12, 44A10, 35K45

1 Introduction

Recently, a new method for the detection of material defects by thermal measurements has been investigated by [8, 15, 22]. This method consists in placing heat sources at the surface of a sample and measuring the temperature at

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the surface. We assume that the sample is described by the half-space

$$\mathbb{R}^d_- := \{(x_1, \ldots, x_d) : x_d < 0\}, \qquad d = 2, 3.$$

Some bounded part $\Omega_- \subset \mathbb{R}^d$ of the sample is occupied by a material with diffusivity $\kappa_- > 0$ (diffusivity equals conductivity divided by density and specific heat) which differs from the diffusivity $\kappa_+ > 0$ in the exterior domain $\Omega_+ := \mathbb{R}^d_- \setminus \Omega_-$. For a homogeneous material, i.e. $\Omega_- = \emptyset$, the heat sources at the boundary $H := \mathbb{R}^{d-1} \times \{0\}$ of the sample would give rise to a temperature distribution $u_{\rm hom}(\mathbf{x}, t)$ satisfying the heat equation $\partial_t u_{\rm hom} = \kappa_+ \Delta u_{\rm hom}$ in $\mathbb{R}^d_-$. In the presence of an inclusion at Ω_-, the temperature distribution is given by $u_{\rm hom} + u_+$ in the exterior and by u_- in interior domina where the fields u_+ and u_- satisfy the differential equations

$$\partial_t u_+ = \kappa_+ \Delta u_+, \qquad \text{in } \Omega_+ \times (0, \infty), \tag{1a}$$

$$\partial_t u_- = \kappa_- \Delta u_-, \qquad \text{in } \Omega_- \times (0, \infty). \tag{1b}$$

We will use the notation

$$u(\mathbf{x}, t) = \begin{cases} u_+(\mathbf{x}, t) & \text{in } \Omega_+ \times (0, \infty), \\ u_-(\mathbf{x}, t), & \text{in } \Omega_- \times (0, \infty). \end{cases}$$

Let Γ denote the boundary of the inclusion Ω_- and ν the unit normal vector on Γ pointing to the exterior of Ω_-. The heat flux $\partial_\nu u_-$ through the boundary Γ is proportional to the difference of the inside temperature $u_-|_\Gamma$ and the outside temperature $u_+|_\Gamma + u_{\rm hom}|_\Gamma$,

$$u_+ + u_{\rm hom} = u_- + f \partial_\nu u_- \qquad \text{on } \Gamma \times (0, \infty). \tag{1c}$$

The proportionality constant $f(\mathbf{x})$, $\mathbf{x} \in \Gamma$ depends on the level of corrosion between the two materials and is the unknown for the inverse problem. This kind of transmission condition is often referred to as an Engquist–Nédélec condition. Moreover, we have the boundary condition

$$\partial_\nu u_+ + \partial_\nu u_{\rm hom} = \alpha\, \partial_\nu u_- \qquad \text{on } \Gamma \times (0, \infty) \tag{1d}$$

with a known parameter $\alpha > 0$, equalling the ratio of interior and exterior conductivities. We assume an adiabatic condition on the top boundary, i.e. all the heat transfer between the exterior and the material is that produced by the heat source. This amounts to

$$\partial_\nu u_+|_H = 0. \tag{1e}$$

Finally, we assume that the initial temperature is zero,

$$u_+(\,\cdot\,, 0) = 0, \qquad u_-(\,\cdot\,, 0) = 0. \tag{1f}$$

The final aim will be to solve the inverse problem of reconstructing the corrosion function $f : \Gamma \to \mathbb{R}$ from measurements of the temperature $u_+|_H$ at the boundary of the sample. As a first step of independent interest we study here the numerical solution of the forward problem.

Since we are dealing with a boundary value problem in an unbounded domain, boundary integral equation methods are an attractive choice for the numerical solution. Several approaches have been discussed in the literature: One possibility is to use a space-time boundary integral formulation of the problem involving a convolution integral in time with the fundamental solution to the heat equation as kernel (see e.g. Costabel [6], Hsiao & Saranen [9], Kress [10, Ch. 9] and Bamberger & Ha Duong [2,3] for a similar approach for the wave equation). Lubich & Schneider [13] suggested operational quadrature methods to solve the resulting Volterrà–Fredholm integral equations of convolution type. Using linear multistep methods they arrive at a sequence of boundary integral equations involving Laplace transforms of the fundamental solution to the heat equation as kernels. A similar algorithm has been derived by Chapko & Kress [4] starting from a semidiscretization in time based on the implicit Euler method. All these methods need to keep record of all previous time steps to compute the solution at each new time value. We will study a different approach, which has been investigated for finite element methods by Sheen, Sloan & Thomée [19,20]. Compared to time-stepping schemes it has the following advantages: The convergence is exponential instead of polynomial with the number of time-independent boundary value problems, and all boundary value problems can be solved in parallel. As a disadvantage of our method we point out that we only obtain estimates on compact time intervals $[t_0, T] \subset (0, \infty)$ which deteriorate as $T/t_0 \to \infty$.

Our approach is as follows: Let

$$U(\mathbf{x}, s) := \int_0^\infty e^{-st} u(\mathbf{x}, t)\, dt, \qquad \operatorname{Re} s > 0,\, \mathbf{x} \in \Omega_+ \cup \Omega_- \tag{2}$$

denote the Laplace transform of the solution with respect to time. It satisfies the differential equation $(s - \kappa_\pm \Delta) U(\,\cdot\,, s) = 0$ in $\Omega_\pm$ and boundary conditions analogous to (1c)-(1e) (see section 2). This independent characterization of $U(\,\cdot\,, s)$ can be used to define and compute $U(\,\cdot\,, s)$ for all $s \in \mathbb{C} \setminus (-\infty, 0]$. The time dependent solution can be recovered from its Laplace transform by the formula

$$u(\mathbf{x}, t) = \frac{1}{2\pi\imath} \int_{\mathcal{C}} e^{st} U(\mathbf{x}, s)\, ds, \qquad t > 0 \tag{3}$$

where $\mathcal{C}$ is any path connecting $-i\infty$ to $i\infty$. Since $U(\mathbf{x}, s)$ depends holomorphically on s, we have a lot of freedom in the choice of the contour $\mathcal{C}$. The integral in (3) is approximated for some suitable choice of $\mathcal{C}$ by a quadrature rule suggested recently by López-Fernández & Palencia [12]

$$u(\mathbf{x}, t) \approx \sum_{j=-N}^{N} \gamma_j^{(N)} e^{s_j^{(N)} t} U(\mathbf{x}, s_j^{(N)}), \tag{4}$$

which is exponentially convergent as $N \to \infty$ for $0 < t_0 \le t \le T < \infty$. For each quadrature point $s_j^{(N)} \in \mathcal{C}$ we have to evaluate $U(\mathbf{x}, s_j^{(N)})$ by solving a time-independent boundary value problem. This will be done by a boundary integral equation method using Galerkin approximations.

In the context of the inverse problem to recover f from $u(\,\cdot\,,t)|_H$, it is sufficient to consider a compact time interval $[t_0,T]$ since all practical measurements are time-limited and since $u(\mathbf{x},t)$ is almost zero for small t and carries no information about f.

We provide a full numerical analysis of this discretization scheme both in full space and on the top barrier H. The main difficulty in this analysis is to obtain error estimates for the boundary integral equation method which are explicit in s. The problem under investigation contains all typical difficulties, and our results are formulated in a way that they can easily be applied to other parabolic evolution problems.

Notations Throughout the work, $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^d$ or $\mathbb{C}^d$ for $d \geq 1$. We will make extensive use of the classical Sobolev spaces $H^r(\Omega)$ for any open set Ω with $r \geq 0$. Its norm will be denoted $\|\cdot\|_{r,\Omega}$. Also, for a smooth closed curve or surface Γ we will use the Sobolev spaces $H^r(\Gamma)$ for $r \in \mathbb{R}$, with norm denoted $\|\cdot\|_{r,\Gamma}$. See [14] for a detailed introduction to these and for properties relevant to our work.

In the sequel we will denote P_k to a polynomial of degree k or less with coefficients independent on the functions it is multiplied by, possibly different in each occurrence. In the final section the Landau O notation will be used in the standard form.

2 Boundary integral equations in the Laplace domain

2.1 Boundary value problems in the Laplace domain

Let Ω^- be a bounded open set strictly included in the half–space $\mathbb{R}^d_-$ with connected smooth boundary Γ, and denote the corresponding exterior domain by $\Omega^+ := \mathbb{R}^d_- \setminus \overline{\Omega_-}$. We will systematically identify

$$u \in L^2(\mathbb{R}^d_-) \cong L^2(\Omega^-) \times L^2(\Omega^+) \ni (u_-, u_+).$$

We introduce the differential operator

$$\Delta_\pm u := \begin{cases} \kappa_- \Delta u_-, \text{ in } \Omega^-, \\ \kappa_+ \Delta u_+, \text{ in } \Omega^+ \end{cases} \tag{5}$$

with the constants $\kappa_+, \kappa_- > 0$ and the boundary operator

$$\mathcal{B}u := (u_-|_\Gamma + f\,\partial_\nu u_-|_\Gamma - u_+|_\Gamma, \alpha\,\partial_\nu u_-|_\Gamma - \partial_\nu u_+|_\Gamma)^\top$$

with the constant $\alpha > 0$ and the function $f \in \mathcal{C}^\infty(\Gamma)$ satisfying

$$f(\,\cdot\,) \geq f_0 > 0. \tag{6}$$

Here ∂_ν denotes the normal derivative, be it from inside or outside Γ with the normal always pointing exterior to Ω_-. Finally, we write

$$\Pi u := \partial_\nu u|_H.$$

The exterior heating from points on H is described by functions u_{hom} of the general form

$$u_{\mathrm{hom}}(\mathbf{x},t) = t^{-\beta/2}\exp(-m(\mathbf{x})/t), \qquad \mathbf{x}\in\mathbb{R}^d_-, t>0 \tag{7a}$$

where

$$\beta\in\mathbb{N}, \quad \text{and} \quad m\in C^\infty(\mathbb{R}^d_-) \quad \text{with} \quad m(\mathbf{x})>0 \text{ for all } \mathbf{x}\in\mathbb{R}^d_-. \tag{7b}$$

It is assumed that $\kappa_+\Delta u_{\mathrm{hom}} = \partial_t u_{\mathrm{hom}}$ is satisfied for all $t\geq 0$. Examples include point sources at a point $\mathbf{y}\in\mathbb{R}^d$, $y_d\geq 0$ (here $\beta=d$ and $m(\mathbf{x}) = |\mathbf{x}-\mathbf{y}|^2/(4\kappa_+)$) and line sources (e.g. $\beta=1$ and $m(\mathbf{x}) = x_2^2/(4\kappa_+)$ for $d=2$). As discussed in Remark 11, everything below remains valid for superpositions of fields of the form (7).

With these notations the problem we want to solve is to find $u:\mathbb{R}^d_-\times(0,\infty)\to\mathbb{R}$ such that

$$\begin{aligned}
&\partial_t u = \Delta_\pm u,\\
&u(\,\cdot\,,0) = 0,\\
&u(\,\cdot\,,t)\in H^2(\Omega^-\cup\Omega^+), \qquad t\geq 0\\
&\Pi u = 0, \qquad \mathcal{B}u = (u_{\mathrm{hom}}|_\Gamma, \partial_\nu u_{\mathrm{hom}}|_\Gamma)^\top, \qquad t\geq 0.
\end{aligned} \tag{8}$$

Precise interpretations of the regularity needed to understand time derivatives and the initial condition will be given in section 4.

Taking formally the Laplace transform in time in this equation, we find by partial integration that the functions

$$U(\mathbf{x},s) := \int_0^\infty e^{-s\,t}u(\mathbf{x},t)\,\mathrm{d}t, \qquad U_{\mathrm{hom}}(\mathbf{x},s) := \int_0^\infty e^{-s\,t}u_{\mathrm{hom}}(\mathbf{x},t)\,\mathrm{d}t \tag{9}$$

defined for $\operatorname{Re} s>0$ satisfy the boundary value problem

$$\begin{aligned}
&\Delta_\pm U - s\,U = 0,\\
&U(\,\cdot\,,s)\in H^2(\Omega^-\cup\Omega^+),\\
&\Pi U(\,\cdot\,,s) = 0, \qquad \mathcal{B}U(\,\cdot\,,s) = \boldsymbol{g}(s).
\end{aligned} \tag{10}$$

for $U(\,\cdot\,,s)$ with boundary data $\mathbf{g}(s) := (U_{\mathrm{hom}}(\,\cdot\,,s), \partial_\nu U_{\mathrm{hom}}(\,\cdot\,,s))^\top$. We will give a rigorous derivation of these equations for all $s\in\mathbb{C}\setminus(-\infty,0]$ in section 5. The second condition in (10) can be seen as a "boundary condition" at infinity, requiring sufficient decay of the solution. For $s\in(-\infty,0)$ it would have to be replaced by a Sommerfeld radiation condition, but we will not consider this case here.

2.2 Some integral operators and potentials

Consider the fundamental solution to the Helmholtz equation $\Delta + \rho^2$

$$\Phi_\rho(\mathbf{x},\mathbf{y}) := \begin{cases} \frac{\imath}{4} H_0^{(1)}(\rho|\mathbf{x}-\mathbf{y}|), \text{ when } d=2, \\ \dfrac{\exp(\imath\,\rho\,|\mathbf{x}-\mathbf{y}|)}{4\pi\,|\mathbf{x}-\mathbf{y}|}, \text{ when } d=3, \end{cases}$$

where $H_0^{(1)}$ is the Hankel function of the first kind and order zero. The single layer potential associates a density ψ to

$$\mathcal{S}_\rho\psi := \int_\Gamma \Phi_\rho(\,\cdot\,,\mathbf{y})\,\psi(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}) \,:\, \mathbb{R}^d \to \mathbb{C}. \tag{11}$$

We consider the integral operators:

$$V_\rho\psi := \int_\Gamma \Phi_\rho(\,\cdot\,,\mathbf{y})\,\psi(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}) \,:\, \Gamma \to \mathbb{C}, \tag{12}$$

$$J_\rho\psi := \int_\Gamma \frac{\partial\Phi_\rho(\,\cdot\,,\mathbf{y})}{\partial\nu(\,\cdot\,)}\,\psi(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}) \,:\, \Gamma \to \mathbb{C}. \tag{13}$$

Given $\mathbf{x} \in \mathbb{R}^d$ we denote by $\widetilde{\mathbf{x}}$ the point reflected from $\mathbf{x}$ with respect to H, i.e., in three space dimensions

$$\mathbf{x} = (x_1, x_2, x_3) \qquad \longmapsto \qquad \widetilde{\mathbf{x}} = (x_1, x_2, -x_3)$$

and similarly in two dimensions. Then we consider the reflected fundamental solution

$$\widetilde{\Phi}_\rho(\mathbf{x},\mathbf{y}) := \Phi_\rho(\mathbf{x},\mathbf{y}) + \Phi_\rho(\mathbf{x},\widetilde{\mathbf{y}}).$$

With this we define the corresponding single layer potential $\widetilde{\mathcal{S}}_\rho$ and the integral operators $\widetilde{V}_\rho$ and $\widetilde{J}_\rho$ by writing $\widetilde{\Phi}$ instead of Φ in eq. (11)-(13). Notice that we always have $\Pi\widetilde{\mathcal{S}}_\rho\psi = 0$.

Given two values $\mu, \lambda \in \mathbb{C}$ we consider the matrix of boundary integral operators

$$\mathcal{W}_{\mu,\lambda} := \begin{bmatrix} f\,(\frac{1}{2}I + J_\mu) + V_\mu & -\widetilde{V}_\lambda \\ \alpha(\frac{1}{2}I + J_\mu) & \frac{1}{2}I - \widetilde{J}_\lambda \end{bmatrix}$$

and also

$$\mathcal{W}_0 := \begin{bmatrix} \frac{1}{2}f & 0 \\ \frac{\alpha}{2}\,I & \frac{1}{2}\,I \end{bmatrix}. \tag{14}$$

The space $\mathbb{H}^r(\Gamma) := H^r(\Gamma) \times H^r(\Gamma)$ will be equipped with the sum of the inner products in $H^r(\Gamma)$ as inner product. Since the parameter α is fixed throughout, we will not make dependence on it apparent in any definition.

Theorem 1 *For all* $r \in \mathbb{R}$, $\mathcal{W}_{\mu,\lambda} : \mathbb{H}^r(\Gamma) \to \mathbb{H}^r(\Gamma)$ *is bounded. Moreover,* $\mathcal{W}_{\mu,\lambda} - \mathcal{W}_0$ *is compact. Therefore* $\mathcal{W}_{\mu,\lambda}$ *is Fredholm of index zero.*

Proof Boundedness and compactness follow from well–known properties of boundary integral operators (see [5] or [14] for instance). Due to the assumption (6), the operator $\mathcal{W}_0$ is boundedly invertible, and this implies that $\mathcal{W}_{\mu,\lambda}$ is Fredholm of index 0. □

Theorem 2 *Assume that* $\lambda^2, \mu^2 \notin [0,\infty)$ *and take* $(g_0, g_1) \in \mathbb{H}^{k-1/2}(\Gamma)$ *with* $k \in \{0,1\}$. *Then*

$$\begin{aligned} & w \in H^{k+1}(\Omega^- \cup \Omega^+), \\ & \Delta w_- + \mu^2 w_- = 0, \qquad \text{in } \Omega^- \\ & \Delta w_+ + \lambda^2 w_+ = 0, \qquad \text{in } \Omega^+ \\ & \Pi w = 0, \qquad \mathcal{B} w = (g_0, g_1)^\top \end{aligned} \tag{15}$$

if and only if

$$\begin{aligned} w_- &= \mathcal{S}_\mu \psi_-, \\ w_+ &= \widetilde{\mathcal{S}}_\lambda \psi_+, \end{aligned} \qquad \text{with} \qquad \mathcal{W}_{\mu,\lambda} \begin{bmatrix} \psi_- \\ \psi_+ \end{bmatrix} = \begin{bmatrix} g_0 \\ g_1 \end{bmatrix}. \tag{16}$$

Proof Potentials as given in (16) solve (15) as a consequence of the jump relations of the single layer potential and of the behaviour at infinity of potentials. Notice that the hypothesis on λ and μ guarantees that $w \in H^{k+1}(\Omega^- \cup \Omega^+)$.

Solutions of the Helmholtz equation can we written as single–layer potentials (with the reflected fundamental solution in the exterior part to ensure the condition $\Pi w = 0$) for all non–resonant cases, i.e., except when $-\lambda^2$ and $-\mu^2$ are Dirichlet eigenvalues of the Laplacian in Ω^-. With the conditions we have imposed on these parameters in the hypotheses we avoid these singular cases. □

Theorem 3 $\mathcal{W}_{\mu,\lambda}$ *is invertible if and only if Problem* (15) *with* $(g_0, g_1) \equiv 0$ *only admits the trivial solution. In particular, when* $\lambda^2, \mu^2 \notin [0,\infty)$ *and* $\lambda/\mu \in \mathbb{R}$, *there is uniqueness of solution to* (15).

Proof The first part of the statement is a simple consequence of the fact that $\mathcal{W}_{\mu,\lambda}$ is Fredholm of index zero (Theorem 1) and of Theorem 2. To prove uniqueness we just have to: (a) apply a simple reflection argument to study a transmission problem in the whole of $\mathbb{R}^d$ (see [18, Proposition 2.1]); (b) use the same kind of arguments as those given in [11]. □

2.3 Boundary integral formulation in the Laplace domain

Once we have the single–layer potentials and boundary integral operators, Theorem 2 allows us to write each transmission problem (10) as an equivalent system of boundary integral equations.

Let

$$\mathcal{P}(s) := \begin{bmatrix} \mathcal{S}_{\mu(s)} & 0 \\ 0 & \widetilde{\mathcal{S}}_{\lambda(s)} \end{bmatrix}, \qquad \mu(s)^2 = -s/\kappa_-, \qquad \lambda(s)^2 = -s/\kappa_+$$

and

$$\mathcal{W}(s) := \mathcal{B}\mathcal{P}(s) = \mathcal{W}_{\mu(s),\lambda(s)}.$$

For simplicity we will write

$$\mathcal{P}_1 := \mathcal{P}(1), \qquad \mathcal{W}_1 := \mathcal{W}(1),$$

which are related to the differential operator $\Delta_\pm - I$ in $\Omega^- \cup \Omega^+$. Let

$$\mathcal{U} := \mathbb{C} \setminus (-\infty, 0], \tag{17}$$

let $\mathcal{L}(X,Y)$ denote the space of bounded linear operators between two Banach spaces X and Y, and $\mathcal{L}(X) := \mathcal{L}(X,X)$.

Theorem 4 *For all $r \in \mathbb{R}$ and all $s \in \mathcal{U}$ the inverse $\mathcal{W}(s)^{-1}$ is well-defined, and $\mathcal{W}(s), \mathcal{W}(s)^{-1}$ belong to $\mathcal{L}(\mathbb{H}^r(\Gamma))$. Moreover, the operator $\mathcal{P}(s)$ belongs to $\mathcal{L}(\mathbb{H}^r(\Gamma), H^{r+3/2}(\Omega^- \cup \Omega^+))$ for all $r > -1$ and $s \in \mathcal{U}$.*

Proof The statement for $\mathcal{W}(s)$ is a particular case of Theorem 1. The statement for $\mathcal{W}(s)^{-1}$ is a consequence of Theorem 3 and the Fredholmness of $\mathcal{W}(s)$. The last statement follows from regularity theorems for elliptic equations on domains with smooth boundaries, from the boundedness of $\mathcal{W}(s)$, and from behaviour at infinity of single–layer potentials. □

Hence, for all $s \in \mathcal{U}$ we can solve (10) by solving the boundary integral system

$$\mathcal{W}(s)\boldsymbol{\psi}(\,\cdot\,, s) = \boldsymbol{g}(\,\cdot\,, s),$$

and then writing $U(\,\cdot\,, s) = \mathcal{P}(s)\boldsymbol{\psi}(\,\cdot\,, s)$.

3 Numerical approximation

We will now describe out method to solve the parabolic problem (8) With a slight abuse of notation we will write $u(t) = u(\,\cdot\,, t)$ where u is now considered as a mapping

$$u : [0,\infty) \to X, \qquad X := H^k(\Omega_+ \cup \Omega_-), \qquad k = 0, 1, 2, \ldots.$$

If u is bounded, its Laplace transform $U(s) := \int_0^\infty e^{-st} u(t)\, dt$ is well defined for $\operatorname{Re} s > 0$. By the Fourier inversion theorem, u can be recovered from U by the formula $u(t) = \frac{1}{\pi} \int_{-i\infty+1}^{i\infty+1} e^{st} U(s)\, ds$. We will show in section 5 that U admits a holomorphic extension

$$U : \mathcal{U} \to X$$

(recall the definition of $\mathcal{U}$ in (17)) and that there exists a constants $M > 0$ and $\delta \in (0, \frac{\pi}{2})$ such that

$$\|U(s)\|_X \leq \frac{M}{|s|} \qquad \text{for all } s \in \mathbb{C} \text{ s.t. } |s| \geq 1,\ |\arg(-s)| \geq \delta. \tag{18}$$

Under these assumptions the integration path can be deformed to a contour which asymptotically forms an acute angle with the negative real axis or is even parallel to the negative real axis (see [16]). López-Fernández and Palencia [12] suggested to use the hyperbola parameterized by

$$\gamma(\omega) = \lambda(1 - \sin(\alpha + \imath\omega)), \qquad \omega \in \mathbb{R} \tag{19}$$

where $\lambda > 0$ and $0 < \alpha < \pi/2$ are geometrical parameters. This leads to the formula

$$u(t) = -\frac{1}{2\pi\imath} \int_{-\infty}^{\infty} e^{t\gamma(\omega)} U(\gamma(\omega))\gamma'(\omega)\, d\omega,$$

(cf. (3)) which is approximated by the trapezoidal rule

$$(T_N U)(t) := \frac{h_N}{2\pi\imath} \sum_{j=-N}^{N} e^{t\gamma(\omega_j^{(N)})} U(\gamma(\omega_j^{(N)}))\gamma'(\omega_j^{(N)}) \tag{20}$$

with step size $h_N := \ln N/N$ and quadrature points $\omega_j^{(N)} := h_N j$. This may alternatively be written in the form (4) with the quadrature points $s_j^{(N)} := \gamma(\omega_j^{(N)})$ and the quadrature weights $\gamma_j^{(N)} := h_N \gamma'(\omega_j^{(N)})$. They established an error bound of the form

$$\|u(t) - (T_N U)(t)\|_X = O(e^{-cN/\ln N}), \qquad N \to \infty \tag{21}$$

uniformly for $t \in [t_0, T] \subset (0, \infty)$ with explicit constants, which can be used to tune the parameters λ and α in (19). This improves error bounds by Talbot [21] of the form $O(e^{-c\sqrt{N}})$ (although it is not quite clear if his proof is valid for the present situation) and super-algebraic error bounds by Sheen, Sloan & Thomée [20] involving derivatives of U.

We will compute $U_h(s_j^{(N)}) \approx U(s_j^{(N)})$ by a boundary integral equation method using a Galerkin approximation with grid size parameter h. The following lemma provides a bound for the effect of the space discretization error on the solution in the time domain:

Lemma 5 *There exists a constant C_t, which is uniformly bounded for t in compact subintervals of $(0, \infty)$ such that*

$$\|(T_N E)(t)\|_X \leq C_t \sup_{j=-N,\ldots,N} \|E(s_j^{(N)})\|_X \tag{22}$$

for all $N \in \mathbb{N}$ and all (not necessarily holomorphic) functions $E : \mathcal{T} \to X$.

Proof Since $\operatorname{Re}\gamma(\omega) = \lambda - \lambda \sin\alpha \cosh\omega$ and $|\gamma'(\omega)| = \lambda|\cos(\alpha + \imath\omega)| \leq \lambda \cosh(\omega)$, we have

$$\|(T_N E)(t)\|_X \leq \frac{h_N}{2\pi} \sum_{j=-N}^{N} \left| e^{t\gamma(\omega_j^{(N)})} \gamma'(\omega_j^{(N)}) \right| \sup_{j=-N,\dots,N} \|E(s_j^{(N)})\|_X$$
$$\leq \frac{h_N}{2\pi} \lambda e^{\lambda t} \sum_{j=-N}^{N} e^{-(\lambda t \sin\alpha)\cosh(\omega_j^{(N)})} \cosh(\omega_j^{(N)}) \sup_{j=-N,\dots,N} \|E(s_j^{(N)})\|_X .$$

Interpreting the sum as a Riemann sum and using the fast decay of the integrand, we obtain

$$h_N \sum_{j=-N}^{N} e^{-\tau \cosh(\omega_j^{(N)})} \cosh(\omega_j^{(N)}) \leq h_N \sum_{j=-\infty}^{\infty} e^{-\tau \cosh(\omega_j^{(N)})} \cosh(\omega_j^{(N)})$$
$$\overset{N\to\infty}{\to} \int_{-\infty}^{\infty} e^{-\tau \cosh(\omega)} \cosh(\omega)\, \mathrm{d}\omega = \int_{-\infty}^{\infty} e^{-\tau\sqrt{1+u^2}}\, \mathrm{d}u < \infty$$

with $\tau := \lambda t \sin\alpha$ using the substitution $u = \sinh\omega$. This implies the assertion. □

Corollary 6 *For all compact intervals $[t_0, T] \subset (0, \infty)$ there exist constants C_1 and C_2 such that the total error is bounded by*

$$\|u(t) - (T_N U_h)(t)\|_X \leq C_1 e^{-cN/\ln N} + C_2 \sup_{j=-N,\dots,N} \|U(s_j^{(N)}) - U_h(s_j^{(N)})\|_X \tag{23}$$

for $t \in [t_0, T]$.

Proof As $\|u(t) - (T_N U_h)(t)\|_X \leq \|u(t) - (T_N U)(t)\|_X + \|(T_N(U - U_h))(t)\|_X$, this follows from (21) and (22). □

In order to estimate the second term in (23), we have to derive bounds on the space discretization error which are explicit with respect to s.

4 Operator form of the parabolic equation

In $L^2(\mathbb{R}^d_-) \cong L^2(\Omega^-) \times L^2(\Omega^+)$ we consider the inner product

$$\langle u, v \rangle := \int_{\Omega_-} (\alpha/\kappa_-) u_- \overline{v}_- + \int_{\Omega_+} (1/\kappa_+) u_+ \overline{v}_+$$

and write $\|u\| := \langle u, u\rangle^{1/2}$. This norm, which is equivalent to the usual one in $L^2(\mathbb{R}^d_-)$, is denoted by $\|\cdot\|_{0,\Omega^-\cup\Omega^+}$. Moreover, we introduce the operator $\mathcal{A} := \Delta_\pm$ defined on the domain

$$D(\mathcal{A}) := \{u \in H^2(\Omega^- \cup \Omega^+) \,|\, \Pi u = 0, \quad \mathcal{B}u = 0\}.$$

Proposition 7 *For all $u, v \in D(\mathcal{A})$*

$$\langle \mathcal{A}u, v\rangle = \langle u, \mathcal{A}v\rangle \qquad \textit{and} \qquad \langle \mathcal{A}u, u\rangle \le 0.$$

Proof Applying Green's formula (it is straightforward to verify that we can apply it in the exterior domain) we obtain

$$\begin{aligned}
\langle \mathcal{A}u, v\rangle &= \int_{\Omega_-} \alpha\, \Delta u_- \,\overline{v}_- + \int_{\Omega_+} \Delta u_+ \,\overline{v}_+ \\
&= -\int_{\Omega_-} \alpha \nabla u_- \cdot \nabla \overline{v}_- + \int_{\Gamma} \alpha\, \partial_\nu u_-|_\Gamma \,\overline{v}_-|_\Gamma \\
&\quad - \int_{\Omega_+} \nabla u_+ \cdot \nabla \overline{v}_+ - \int_{\Gamma} \partial_\nu u_+|_\Gamma \,\overline{v}_+|_\Gamma \\
&= -\int_{\Omega_-} \alpha\, \nabla u_- \cdot \nabla \overline{v}_- - \int_{\Omega_+} \nabla u_+ \cdot \nabla \overline{v}_+ - \int_{\Gamma} (f/\alpha)\, \partial_\nu u_+|_\Gamma \partial_\nu \,\overline{v}_+|_\Gamma .
\end{aligned}$$

The result is then straightforward. □

Proposition 8 *The operator $\mathcal{I} - \mathcal{A} : D(\mathcal{A}) \to L^2(\mathbb{R}^d_-)$ is onto.*

Proof Let $f \in L^2(\mathbb{R}^d_-)$. As a first step we construct $w \in H^2(\Omega^- \cup \Omega^+)$ satisfying

$$\Delta_\pm w - w = f, \qquad \Pi w = 0.$$

To find w_+ we define $\widetilde{f}_+$ by extending f_+ to zero in Ω_- and to the upper part of the space by reflection, i.e., demanding that $\widetilde{f}_+(\widetilde{\mathbf{x}}) = \widetilde{f}_+(\mathbf{x})$. Then there exists a unique $w_+ \in H^2(\mathbb{R}^d)$ such that $-\kappa_+ \Delta_+ w_+ + w_+ = \widetilde{f}_+$ in $\mathbb{R}^d$. This function satisfies $\partial_\nu w_+|_H = 0$ by symmetry. A function $w_- \in H^2(\Omega_-)$ satisfying $-\kappa_- \Delta_- w_- + w_- = f_-$ can be constructed similarly.

As a second step we define

$$v := \mathcal{P}_1 \boldsymbol{\psi}, \qquad \text{where} \quad \mathcal{W}_1 \boldsymbol{\psi} = -\mathcal{B}w.$$

Since $w \in H^2(\Omega^- \cup \Omega^+)$, then $\mathcal{B}w \in \mathbb{H}^{1/2}(\Gamma)$ and therefore $\boldsymbol{\psi} \in \mathbb{H}^{1/2}(\Gamma)$. Hence $v \in H^2(\Omega^- \cup \Omega^+)$. Finally $u := w + v \in D(\mathcal{A})$ satisfies $u - \mathcal{A}u = f$. □

By Propositions 7 and 8, $\mathcal{A}$ is symmetric and maximally dissipative. Therefore, $\mathcal{A}$ is self–adjoint and is the infinitesimal generator of a contractive semigroup (see [16, Chapter 1]). Moreover $(s\mathcal{I} - \mathcal{A})^{-1}$ exists for all $s \in \mathcal{U}$. If we define

$$\delta(s) := \operatorname{dist}(s, (-\infty, 0]) = \begin{cases} |s|, & \text{if Re } s \ge 0, \\ \text{Im} s, & \text{if Re } s < 0, \end{cases}$$

then (see [16, Chapter 1, Theorem 3.9])

$$\|(s\mathcal{I} - \mathcal{A})^{-1} f\| \le \frac{1}{\delta(s)} \|f\|, \qquad \forall f \in L^2(\mathbb{R}^d_-). \tag{24}$$

Proposition 9 *There exists a polynomial P_1 of degree 1 such that*

$$\|(s\mathcal{I}-\mathcal{A})^{-1}f\|_{2,\Omega^-\cup\Omega^+} \le \frac{P_1(|s|)}{\delta(s)}\,\|f\| \qquad \text{for all } f\in L^2(\mathbb{R}^d_-).$$

Proof The space $D(\mathcal{A})$ is closed with respect to the norm of $H^2(\Omega^-\cup\Omega^+)$. Since $\mathcal{I}-\mathcal{A}: D(\mathcal{A})\to L^2(\mathbb{R}^d_-)$ is bounded (with respect to the norm in $D(\mathcal{A})$) and invertible, it has a bounded inverse, so

$$\|(\mathcal{I}-\mathcal{A})^{-1}f\|_{2,\Omega^-\cup\Omega^+} \le C\|f\| \qquad \text{for all } f\in L^2(\mathbb{R}^d_-). \tag{25}$$

Finally, $(s\mathcal{I}-\mathcal{A})u=f$ if and only if

$$u=(\mathcal{I}-\mathcal{A})^{-1}(f+(1-s)\,u)$$

and therefore (24), (25) prove the result. □

We now formalise the parabolic problem (8) using these elements. We decompose

$$u=v+w \tag{26}$$

where $v:[0,\infty)\to L^2(\mathbb{R}^d_-)$ given below and $w:[0,\infty)\to D(\mathcal{A})\subset L^2(\mathbb{R}^d_-)$ solves the non–homogeneous Cauchy problem

$$\begin{aligned} w' &= \mathcal{A}w+g,\\ w(0)&=0, \end{aligned} \tag{27}$$

with

$$g(t):=v(t)-v'(t). \tag{28}$$

The function $v:[0,\infty)\to L^2(\mathbb{R}^d_-)$ is defined for each value of t as the solution to the steady–state problem

$$\begin{aligned} &\Delta_\pm v(t)-v(t)=0,\\ &v(t)\in H^2(\Omega^-\cup\Omega^+),\\ &\Pi v(t)=0, \qquad \mathcal{B}v(t)=(u_{\mathrm{hom}}|_\Gamma,\partial_\nu u_{\mathrm{hom}}|_\Gamma)^\top. \end{aligned} \tag{29}$$

This function serves to homogenize the boundary conditions and is used only for theoretical purposes: the decomposition (26) will not be computed. Notice that for any u_{hom} of the form (7), the function

$$t\longmapsto \boldsymbol{a}(t):=(u_{\mathrm{hom}}|_\Gamma,\partial_\nu u_{\mathrm{hom}}|_\Gamma)^\top$$

satisfies $\boldsymbol{a}\in\mathcal{C}^\infty([0,\infty),\mathbb{H}^r(\Gamma))$ for any $r\ge 0$ and $\boldsymbol{a}^{(k)}(0)=0$ for all $k\ge 0$. By (29) and Theorem 2,

$$v(t)=\mathcal{P}_1\mathcal{W}_1^{-1}\boldsymbol{a}(t) \tag{30}$$

and hence $v\in\mathcal{C}^\infty([0,\infty),H^2(\Omega^-\cup\Omega^+))$. If we define g by (28), then g has the same regularity. Also

$$g^{(k)}(0)=v^{(k)}(0)=0 \qquad \text{for all } k\ge 0. \tag{31}$$

The function w is constructed so that u solves the original parabolic equation (8).

We finally remark that (27) has a unique solution (see [16, Chapter 4]) and that $w\in\mathcal{C}^\infty([0,\infty),H^2(\Omega^-\cup\Omega^+))$.

5 Justification of forward and inverse Laplace transform

After the preparations in sections 2 and 4 we can now give a rigorous derivation of the Laplace transformed problem (10) formally derived in section 2. Moreover, we verify the hypothesis (18) in section 3 which allows us to return from the Laplace to the time domain in a stable and numerically efficient manner.

First we consider the Laplace transforms $U_{\mathrm{hom}}(s,x)$ of the fields $u_{\mathrm{hom}}(x,t)$ generated by the heat sources in a homogeneous medium given in (7).

Lemma 10 *Every function u_{hom} of the form (7) has a Laplace transform $U_{\mathrm{hom}}(\mathbf{x},s)$ defined for $\operatorname{Re} s>0$ in (9), which has a holomorphic extension to $s\in\mathcal{U}$. Moreover, for all $k\in\mathbb{N}_0$ the mappings $\mathcal{U}\to H^k(\Gamma)$, $s\mapsto U_{\mathrm{hom}}(\,\cdot\,,s)|_\Gamma$ and $s\mapsto\partial_\nu U_{\mathrm{hom}}(\,\cdot\,,s)|_\Gamma$ are holomorphic, and there exists a constant $C>0$ such that for all $s\in\mathcal{U}$, $|s|\geq 1$*

$$\|U_{\mathrm{hom}}(\,\cdot\,,s)\|_{k,\Gamma}\leq C|s|^{\gamma_1}\exp(-2\sqrt{m_0}\operatorname{Re}\sqrt{s}), \tag{32a}$$

$$\|\partial_\nu U_{\mathrm{hom}}(\,\cdot\,,s)\|_{k,\Gamma}\leq C|s|^{\gamma_2}\exp(-2\sqrt{m_0}\operatorname{Re}\sqrt{s}) \tag{32b}$$

with $\gamma_1=\beta/4+k/2-3/4$ and $\gamma_2=\beta/4+k/2-1/4$ if β is odd and $\gamma_1=\beta/4+k/2-1/2$, $\gamma_2=\beta/4+k/2$ if β is even. Here the constant $m_0:=\inf_{\mathbf{x}\in\Gamma}m(\mathbf{x})$ is strictly positive.

Proof First note that $m_0>0$ since the continuous functions m attains its infinimum on the compact set $\Gamma\subset\mathbb{R}^d_-$. To indicate the dependence on β we write $u_\beta=u_{\mathrm{hom}}$ and $U_\beta:=U_{\mathrm{hom}}$ in this proof. From the identity

$$\partial_t u_\beta(\mathbf{x},t)=-\frac{\beta}{2}u_{\beta+2}(\mathbf{x},t)+m(\mathbf{x})u_{\beta+4}(\mathbf{x},t)$$

we obtain $sU_\beta(\mathbf{x},s)-u_\beta(\mathbf{x},0)=-\beta/2U_{\beta+2}(\mathbf{x},s)+m(\mathbf{x})U_{\beta+4}(\mathbf{x},s)$ for $\beta\in\mathbb{N}$, which yields the two term recursion

$$U_{\beta+4}(\mathbf{x},s)=\frac{1}{m(\mathbf{x})}\left(\frac{\beta}{2}U_{\beta+2}(\mathbf{x},s)+sU_\beta(\mathbf{x},s)\right),\qquad\beta\in\mathbb{N}. \tag{33}$$

From tables of Laplace transforms we find that

$$U_1(\mathbf{x},s)=\sqrt{\pi/s}\,\exp\left(-2\sqrt{m(\mathbf{x})s}\right),$$
$$U_2(\mathbf{x},s)=2K_0\left(2\sqrt{m(\mathbf{x})s}\right),$$
$$U_3(\mathbf{x},s)=\sqrt{\pi/m(\mathbf{x})}\,\exp\left(-2\sqrt{m(\mathbf{x})s}\right),$$
$$U_4(\mathbf{x},s)=2\sqrt{s/m(\mathbf{x})}\,K_1\left(2\sqrt{m(\mathbf{x})s}\right)$$

where K_0 and K_1 denote the modified Bessel functions (or MacDonald's functions) of order 0 and 1. It follows by induction from eq. (33) that there exist functions $f_{\beta,j},g_{\beta,j},h_{\beta,j}\in C^\infty(\mathbb{R}^d_-)$ such that

$$U_\beta(\mathbf{x},s)=\sum_{j=0}^{(\beta-1)/2}f_{\beta,j}(\mathbf{x})s^{(j-1)/2}\exp\left(-2\sqrt{m(\mathbf{x})s}\right)$$

for β odd and

$$U_\beta(\mathbf{x},s) = \sum_{j=0}^{(\beta-2)/2} s^{j/2}\left(g_{\beta,j}(\mathbf{x})K_0\left(2\sqrt{m(\mathbf{x})s}\right) + h_{\beta,j}(\mathbf{x})K_1\left(2\sqrt{m(\mathbf{x})s}\right)\right)$$

for β even. Choosing $(-\infty,0]$ as branch cut of the square root function, it follows that the functions $U_\beta(\mathbf{x},\cdot\,)$ have a holomorphic extension to $s\in\mathcal{U}$ for fixed $\mathbf{x}$. Let $\alpha\in\mathbb{N}_0^d$ be a multi-index and $|\alpha| := \alpha_1+\cdots+\alpha_d$. Differentiating the formulas for U_β with respect to $\mathbf{x}$ and using the asymptotic behavior of the modified Bessel functions (see [1])

$$K_\nu^{(j)}(z) = (-1)^j\left(\frac{\pi}{2z}\right)^{1/2} e^{-z}\left(1+O(|z|^{-1})\right), \qquad |z|\to\infty, |\arg(z)| < \frac{3}{2}\pi,$$

with $\nu=0,1$, it follows that there exist constants $C_{\alpha,\beta}$ such that

$$\sup_{\mathbf{x}\in\Gamma}\left|\frac{\partial^\alpha U_\beta(\mathbf{x},s)}{\partial\mathbf{x}^\alpha}\right| \le C_{\alpha,\beta}|s|^\gamma \exp(-2\sqrt{m_0}\,\mathrm{Re}\,\sqrt{s}),$$
$$\gamma = (\beta-3)/4+|\alpha|/2 \text{ for } \beta \text{ odd }, \qquad \gamma=(\beta-2)/4+|\alpha|/2 \;\text{ for } \beta \text{ even}$$

for all $s\in\mathcal{U}$ with $|s|\ge 1$. This implies the bounds (32). The differentiability of the mappings $s\mapsto U_{\mathrm{hom}}(\,\cdot\,,s)|_\Gamma$ and $s\mapsto \partial_\nu U_{\mathrm{hom}}(\,\cdot\,,s)|_\Gamma$ with respect to the H^k-norm is a simple consequence of the local boundedness of all derivatives of $U_{\mathrm{hom}}(\mathbf{x},s)$ with respect to both $\mathbf{x}$ and s. □

To show that the solution u constructed in section 4 has a Laplace transform which has a holomorphic extension to $\mathcal{U}$, we consider the decomposition (26) and prove the same statement for v and w. Due to (30) and Lemma 10, the function v has a Laplace transform with a holomorphic extension $V:\mathcal{U}\to L^2(\Omega^-\cup\Omega^+)$ given by

$$V(s) = \mathcal{P}_1\mathcal{W}_1^{-1}(U_{\mathrm{hom}}(s), \partial_\nu U_{\mathrm{hom}}(s))^\top,$$

and it is bounded by

$$\|V(s)\|_{0,\Omega^-\cup\Omega^+} \le C|s|^\gamma \exp(-2\sqrt{m_0}\,\mathrm{Re}\,\sqrt{s}) \tag{34}$$

for some constants $C,\gamma>0$. Using (27), (28), and (31) we obtain that w has a Laplace transform given by

$$W(s) = (s\mathcal{I}-\mathcal{A})^{-1}(V(s)-sV(s)), \qquad \mathrm{Re}\,s>0.$$

Since the resolvent of $\mathcal{A}$ is holomorphic on its domain of definition, W has a holomorphic extension to $W:\mathcal{U}\to L^2(\Omega^-\cup\Omega^+)$. Therefore, $U:\mathcal{U}\to L^2(\Omega^-\cup\Omega^+)$,

$$U(s) := V(s)+W(s) \tag{35}$$

is well-defined. Together with the bound (24) on the resolvent of $\mathcal{A}$ we obtain the bound (18) on U from section 3 in $L^2(\Omega^-\cup\Omega^+)$. To obtain the stronger bound in $H^2(\Omega^-\cup\Omega^+)$, we derive a bound like (34) in $H^2(\Omega^-\cup\Omega^+)$ from Lemma 10 and use Proposition 9.

The following computations show that U defined by (35) satisfies the boundary value problem (10):

$$(s\mathcal{I} - \Delta_\pm)U = (s\mathcal{I} - \Delta_\pm)V + (s\mathcal{I} - \mathcal{A})W = sV - \Delta_\pm V + V - sV \overset{(29)}{=} 0,$$
$$\mathcal{B}U = \mathcal{B}V = \mathbf{g}, \qquad \Pi U = 0.$$

Remark 11 We can also consider superpositions of functions of the form (7) describing spread heat sources and the temporal process of heating. Let $\Upsilon(x,t)$ denote the right-hand side of (7) extended by 0 for $t \le 0$ and consider an incident field of the form

$$u_{\mathrm{hom}}(\mathbf{x},t) = \int_0^\infty \int_H \zeta(\mathbf{y},\tau)\Upsilon(\mathbf{x}-\mathbf{y},t-\tau)\,\mathrm{d}\mathbf{y}\,\mathrm{d}\tau, \qquad \mathbf{x} \in \mathbb{R}^d_-, t > 0$$

with a bounded measurable heat source density ζ that is either compactly supported or decays sufficiently rapidly as $|\mathbf{y}|, \tau \to \infty$. Since the Laplace transform $\hat{\Upsilon}(x,s)$ of Υ with respect to t satisfies the bounds (32), it is easy to see that

$$U_{\mathrm{hom}}(\mathbf{x},s) = \int_0^\infty \int_H \zeta(\mathbf{y},\tau)e^{-s\tau}\hat{\Upsilon}(\mathbf{x}-\mathbf{y},s)\,\mathrm{d}\mathbf{y}\,\mathrm{d}\tau$$

satisfies the same kind of bounds (32).

6 Bounds in the Laplace domain

In this section we bound the quantities

$$C_r(s) := \|\mathcal{W}(s)\|_{\mathcal{L}(\mathbb{H}^r(\Gamma))}, \qquad D_r(s) := \|\mathcal{W}(s)^{-1}\|_{\mathcal{L}(\mathbb{H}^r(\Gamma))} \tag{36}$$

for several relevant values of r. These bounds are necessary to keep track of the dependence of s in bounds related to discretization of the system of boundary integral equations. Bounds on the single layer potential operator $V(s) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ and its inverse have been derived by Lubich & Schneider [13] using estimates of the kernels and parameter-dependent pseudodifferential calculus. Here we follow a different approach using bounds on the solution of the transmission problem

$$\Delta_\pm u - s\,u, \qquad \mathcal{B}u = \boldsymbol{g}, \qquad \Pi u = 0$$

depending on s. (In this and the following section we will use small letters to denote solutions of the Laplace transformed problems!) As pointed out by a referee, related results concerning parametric dependence of $\|V(s)\|$ and $\|V^{-1}(s)\|$ in the natural spaces $H^{\pm 1/2}(\Gamma)$ have also been obtained by Bamberger and Ha Duong [2] to prove existence and uniqueness of retarded potentials for the wave equation.

6.1 Transmission problem

Throughout this section, in addition to the sets $\Omega^{\pm}$ we will also consider

$$\widetilde{\Omega}^- := \{\mathbf{x} \in \mathbb{R}^d \,|\, \widetilde{\mathbf{x}} \in \Omega^-\}, \qquad \mathcal{O}^- := \Omega^- \cup \widetilde{\Omega}^-, \qquad \mathcal{O}^+ := \mathbb{R}^d \setminus \overline{\mathcal{O}^-}.$$

The common boundary of $\mathcal{O}^- \cup \mathcal{O}^+$ will be denoted Υ. We will use the identification $L^2(\mathbb{R}^d) \cong L^2(\mathcal{O}^-) \times L^2(\mathcal{O}^+)$, the transmission operator $\mathcal{B}$ (now traces take place in Υ) is the same and $\Delta_{\pm}$ is defined by adapting (5) to this new situation.

Lemma 12 *For any $k \geq 1$, if $u \in H^k(\mathcal{O}^- \cup \mathcal{O}^+)$, $\Delta_{\pm} u \in H^k(\mathcal{O}^- \cup \mathcal{O}^+)$ and $\mathcal{B}u = 0$, then $u \in H^{k+2}(\mathcal{O}^- \cup \mathcal{O}^+)$.*

Proof If $u \in H^k(\mathcal{O}^- \cup \mathcal{O}^+)$, the we can solve the equations $\mathcal{B}u = 0$ for $\partial_\nu u_{\pm}|_{\Upsilon}$ and obtain $\partial_\nu u_{\pm}|_{\Upsilon} \in H^{k-1/2}(\Upsilon)$. Since $\Delta_{\pm} u - u \in H^{k-1}(\mathcal{O}^- \cup \mathcal{O}^+)$ by regularity of elliptic problems we have that $u \in H^{k+1}(\mathcal{O}^- \cup \mathcal{O}^+)$. Hence $\partial_\nu u_{\pm}|_{\Upsilon} \in H^{k+1/2}(\Upsilon)$ and we can use the same argument to show that $u \in H^{k+2}(\mathcal{O}^- \cup \mathcal{O}^+)$. □

Proposition 13 *Let $k \geq 0$, $f \in H^k(\mathcal{O}^- \cup \mathcal{O}^+)$ and $\boldsymbol{g} \in \mathbb{H}^{k+1/2}(\Upsilon)$. Then the unique solution of*

$$\Delta_{\pm} u - u = f, \qquad \mathcal{B}u = \boldsymbol{g} \tag{37}$$

is in $H^{k+2}(\mathcal{O}^- \cup \mathcal{O}^+)$. Moreover, there exists $C > 0$ such that

$$\|u\|_{k+2,\mathcal{O}^- \cup \mathcal{O}^+} \leq C\big(\|f\|_{k,\mathcal{O}^- \cup \mathcal{O}^+} + \|\boldsymbol{g}\|_{k+1/2,\Upsilon}\big). \tag{38}$$

Proof Notice first that if $v \in H^1(\mathcal{O}^- \cup \mathcal{O}^+)$ satisfies

$$\Delta_{\pm} v - v = f \in H^k(\mathcal{O}^- \cup \mathcal{O}^+), \qquad \mathcal{B}v = 0$$

($\partial_\nu v_{\pm}|_{\Upsilon}$ makes sense in a weak form since $\Delta_{\pm} v \in L^2(\mathcal{O}^- \cup \mathcal{O}^+)$). A repeated application of Lemma 12 proves then that $v \in H^{k+2}(\mathcal{O}^- \cup \mathcal{O}^+)$. Clearly, $u = v + \mathcal{P}_1 \mathcal{W}_1^{-1} \boldsymbol{g}$. The argument above and Theorem 4 show that $u \in H^{k+2}(\mathcal{O}^- \cup \mathcal{O}^+)$. Therefore, the bounded linear map

$$(\Delta_{\pm} - I, \mathcal{B}) : H^{k+2}(\mathcal{O}^- \cup \mathcal{O}^+) \to H^k(\mathcal{O}^- \cup \mathcal{O}^+) \times \mathbb{H}^{k+1/2}(\Upsilon)$$

is onto. It is also trivially injective. Therefore, by the open mapping theorem, its inverse is bounded and we have (38). □

Given a function $u : \mathbb{R}^d_- \to \mathbb{C}$ we define

$$\widetilde{u}(\mathbf{x}) := \begin{cases} u(\mathbf{x}), \text{ if } \mathbf{x} \in \mathbb{R}^d_-, \\ u(\widetilde{\mathbf{x}}), \text{ otherwise.} \end{cases}$$

The proof of the following result is straightforward. Notice that condition (39) can be simplified to include only derivatives with respect to the $d-$th variable, but it is like this that we will be using it.

Lemma 14 *Let $k \geq 0$ and $f \in H^k(\mathbb{R}^d_-)$. Then $\widetilde{f} \in H^k(\mathbb{R}^d)$ if and only if*

$$\Pi \Delta^j f = 0 \qquad \text{for all } j \quad \text{s.t.} \quad 2j + 2 \leq k. \tag{39}$$

Proposition 15 *Let $k \geq 0$, $f \in H^k(\Omega^- \cup \Omega^+)$, satisfying (39) and $\boldsymbol{g} \in \mathbb{H}^{k+1/2}(\Gamma)$. Then the solution to*

$$\Delta_\pm u - u = f, \qquad \mathcal{B}u = \boldsymbol{g}, \qquad \Pi u = 0$$

is in $H^{k+2}(\Omega^- \cup \Omega^+)$. Moreover there exists $C_k > 0$ such that

$$\|u\|_{k+2,\Omega^-\cup\Omega^+} \leq C_k\big(\|f\|_{k,\Omega^-\cup\Omega^+} + \|\boldsymbol{g}\|_{k+1/2,\Gamma}\big). \tag{40}$$

Proof We can use a reflection argument to solve a transmission problem in $\mathcal{O}^- \cup \mathcal{O}^+$, with symmetric data. Condition (39) guarantees that $\widetilde{f} \in H^k(\mathcal{O}^- \cup \mathcal{O}^+)$ by Lemma 14. The symmetry of the data proves easily that $\Pi u = 0$. The result is then a trivial consequence of Proposition 13. □

Theorem 16 *Let $k \geq -1$ and $m = \lfloor (k+1)/2 \rfloor \geq 0$. If $\boldsymbol{g} \in \mathbb{H}^{k+1/2}(\Gamma)$, then the solution to*

$$\Delta_\pm u - s\,u = 0, \qquad \mathcal{B}u = \boldsymbol{g}, \qquad \Pi u = 0$$

belongs to $H^{k+2}(\Omega^- \cup \Omega^+)$ and we have a bound

$$\|u\|_{k+2,\Omega^-\cup\Omega^+} \leq \frac{P_{m+2}(|s|)}{\delta(s)} \|\boldsymbol{g}\|_{k+1/2,\Gamma}.$$

Proof For $k = -1, 0$ ($m = 0$) we decompose

$$u = \mathcal{P}_1 \mathcal{W}_1^{-1} \boldsymbol{g} + (s-1)(\mathcal{A} - s\mathcal{I})^{-1} \mathcal{P}_1 \mathcal{W}_1^{-1} \boldsymbol{g}. \tag{41}$$

Here $\mathcal{P}_1 \mathcal{W}_1^{-1} \boldsymbol{g} \in H^{k+2}(\Omega^- \cup \Omega^+) \subset L^2(\mathbb{R}^d_-)$ and we can use Theorem 4 and Proposition 9, obtaining

$$\|u\|_{k+2,\Omega^-\cup\Omega^+} \leq C \left(\|\boldsymbol{g}\|_{k+1/2,\Gamma} + (1+|s|) \frac{P_1(|s|)}{\delta(s)} \|\mathcal{P}_1 \mathcal{W}_1^{-1} \boldsymbol{g}\|_{k+2,\Omega^-\cup\Omega^+} \right), \tag{42}$$

for $k = -1, 0$, from where the result follows readily in those cases.

If $k \geq 1$ we notice that

$$\Delta_\pm u - u = (s-1)\,u, \qquad \mathcal{B}u = \boldsymbol{g}, \qquad \Pi u = 0.$$

A recurrent application of Proposition 15 proves that $u \in H^{k+2}(\Omega^- \cup \Omega^+)$. We remark that, seen as right–hand side $(s-1)\,u$ satisfies (39) as far as needed by induction, using that $\Pi u = 0$ and that $\Delta^j_\pm u = s \Delta^{j-1}_\pm u$. The bound follows by induction using (40) and cases $k = -1, 0$. □

6.2 Bounds for $\mathcal{W}(s)^{-1}$

Proposition 17 *Let $k \geq -1$ and $m = \lfloor (k+1)/2 \rfloor \geq 0$. Let u be the solution of the interior–exterior Dirichlet problem*

$$\kappa_+ \Delta u - s\, u = 0, \qquad \text{in } \Omega^- \cup \Omega^+,$$

$$u|_\Gamma = h, \qquad \Pi u = 0,$$

with $h \in H^{k+3/2}(\Gamma)$. Then $u \in H^{k+2}(\Omega^- \cup \Omega^+)$ and

$$\|u\|_{k+2,\Omega^- \cup \Omega^+} \leq \frac{P_{m+2}(|s|)}{\delta(s)} \|h\|_{k+3/2,\Gamma}. \tag{43}$$

Also

$$\|u\|_{0,\Omega^- \cup \Omega^+} \leq \frac{P_1(|s|)}{\delta(s)} \|h\|_{1/2,\Gamma}. \tag{44}$$

Proof The proof is very similar to the one given for transmission problems in Theorem 16. We simply give a sketch of it.

We consider the set $D(\Delta_+) := \{u \in H^2(\Omega^- \cup \Omega^+) \,|\, u|_\Gamma = 0, \Pi u = 0\}$ and the operator $\Delta_+ : D(\Delta_+) \to L^2(\mathbb{R}^d_-)$ defined by $\Delta_+ := \kappa_+ \Delta$, applied in $\Omega^- \cup \Omega^+$. The results of Section 4 apply to this operator. If $\rho^2 = -1/\kappa_+$, then u admits the decomposition

$$u = (\mathcal{I} + (s-1)(\Delta_+ - s\mathcal{I})^{-1}) \widetilde{\mathcal{S}}_\rho \widetilde{V}_\rho^{-1} h$$

(compare with (41)). With this and the equivalent to Proposition 9, we can easily prove the result for $k = -1$ and $k = 0$. With the equivalent to (24) we can also prove (44).

Now we prove that if $f \in H^k(\Omega^- \cup \Omega^+)$ satisfies (39) and $h \in H^{k+3/2}(\Gamma)$, then the solution to

$$\begin{aligned} &\kappa_+ \Delta u - u = f, \qquad \text{in } \Omega^- \cup \Omega^+, \\ &u|_\Gamma = h, \qquad \Pi u = 0, \end{aligned} \tag{45}$$

admits a bound

$$\|u\|_{k+2,\Omega^- \cup \Omega^+} \leq C \left(\|f\|_{k,\Omega^- \cup \Omega^+} + \|h\|_{k+3/2,\Gamma} \right) \tag{46}$$

by repeating the arguments of Proposition 15. The remaining cases are proven by induction taking $f = (s-1)\, u$ in (45) and using (46). □

We recall that if $\mathcal{S}_\rho \psi = v : \mathbb{R}^d \to \mathbb{C}$, then $\psi = [\partial_\nu v] = \partial_\nu v_-|_\Gamma - \partial_\nu v_+|_\Gamma$ and hence

$$\|\psi\|_{k+1/2,\Gamma} \leq C \|v\|_{k+2,\Omega^- \cup \Omega^+}. \tag{47}$$

This bound is valid for $k \geq 0$. The case $k = -1$ requires using that $\Delta v = -\rho^2 v$ in $\Omega^- \cup \Omega^+$ and yields

$$\begin{aligned} \|\psi\|_{-1/2,\Gamma} &\leq C \left(\|v\|_{1,\Omega^- \cup \Omega^+} + \|\Delta v\|_{0,\Omega^- \cup \Omega^+} \right) \\ &\leq C' \left(\|v\|_{1,\Omega^- \cup \Omega^+} + |\rho|^2 \|v\|_{0,\Omega^- \cup \Omega^+} \right). \end{aligned} \tag{48}$$

Proposition 18 *Let $k \geq -1$ and $m = \lfloor (k+1)/2 \rfloor$. Let $\boldsymbol{\psi} \in \mathbb{H}^{k+1/2}(\Gamma)$ and $u = \mathcal{P}(s)\boldsymbol{\psi}$. Then*

$$\|\boldsymbol{\psi}\|_{k+1/2,\Gamma} \leq \frac{P_{m+2}(|s|)}{\delta(s)} \|u\|_{k+2,\Omega^- \cup \Omega^+}.$$

Proof Let $\boldsymbol{\psi} = (\psi^-, \psi^+)$. The function $\widetilde{u}_+ = \widetilde{\mathcal{S}}_{\lambda(s)}\psi^+$ is a $H^1(\mathbb{R}^d_-)-$extension of u_+ to the interior domain Ω^-. Then, for $k \geq 0$, by (47) and Proposition 17

$$\begin{aligned}\|\psi^+\|_{k+1/2,\Gamma} &\leq C\|\widetilde{u}_+\|_{k+2,\Omega^-\cup\Omega^+} \leq \frac{P_{m+2}(|s|)}{\delta(s)} \|\gamma \widetilde{u}_+\|_{k+3/2,\Gamma} \\ &\leq C\,\frac{P_{m+2}(|s|)}{\delta(s)} \|u_+\|_{k+2,\Omega^+}.\end{aligned}$$

For $k = -1$, we have to use (48) with $\rho^2 = s/\kappa_+$ as well as (43) with $k = -1$ ($m = 0$) and (44).

Finally, $\psi^- = [\partial_\nu \widetilde{u}_-]$, where $\widetilde{u}_- = \mathcal{S}_{\mu(s)}\psi_-$. Bounds similar to those of Proposition 17 hold for the problem in $\mathbb{R}^d$ without the condition $\Pi u = 0$. Their proofs are essentially identical to those of the half space. With these we can bound ψ_- in terms of u_-. □

Theorem 19 *Let $k \geq -1$ and $m = \lfloor (k+1)/2 \rfloor$. Then*

$$D_{k+1/2}(s) = \|\mathcal{W}(s)^{-1}\|_{\mathcal{L}(\mathbb{H}^{k+1/2}(\Gamma))} \leq \frac{P_{2m+4}(|s|)}{\delta(s)^2}. \tag{49}$$

Proof If $\mathcal{W}(s)\boldsymbol{\psi} = \boldsymbol{g}$, then $u = \mathcal{P}(s)\boldsymbol{\psi}$ and u satisfies

$$\Delta_\pm u - s\,u = 0, \qquad \mathcal{B}u = \boldsymbol{g}, \qquad \Pi u = 0.$$

We then just have to apply Proposition 18 to bound $\boldsymbol{\psi}$ in terms of u and Theorem 16 to bound u in terms of $\boldsymbol{g}$. □

6.3 Bounds for $\mathcal{W}(s)$

We recall the notation $[\partial_\nu v] = \partial_\nu v_-|_\Gamma - \partial_\nu v_+|_\Gamma$ for the jump of the normal derivative accross Γ.

Proposition 20 *Let $\psi \in H^{k-3/2}(\Gamma)$, $k \in \{1, 2\}$ and $u \in H^k(\Omega^- \cup \Omega^+)$ be the unique solution to*

$$\begin{aligned}&\kappa_+ \Delta u - s\,u = 0, \qquad \text{in } \Omega^- \cup \Omega^+,\\ &[u] = 0, \qquad [\partial_\nu u] = \psi, \qquad \Pi u = 0.\end{aligned}$$

Then

$$\|u\|_{k,\Omega^-\cup\Omega^+} \leq \frac{P_2(|s|)}{\delta(s)} \|\psi\|_{k-3/2,\Gamma}.$$

Also

$$\|u\|_{0,\Omega^-\cup\Omega^+} \leq \frac{P_1(|s|)}{\delta(s)} \|\psi\|_{-1/2,\Gamma}$$

Proof Notice that $u = \widetilde{\mathcal{S}}_{\lambda(s)}\psi$, with $\lambda(s)^2 = -s/\kappa_+$. Let $\rho^2 = -1/\kappa_+$, $v := \widetilde{\mathcal{S}}_\rho\psi$ and $w := (s-1)(\Delta_+ - \mathcal{I})^{-1}v$, where $\Delta_+ = \kappa_+\Delta$ with $\mathcal{D}(\Delta_+) = \{u \in H^1(\mathbb{R}^d) \cap H^2(\Omega^- \cup \Omega^+) : \Pi u = 0\}$. Therefore

$$\|w\|_{2,\Omega^-\cup\Omega^+} \le \frac{P_2(|s|)}{\delta(s)}\|v\|_{0,\Omega^-\cup\Omega^+}, \qquad \|w\|_{0,\Omega^-\cup\Omega^+} \le \frac{C}{\delta(s)}\|v\|_{0,\Omega^-\cup\Omega^+}.$$

The result is then a simple consequence of the continuity of $\widetilde{\mathcal{S}}_\rho$. □

Theorem 21 *Let $r \in \{-1/2, 1/2\}$. Then*

$$C_r(s) = \|\mathcal{W}(s)\|_{\mathcal{L}(\mathbb{H}^r(\Gamma))} \le \frac{P_2(|s|)}{\delta(s)}. \tag{50}$$

Proof By Proposition 20 and a similar result in the whole space without the condition $\Pi u = 0$ it is clear that

$$\|\mathcal{P}(s)\boldsymbol{\psi}\|_{k,\Omega^-\cup\Omega^+} \le \frac{P_2(|s|)}{\delta(s)}\|\boldsymbol{\psi}\|_{k-3/2,\Gamma}, \qquad \forall\boldsymbol{\psi} \in \mathbb{H}^{k-3/2}(\Gamma), k \in \{1,2\} \tag{51}$$

and

$$\|\mathcal{P}(s)\boldsymbol{\psi}\|_{0,\Omega^-\cup\Omega^+} \le \frac{P_1(|s|)}{\delta(s)}\|\boldsymbol{\psi}\|_{-1/2,\Gamma}, \qquad \forall\boldsymbol{\psi} \in \mathbb{H}^{1/2}(\Gamma). \tag{52}$$

Since $\mathcal{W}(s) = \mathcal{B}\,\mathcal{P}(s)$, the result follows readily for $r = 1/2$ by the continuity of $\mathcal{B} : H^2(\Omega^- \cup \Omega^+) \to \mathbb{H}^{1/2}(\Gamma)$. For $r = -1/2$, we use the fact that

$$\|\mathcal{B}u\|_{-1/2,\Gamma} \le C\left(\|u\|_{1,\Omega^-\cup\Omega^+} + |s|\,\|u\|_{0,\Omega^-\cup\Omega^+}\right)$$

if $\Delta_\pm u - s\,u = 0$ and apply the inequalities above. □

7 Space discretization

We will deal with two different Galerkin schemes for discretization of the system of integral equations

$$\mathcal{W}(s)\boldsymbol{\psi} = \boldsymbol{g}. \tag{53}$$

For both we consider a triangulation of Γ. In two dimensions, this is just a choice of nodes in the boundary and the separation of arcs between consecutive nodes. In three dimensions, we consider a polyhedron with triangular faces and nodes on Γ and an inherited partition of Γ in curved triangles. This kind of partition is explained in detail in [7, Section 2]. When we refer to polynomial functions on an element we understand polynomials on the corresponding straight element transformed to the curved element by the mapping that parameterizes the curved element from the straight one. The parameter h is the diameter of the partition.

In the first situation we consider a class of spaces $X_h \subset H^{-1/2}(\Gamma)$ of piecewise polynomial functions of degree $k \geq 0$. They can be discontinuous (which is necessary to have a nontrivial space when $k = 0$) or not. It is well-known that

$$\inf_{\psi_h \in X_h} \|\psi - \psi_h\|_{0,\Gamma} \leq C h^{k+1} \|\psi\|_{k+1,\Gamma} \qquad \text{for all } \psi \in H^{k+1}(\Gamma), \tag{54a}$$

$$\inf_{\psi_h \in X_h} \|\psi - \psi_h\|_{0,\Gamma} \stackrel{h \to 0}{\to} 0 \qquad \text{for all } \psi \in H^0(\Gamma), \tag{54b}$$

the second assertion being a consequence of the first one and the Banach-Steinhaus Theorem. The discrete method is then a Galerkin scheme in $\mathbb{X}_h := X_h \times X_h$:

$$\text{Find } \boldsymbol{\psi}_h \in \mathbb{X}_h \text{ s.t.} \quad \int_\Gamma \boldsymbol{\varphi}_h \cdot \mathcal{W}(s) \boldsymbol{\psi}_h = \int_\Gamma \boldsymbol{\varphi}_h \cdot \boldsymbol{g} \qquad \text{for all } \boldsymbol{\varphi}_h \in \mathbb{X}_h. \tag{55}$$

In the second situation we consider a class of spaces $Y_h \subset H^{-1/2}(\Gamma)$ of continuous piecewise polynomial functions of degree $k \geq 1$, and we assume the triangulation to be quasi–uniform. Then there exists a projection $\pi_h : H^0(\Gamma) \to Y_h$ and a constant $C > 0$ such that

$$\|\psi - \pi_h \psi\|_{r,\Gamma} \leq C h^{\tau - r} \|\psi\|_{\tau,\Gamma} \qquad \text{for all } \psi \in H^\tau(\Gamma) \tag{56}$$

for $0 \leq r \leq \tau \leq 1$. Also, for $-1 \leq r \leq 1$,

$$\inf_{\psi_h \in Y_h} \|\psi - \psi_h\|_{r,\Gamma} \leq C h^{k+1-r} \|\psi\|_{k+1,\Gamma} \qquad \text{for all } \psi \in H^{k+1}(\Gamma). \tag{57}$$

Finally, for $0 \leq r \leq \tau \leq 1$, the inverse inequality

$$\|\psi_h\|_{\tau,\Gamma} \leq C h^{r-\tau} \|\psi_h\|_{r,\Gamma} \qquad \text{for all } \psi_h \in Y_h \tag{58}$$

holds true. Detailed proofs of these inequalities in the two–dimensional case can be found in [17]. The same kind of arguments apply for the three dimensional case. The corresponding discretization of (53) is similar to (55) changing $\mathbb{X}_h$ to $\mathbb{Y}_h := Y_h \times Y_h$:

$$\text{Find } \boldsymbol{\psi}_h \in \mathbb{Y}_h \text{ s.t.} \quad \int_\Gamma \boldsymbol{\varphi}_h \cdot \mathcal{W}(s) \boldsymbol{\psi}_h = \int_\Gamma \boldsymbol{\varphi}_h \cdot \boldsymbol{g} \qquad \text{for all } \boldsymbol{\varphi}_h \in \mathbb{Y}_h. \tag{59}$$

Proposition 22 *For all $s \in \mathcal{U}$ there exists a constant $h_0(s)$ such that the discrete problem* (55) *is uniquely solvable for $h \leq h_0(s)$, and*

$$\|\boldsymbol{\psi} - \boldsymbol{\psi}_h\|_{0,\Gamma} \leq C_0(s)\, D_0(s)\, C \inf_{\boldsymbol{\varphi}_h \in \mathbb{X}_h} \|\boldsymbol{\psi} - \boldsymbol{\varphi}_h\|_{0,\Gamma}.$$

Moreover, the same $h_0(s) = h_0(\mathcal{K})$ can be chosen for s in any compact subset $\mathcal{K} \subset \mathcal{U}$.

Proof For the operator $\mathcal{W}_0$ defined in (14) it is straightforward to prove that there exists $C > 0$ such that

$$\sup_{\boldsymbol{\varphi}_h \in \mathbb{X}_h \setminus \{0\}} \frac{1}{\|\boldsymbol{\varphi}_h\|_{0,\Gamma}} \left| \int_\Gamma \boldsymbol{\varphi}_h \cdot \mathcal{W}_0 \boldsymbol{\psi}_h \right| \geq C \|\boldsymbol{\psi}_h\|_{0,\Gamma} \qquad \text{for all } \boldsymbol{\psi}_h \in \mathbb{X}_h. \tag{60}$$

Since $\mathcal{W}(s) - \mathcal{W}_0$ is compact and since $\inf_{\boldsymbol{\psi}_h \in X_h} \|\boldsymbol{\psi} - \boldsymbol{\psi}_h\|_{0,\Gamma} \to 0$ for all $\boldsymbol{\psi} \in \mathbb{H}^0(\Gamma)$, (60) proves that there exist constants $C', h_0(s) > 0$ such that for all $h \leq h_0(s)$

$$\sup_{\boldsymbol{\varphi}_h \in \mathbb{X}_h \setminus \{0\}} \frac{1}{\|\boldsymbol{\varphi}_h\|_{0,\Gamma}} \left| \int_\Gamma \boldsymbol{\varphi}_h \cdot \mathcal{W}(s) \boldsymbol{\psi}_h \right| \geq \frac{C'}{D_0(s)} \|\boldsymbol{\psi}_h\|_{0,\Gamma} \qquad \text{for all } \boldsymbol{\psi}_h \in \mathbb{X}_h,$$

by an argument valid for compact perturbations of operator equations [10, Theorem 13.7]. The equivalence of stability, inf–sup conditions and Céa type estimates (see [10] and [23]) proves the first statement.

The second statement follows by a simple argument using continuous dependence of the operator on s. □

Proposition 23 *For all $s \in \mathcal{U}$ there exists a constant $h_0(s)$ such that the discrete problem* (59) *is uniquely solvable for $h \leq h_0(s)$, and*

$$\|\boldsymbol{\psi} - \boldsymbol{\psi}_h\|_{\pm 1/2,\Gamma} \leq C_{\pm 1/2}(s)\, D_{\pm 1/2}(s) C \inf_{\boldsymbol{\varphi}_h \in \mathbb{Y}_h} \|\boldsymbol{\psi} - \boldsymbol{\varphi}_h\|_{\pm 1/2,\Gamma}.$$

Moreover, the same $h_0(s) = h_0(\mathcal{K})$ can be chosen for s in any compact subset $\mathcal{K} \subset \mathcal{U}$.

Proof The key to the proof is the following inequality: if $\eta \in \mathcal{C}^1(\Gamma)$ is strictly positive, then there exists $C > 0$ such that

$$\sup_{\varphi_h \in Y_h \setminus \{0\}} \frac{1}{\|\varphi_h\|_{-1,\Gamma}} \left| \int_\Gamma \varphi_h \, \eta \, \psi_h \right| \geq C \|\psi_h\|_{1,\Gamma} \qquad \text{for all } \psi_h \in Y_h. \tag{61}$$

Once we have this, we use the special form of $\mathcal{W}_0$ and its adjoint to prove that

$$\sup_{\boldsymbol{\varphi}_h \in \mathbb{Y}_h \setminus \{0\}} \frac{1}{\|\boldsymbol{\varphi}_h\|_{-r,\Gamma}} \left| \int_\Gamma \boldsymbol{\varphi}_h \cdot \mathcal{W}_0 \boldsymbol{\psi}_h \right| \geq C \|\boldsymbol{\psi}_h\|_{r,\Gamma} \qquad \text{for all } \boldsymbol{\psi}_h \in \mathbb{Y}_h \tag{62}$$

and $r = \pm 1$. Notice that this result also holds with $r = 0$ as we saw in (60). Now the case $r = \pm 1/2$ can be shown by interpolation. From this inequality the result follows with the same argument as in the proof of Proposition 22.

It remains then to prove (61), which follows from a standard argument. Given $\psi \in H^1(\Gamma)$, we take the unique $\psi_h \in Y_h$ satisfying

$$\int_\Gamma \varphi_h \, \eta \, (\psi - \psi_h) = 0 \qquad \text{for all } \varphi_h \in Y_h.$$

Then

$$\begin{aligned}\|\psi-\psi_h\|_{1,\Gamma} &\le \|\psi-\pi_h\psi\|_{1,\Gamma}+\|\pi_h\psi-\psi_h\|_{1,\Gamma}\\ &\le C\left[\|\psi\|_{1,\Gamma}+h^{-1}\|\pi_h\psi-\psi_h\|_{0,\Gamma}\right]\\ &\le C'\left[\|\psi\|_{1,\Gamma}+h^{-1}\|\pi_h\psi-\psi\|_{0,\Gamma}\right]\le C''\|\psi\|_{1,\Gamma}\end{aligned}$$

by (56) and (58). This last bound means that computation of ψ_h from ψ is stable in $H^1(\Gamma)$. Since stability for Petrov-Galerkin schemes is equivalent to inf-sup conditions, the previous assertion implies that (61) holds. Again, the last statement follows from continuous dependence of the operator on s. □

Proposition 24 *Let $\boldsymbol{\psi}_h$ be the solution of* (55) *or* (59)*. Then*

$$\|\boldsymbol{\psi}-\boldsymbol{\psi}_h\|_{-k-1,\Gamma}\le C(s)\,h^{2k+2}\|\boldsymbol{\psi}\|_{k+1,\Gamma}$$

where $C(s)\le C\,C_0(s)^3\,D_0(s)^2\,D_{k+1}(s)$.

Proof The proof is based on the Aubin–Nitsche technique. Notice first that Proposition 22 is valid for both (55) and (59). It follows from Proposition 22 and the approximation properties (54a) and (57) that

$$\|\boldsymbol{\psi}-\boldsymbol{\psi}_h\|_{0,\Gamma}\le C_0(s)\,D_0(s)\,Ch^{k+1}\|\boldsymbol{\psi}\|_{k+1,\Gamma}. \tag{63}$$

Let $\mathcal{W}^*(s)$ be the adjoint of $\mathcal{W}(s)$. For arbitrary $\boldsymbol{\varphi}\in\mathbb{H}^{k+1}(\Gamma)$ we define $\boldsymbol{\rho}\in\mathbb{H}^{k+1}(\Gamma)$ satisfying $\mathcal{W}^*(s)\boldsymbol{\rho}=\boldsymbol{\varphi}$ and

$$\boldsymbol{\rho}_h\in\mathbb{X}_h\ (\text{rsp. }\mathbb{Y}_h)\ \text{s.t.}\quad \int_\Gamma \boldsymbol{\xi}_h\cdot\mathcal{W}^*(s)(\boldsymbol{\rho}-\boldsymbol{\rho}_h)=0\quad \text{for all }\boldsymbol{\xi}_h\in\mathbb{X}_h\ (\text{rsp. }\mathbb{Y}_h).$$

Then

$$\begin{aligned}\|\boldsymbol{\rho}-\boldsymbol{\rho}_h\|_{0,\Gamma} &\le C_0(s)\,D_0(s)\,Ch^{k+1}\|\boldsymbol{\rho}\|_{k+1,\Gamma}\\ &\le C_0(s)\,D_0(s)\,D_{k+1}(s)\,Ch^{k+1}\|\boldsymbol{\varphi}\|_{k+1,\Gamma}\end{aligned}$$

and therefore

$$\begin{aligned}\|\boldsymbol{\psi}-\boldsymbol{\psi}_h\|_{-k-1,\Gamma} &= \sup_{\boldsymbol{\varphi}\in\mathbb{H}^{k+2}(\Gamma)}\frac{1}{\|\boldsymbol{\varphi}\|_{k+1,\Gamma}}\left|\int_\Gamma(\boldsymbol{\psi}-\boldsymbol{\psi}_h)\cdot\mathcal{W}^*(s)\boldsymbol{\rho}\right|\\ &\le \sup_{\boldsymbol{\varphi}\in\mathbb{H}^{k+2}(\Gamma)}\frac{1}{\|\boldsymbol{\varphi}\|_{k+1,\Gamma}}\left|\int_\Gamma\mathcal{W}(s)(\boldsymbol{\psi}-\boldsymbol{\psi}_h)\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}_h)\right|\\ &\le \|\boldsymbol{\psi}-\boldsymbol{\psi}_h\|_{0,\Gamma}\,C\,h^{k+1}C_0(s)^2\,D_0(s)\,D_{k+1}(s).\end{aligned}$$

This and (63) prove the result. □

8 Full analysis

We are now in a position to give bounds for the term $\|T_N(U-U_h)(t)\|_X$ in the total error bound (23) for several choices of X. The exact integral system to be solved is $\mathcal{W}(s)\boldsymbol{\psi}(s)=\boldsymbol{g}(s)$ with the right hand side $\boldsymbol{g}(s)$ defined after (10). The solution $\boldsymbol{\psi}(s)$ is plugged into the corresponding potential $U(s)=\mathcal{P}(s)\boldsymbol{\psi}(s)$. This has to be done for the values $s_j^{(N)}=\gamma(j\,h_N)\in\mathcal{T}:=\{\gamma(\omega)\,|\,\omega\in\mathbb{R}\}$. We will also use the notation $\mathcal{T}_N:=\{\gamma(\omega)\,|\,\omega_{-N}^{(N)}\le\omega\le\omega_N^{(N)}\}$. The numerical solution $\psi_h(s)$, be it in $\mathbb{X}_h$ or $\mathbb{Y}_h$, is also the input in the approximate potential $U_h(s)=\mathcal{P}(s)\boldsymbol{\psi}_h(s)$. Notice that for points in the contour $\mathcal{T}$, $1/\delta(s)=O(|s|^{-1})$ and that $P_k(|s|)=O(|s|^k)$.

Lemma 25 *For $s\in\mathcal{T}$, $C_r(s)=O(|s|)$ for all $r\in[-1/2,1/2]$. Also $D_j(s)=O(|s|^{j+2})$ for all integers $j\ge0$.*

Proof Since $C_{\pm1/2}(s)=O(|s|)$ by Theorem 21, the first result follows by interpolation. The second one can be shown as follows using Theorem 19:

$$D_j(s)\le D_{j-1/2}(s)^{1/2}D_{j+1/2}(s)^{1/2}=O(|s|^{\lfloor\frac{j}{2}\rfloor+\lfloor\frac{j+1}{2}\rfloor+2})=O(|s|^{j+2}).$$

□

Theorem 26 *Let $[t_0,T]\subset(0,\infty)$ be a compact interval, $m\in\{1,2\}$, and $k\in\mathbb{N}$. Moreover, let $\boldsymbol{\psi}_h(s)\in\mathbb{Y}_h$ be the Galerkin approximation to $\boldsymbol{\psi}(s)$ and $U_h(s)=\mathcal{P}(s)\boldsymbol{\psi}_h(s)$. Then there exist constants $C_1,C_2>0$ such that*

$$\|u(t)-(T_NU_h)(t)\|_{m,\Omega^-\cup\Omega^+}\le C_1e^{-c\,N/\ln N}+C_2\,h^{k+5/2-m},\qquad t\in[t_0,T]\tag{64}$$

for all $N\in\mathbb{N}$ and all $h\le h_0(\mathcal{T}_N)$.

Proof Applying (51), Proposition 23, Lemma 25 and the approximation property (57), we can prove the following chain of inequalities, valid for $s\in\{s_j^{(N)},j=-N,\dots,N\}$

$$\begin{aligned}\|U(s)-U_h(s)\|_{2,\Omega^-\cup\Omega^+}&\le O(|s|)\,\|\boldsymbol{\psi}(s)-\boldsymbol{\psi}_h(s)\|_{1/2,\Gamma}\\&\le O(|s|^4)\inf_{\boldsymbol{\varphi}_h\in\mathbb{Y}_h}\|\boldsymbol{\psi}(s)-\boldsymbol{\varphi}_h\|_{1/2,\Gamma}\\&\le O(|s|^4)\,h^{k+1/2}\|\boldsymbol{\psi}(s)\|_{k+1,\Gamma}\\&\le O(|s|^{k+7})h^{k+1/2}\|\boldsymbol{g}(s)\|_{k+1,\Gamma}.\end{aligned}$$

With this bound, the result with $m=2$ is a simple consequence of Lemma 10 and Corollary 6. The case $m=1$ is similar. □

Theorem 27 *Let $[t_0,T]\subset(0,\infty)$ be a compact interval and $k\in\mathbb{N}$. Let $U_h(s)=\mathcal{P}(s)\boldsymbol{\psi}_h(s)$ with $\boldsymbol{\psi}_h(s)\in\mathbb{X}_h$ the corresponding Galerkin approximation to $\boldsymbol{\psi}(s)$. Then there exist constants $C_1,C_2>0$ such that*

$$\|u(t)-(T_NU_h)(t)\|_{1,\Omega^-\cup\Omega^+}\le C_1e^{-c\,N/\ln N}+C_2\,h^{k+1},\qquad t\in[t_0,T]$$

for all $N\in\mathbb{N}$ and all $h\le h_0(\mathcal{T}_N)$.

Proof In this case we begin with the rougher estimate

$$\|U(s) - U_h(s)\|_{2,\Omega^- \cup \Omega^+} \le O(|s|)\, \|\boldsymbol{\psi}(s) - \boldsymbol{\psi}_h(s)\|_{0,\Gamma}$$

and use then Proposition 22 instead of Proposition 23. Now we obtain that $\sup_{j=-N,\cdots,N} \|U(s_j^{(N)}) - U_h(s_j^{(N)})\|_{2,\Omega^- \cup \Omega^+} = O(h^{k+1})$ using the same argument as in the proof of Theorem 26. Hence, the result follows from Corollary 6. □

Notice that the result for $\mathbb{X}_h$ is worse, since we have only used stability in $\mathbb{H}^0(\Gamma)$ of the Galerkin approximation. This however allows for general meshes and discontinuous boundary elements. Finally, we show a faster rate of convergence on the top boundary H, which is important for the solution of the inverse problem mentioned in the introduction.

Theorem 28 *Let $[t_0, T] \subset (0, \infty)$ be a compact interval and $k \in \mathbb{N}$. Moreover, let $U_h(s) = \mathcal{P}(s)\boldsymbol{\psi}_h(s)$ with $\boldsymbol{\psi}_h(s) \in \mathbb{X}_h$ or $\mathbb{Y}_h$ be the corresponding Galerkin approximation to $\boldsymbol{\psi}(s)$. Then there exist constants $C_1, C_2 > 0$ such that*

$$\|u(t) - (T_N U_h)(t)\|_{L^\infty(H)} \le C_1 e^{-cN/\ln N} + C_2\, h^{2k+2}, \qquad t \in [t_0, T]$$

for all $N \in \mathbb{N}$ and all $h \le h_0(\mathcal{T}_N)$.

Proof Since $U(s) - U_h(s) = \widetilde{\mathcal{S}}_{\lambda(s)}(\psi^+(s) - \psi_h^+(s))$, with $\lambda(s)^2 = -s/\kappa_+$, it follows readily that

$$\|U(s) - U_h(s)\|_{L^\infty(H)} \le \sup_{\mathbf{x} \in H} \|\Phi_{\lambda(s)}(\mathbf{x}, \cdot)\|_{k+1,\Gamma}\, \|\boldsymbol{\psi}(s) - \boldsymbol{\psi}_h(s)\|_{-k-1,\Gamma}.$$

For points $s \in \mathcal{T}_N$ we can give a polynomial bound for the first term in the preceding inequality. By Proposition 24 and the same arguments as those given in Theorems 26 and 27, we can easily prove that $\sup_{j=-N,\ldots,N} \|(U - U_h)(s_j^{(N)})\|_{L^\infty(H)} = O(h^{2k+2})$. Finally, we need a bound like (18) with $X = L^\infty(H)$. This follows from a basic inequality

$$\|U(s)\|_{L^\infty(H)} \le C\, C_{-1/2}(s) \sup_{\mathbf{x} \in H} \|\Phi_{\lambda(s)}(\mathbf{x}, \cdot)\|_{1/2,\Gamma}\, C_{-1/2}(s)\, \|\boldsymbol{g}(s)\|_{-1/2,\Gamma}$$

together with Theorem 21, Lemma 10 and a direct bound for $\Phi_{\lambda(s)}$. □

9 Numerical results

To test the proposed method numerically we have chosen a simpler problem for which we know the exact solution explicitly. We consider the heat equation $\partial_t u = \Delta u$ in a two-dimensional exterior domain shown in Fig. 2 with a heat source $u_{\text{hom}}(x, t) = t^{-1} \exp(-|x - x_0|/t)$ located at a point x_0 in the interior domain, the Dirichlet condition $u = u_{\text{hom}}$ on the boundary, and the initial condition $u(\cdot, 0) = 0$. Obviously, the unique solution is given by $u = u_{\text{hom}}$.

Since the convergence of the space discretization is standard, we only studied the convergence of the time discretization, i.e. the limit $N \to \infty$

N	rel. error
5	3.18 e-4
10	1.27 e-4
15	1.16 e-5
20	1.44 e-6
25	2.55 e-7
30	1.94 e-8
35	5.46 e-9
40	2.93 e-10
45	1.18 e-10
50	5.32 e-12
55	2.98 e-12
60	2.46 e-13

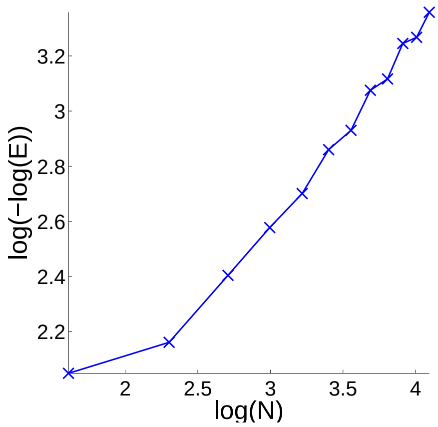

Fig. 1 Time discretization error in dependence of the number $2N+1$ of quadrature points in the Laplace domain for $\lambda = t = 1$.

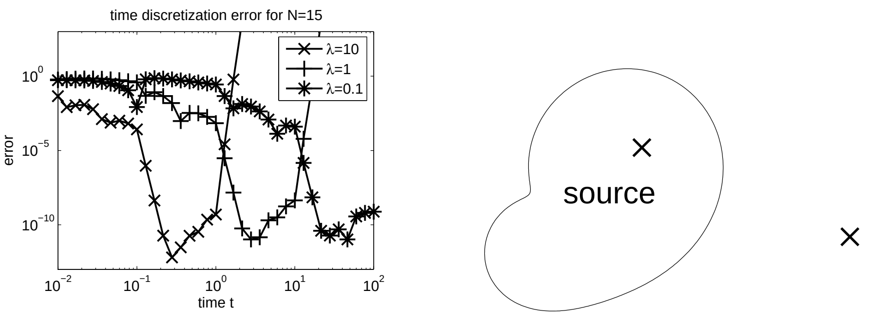

Fig. 2 Left: Time discretization errors for three different values of the parameter λ in (19) with $\alpha = \pi/4$. Right: Geometry of the test problem.

using a very fine space discretization with an extrapolation scheme. Our numerical experiments suggest that $h_0(\mathcal{T}_N)$ depends not or only weakly on N. Due to the symmetry of the quadrature points, $N+1$ stationary boundary value problems have to be solved for a given value of N. We compared the computed solution to the exact solution at the point indicated in the right panel of Fig. 2. Even for small values of N the time discretization errors are very small, and they decay at an exponential rate (see Fig. 1). We have also investigated the dependence of the time discretization error on t for $N = 40$. The results shown in Fig. 2 indicate that with an appropiate choice of the parameter λ in (19) the time discretization errors are almost independent of the values of t_0 and T over many orders of magnitudes, but only depend on T/t_0.

Acknowledgements We would like to thank Dr. María–Luisa Rapún for her generous help with the numerical experiments. F.–J. Sayas was partially supported by MCYT Projects MTM2004-019051 and MAT2002–04153.

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