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Technische Hochschule
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Mathematik

Time discretization of parabolic boundary integral equations

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Abstract

In time-dependent boundary integral equations, a boundary element method in space can be coupled with a different type of discretization in time. For the latter a procedure based on linear multistep methods is proposed, which is applicable whenever the Laplace transform of the fundamental solution is known. The stability properties of the method are obtained from those of the underlying multistep method. In the absence of a space discretization, the numerical solution given by the proposed method is identical to that of a semi-discretization in time of the partial differential equation by the underlying multistep method. The theory is presented for the single layer potential equation of the heat equation. Convergence estimates, which are pointwise in time and expressed in terms of the boundary data, are obtained for full discretizations using Galerkin or collocation boundary element methods in space. Numerical examples are included.

Keywords: boundary integral equation, parabolic differential equation, convolution quadrature, multistep method, boundary element method, Galerkin, collocation, parameter-dependent pseudodifferential calculus

AMS(MOS) Subject Classification: 65R20, 65M10, 47G05, 45A05

1. Introduction

The present article is concerned with numerical methods for boundary integral equations for *parabolic* partial differential equations, and with their analysis. Similarly to the elliptic case, an efficient numerical solution of boundary integral equations is of interest in the following situations: For problems formulated on the boundary of the spatial domain (e.g., to compute the heat flow through the boundary from the given surface temperature), for exterior problems posed on unbounded domains with bounded boundary, and for problems where the solution, or a derivative thereof, is sought only in a small portion of the domain.

The *spatial* discretization by boundary elements can be done for parabolic problems in much the same way as for the elliptic case, but it has to be coupled to a *time discretization.* The latter is the main theme of the present article. We study a class of quadrature methods whose construction is based on a linear multistep method and the Laplace transform of the fundamental solution. The time-dependent fundamental solution need not itself be known explicitly, even though all computations with the boundary data and solution are done in time domain. The computational work is almost linear in the number of time steps, and only one matrix factorization of a boundary element matrix is needed. In the absence of a space discretization, the semi-discrete solution obtained from the proposed time discretization of the boundary integral equation is identical to that of a multistep time discretization of the partial differential equation. The temporal stability properties follow from those of the underlying multistep method, also in the fully discrete case.

Sacrificing generality for concreteness, we have chosen to present the methods and their theory only for the single layer potential equation of the heat equation. This can be extended without new difficulties to other boundary integral equations for the heat equation (see [8]) and, in fact, for quite general linear parabolic differential equations. For example, we expect our techniques to extend rather straightforwardly to boundary integral equations for the nonstationary Stokes problem. While the presented theory only pertains to parabolic problems, the formulation of the method applies equally well to boundary integral equations for the wave equation and for nonstationary equations in elasticity, which have been used in important engineering applications [4]. The analysis of such problems will have to be the subject of further study. A numerical example of the proposed time discretization methods for an integral equation for a time-dependent Schrödinger equation is given in [18].

A solution theory of boundary integral equations for the heat equation has been developed only very recently. A substantial and surprising result, discovered independently by Arnold & Noon [5] and Costabel [8], states that the single layer heat potential operator is *elliptic* in an anisotropic Sobolev space, with exponents $-\frac{1}{2}$ w.r.t. space and $-\frac{1}{4}$ w.r.t. time. The corresponding theory can be viewed as a counterpart of Lions & Magenes' [16] theory of parabolic differential equations in related anisotropic spaces. In contrast, the theory developed here is rather related to the theory of analytic semigroups (e.g. [15]), in that it is based on a Dunford-Taylor operational calculus over sectorial regions of the complex plane, combined with the study of the single layer potential operator for the parameter-dependent

equation $\lambda u - \Delta u = 0$. The latter is done with the help of a parameter-dependent pseudo-differential calculus as developed by Agranovich [2]. This approach allows us to obtain a-priori estimates *pointwise in time*, which would not follow with the theory of [5] and [8]. Apart from these analytical subtleties, the two different approaches to the theory form the basis of two entirely different numerical methods: Galerkin in both space and time as in [5],[8], vs. convolution quadrature in time coupled with a Galerkin or collocation boundary element method in space as considered here. Unlike [5] and [8], our convergence estimates are pointwise in time and are given in terms of the boundary data. This allows us to cover also the case of heat shocks. Estimates in terms of the solution could also have been obtained here, but they appear to be of less interest in view of the generally low regularity of the solution near $t = 0$. We note that our results are shown only for smooth spatial domains, whereas general Lipschitz domains are treated in [8].

An outline of the paper is as follows: In Section 2 we study mapping properties of the single layer heat potential operator. Section 3 deals with the construction of the solution of the heat equation with non-homogeneous Dirichlet boundary conditions via heat potentials. These two sections develop the analytical framework for the numerical methods. Section 4 introduces semi-discretization in time by operational quadrature methods. In Sections 5 and 6 this is coupled with space discretization by Galerkin and collocation boundary element methods, respectively. Section 7 describes the implementation of the proposed methods and reports on numerical experiments.

2. The single layer potential operator for the heat equation

Throughout this paper, Γ will denote the boundary of a smooth bounded domain Ω in $\mathbf{R}^d$, with $d = 2$ or 3, and $I = [0, \overline{t}]$ denotes the time interval. We are interested in solving the equation

$$\mathcal{V}\varphi = g \qquad \text{on } \Gamma \times I \tag{2.1}$$

where $\mathcal{V}$ is the single layer heat potential operator, defined for $\varphi \in C(\Gamma \times I)$ by

$$(\mathcal{V}\varphi)(x,t) = \int_0^t \int_\Gamma k(x-y, t-s)\varphi(y,s)\,dy\,ds\ , \qquad x \in \Gamma\ ,\ 0 \le t \le \overline{t}\ , \tag{2.2}$$

with k denoting the fundamental solution of the heat equation. We shall actually need only the Laplace transform $K(x,\lambda)$ of $k(x,t)$ which is the fundamental solution of the stationary differential equation $\lambda u - \Delta u = 0$:

$$K(x,\lambda) = \begin{cases} \frac{1}{2\pi} K_0(|x| \cdot \sqrt{\lambda}) & d = 2 \\ \frac{1}{4\pi|x|} \exp(-|x| \cdot \sqrt{\lambda}) & d = 3 \end{cases} \tag{2.3}$$

where K_0 denotes the modified Bessel function of order 0. The associated integral operator $V(\lambda)$ given for $\psi \in C(\Gamma)$ by

$$(V(\lambda)\psi)(x) = \int_\Gamma K(x-y,\lambda)\,\psi(y)\,dy\ , \qquad x \in \Gamma \tag{2.4}$$

is thus the single layer potential operator corresponding to the equation $-\Delta u + \lambda u = 0$ on Ω.

Our study of equation (2.1) relies heavily on mapping properties of the operators $V(\lambda)$.

Theorem 2.1. *Let the sectorial region $\Lambda = \{\lambda \in \mathbf{C} : |\arg\lambda| \le \pi - \phi, |\lambda| \ge R\}$, with $0 < \phi < \frac{\pi}{2}$, and sufficiently large R. For $\lambda \in \Lambda$, the operator $V(\lambda)$ defined by (2.4) can be extended to an isomorphism*

$$V(\lambda) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$$

with

$$\begin{aligned} \|V(\lambda)\psi\|_{H^{1/2}} &\le C\,\|\psi\|_{H^{-1/2}} \\ \mathrm{Re}\,\langle V(\lambda)\psi,\psi\rangle &\ge \frac{\alpha}{\sqrt{|\lambda|}}\,\|\psi\|^2_{H^{-1/2}} \qquad \textit{for all } \psi \in H^{-1/2}(\Gamma)\ . \end{aligned}$$

The constants C and $\alpha > 0$ are independent of $\lambda \in \Lambda$. Moreover, the mapping $\lambda \mapsto V(\lambda)$ is analytic.

Proof. We consider first the case of a half-space, $\Omega = \mathbf{R}^d_+ = \{(x', x_d) \in \mathbf{R}^d : x_d > 0\}$. This shows the basic estimates in a nontechnical setting. The powerful machinery of pseudodifferential calculus then allows us to extend the result to general smooth bounded domains Ω.

(a) With $\Omega = \mathbf{R}^d_+$ we have $\Gamma = \mathbf{R}^{d-1} \times 0$, and $V(\lambda)$ is given for $\psi \in C_0^\infty(\Gamma)$ by the relation

$$\mathcal{F}V(\lambda)\psi(\xi) = \tfrac{1}{2}(\lambda + |\xi|^2)^{-1/2} \cdot \mathcal{F}\psi(\xi)$$

where $\mathcal{F}$ denotes the $(d-1)$-dimensional Fourier transform. Since

$$\left|\tfrac{1}{2}\frac{(1+|\xi|^2)^{1/2}}{(\lambda+|\xi|^2)^{1/2}}\right| \le C\ , \qquad \xi \in \mathbf{R}^{d-1}\ ,\ \lambda \in \Lambda\ , \tag{2.5}$$

we have with $\widehat{\psi} = \mathcal{F}\psi$

$$\|V(\lambda)\psi\|_{H^{1/2}} = \|(1+|\xi|^2)^{1/4} \cdot \tfrac{1}{2}(\lambda+|\xi|^2)^{-1/2}\widehat{\psi}\|_{L^2} \le C\,\|(1+|\xi|^2)^{-1/4}\widehat{\psi}\|_{L^2} = C\,\|\psi\|_{H^{-1/2}}\ .$$

In a similar way, since

$$\mathrm{Re}\ \tfrac{1}{2}\frac{(1+|\xi|^2)^{1/2}}{(\lambda+|\xi|^2)^{1/2}} \ge \alpha|\lambda|^{-1/2}\ , \qquad \xi \in \mathbf{R}^{d-1}\ ,\ \lambda \in \Lambda\ , \tag{2.6}$$

holds for some $\alpha > 0$, we have

$$\begin{aligned}\mathrm{Re}\,\langle V(\lambda)\psi,\psi\rangle = \mathrm{Re}\int_{\mathbf{R}^{d-1}} \tfrac{1}{2}(\lambda+|\xi|^2)^{-1/2}|\widehat{\psi}|^2 d\xi = \\ \mathrm{Re}\int_{\mathbf{R}^{d-1}} \tfrac{1}{2}\frac{(1+|\xi|^2)^{1/2}}{(\lambda+|\xi|^2)^{1/2}}\,|(1+|\xi|^2)^{-1/4}\widehat{\psi}|^2\,d\xi \geq \\ \int_{\mathbf{R}^{d-1}} \alpha|\lambda|^{-1/2}\,|(1+|\xi|^2)^{-1/4}\widehat{\psi}|^2\,d\xi = \alpha|\lambda|^{-1/2}\,\|\psi\|^2_{H^{-1/2}}\ .\end{aligned}$$

This establishes the required inequalities in the case $\Omega = \mathbf{R}^d_+$.

(b) When $\Omega \subset \mathbf{R}^d$ is an arbitrary smooth domain with boundary Γ, we use the parameter-dependent pseudodifferential calculus as developed by Agranovich [2], cf. also Shubin [28], Section 9. $V(\lambda)$ can be considered as a pseudodifferential operator of the class $CL_2^{-1}(\Gamma,\Lambda)$ in the notation of [28], p.76, with principal symbol locally of the form

$$v_{-1}(x,\xi,\lambda) = (\lambda+|A(x)\xi|^2)^{-1/2}\ , \qquad x\in\Gamma,\ \xi\in\mathbf{R}^{d-1}\ ,\ \lambda\in\Lambda\ ,$$

where the nonsingular matrix $A(x)$ is the Jacobian of a local coordinate transform. Hence the symbol still satisfies estimates as in (2.5), (2.6). With the Gårding inequality Prop. 2.9 of [2] and with the techniques used in the proofs of its corollaries in [2], one can then conclude the desired estimates of Theorem 2.1 for sufficiently large $|\lambda|$.

(c) The Lax-Milgram lemma then shows that $V(\lambda) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is an isomorphism with

$$\|V(\lambda)^{-1}\|_{H^{-1/2}\leftarrow H^{1/2}} \leq \frac{1}{\alpha}\,|\lambda|^{1/2}\ , \qquad \lambda\in\Lambda\ . \tag{2.7}$$

(d) Finally, to get the analyticity of $\lambda \mapsto V(\lambda)$ we begin with the fact that $\langle V(\lambda)\psi_1,\psi_2\rangle$ is analytic for every $\psi_1,\psi_2 \in C(\Gamma)$, which is seen immediately from (2.4). Since $\|V(\lambda)\|$ is locally bounded, the result is then obtained from Theorem III.3.12 in Kato [15], p.152, and the remark following it. □

With the Laplace inversion formula in mind, we will now express the single layer heat potential operator $\mathcal{V}$ and its inverse in terms of the operators $V(\lambda)$. The construction resembles that of analytic semigroups, cf. e.g. Kato [15], Ch.IX. Our main tool in this construction, and later on in the analysis of the numerical approximation schemes, will be the representation formula given in the following lemma, which we formulate in an abstract setting.

Lemma 2.2. *Let Λ be a sectorial region as in Theorem 2.1. Suppose that $T(\lambda)$, $\lambda\in\Lambda$, is an analytic family of linear operators between Banach spaces E and F, whose operator norms satisfy for some $0\leq\gamma<1$*

$$\|T(\lambda)\| \leq c\cdot|\lambda|^{\gamma}\ , \qquad \lambda\in\Lambda\ . \tag{2.8}$$

(a) For $g \in C^\mu(I,E)$ with $\gamma < \mu \le 1$, the formula

$$(\mathcal{T}g)(t) = \frac{1}{2\pi i}\int_L \lambda^{-1}T(\lambda)\frac{d}{dt}\int_0^t e^{\lambda(t-s)}g(s)\,ds\,d\lambda \ , \tag{2.9}$$

with complex contour $L \subset \Lambda$ parallel to the boundary of Λ, defines $(\mathcal{T}g)(t) \in F$ satisfying

$$\|(\mathcal{T}g)(t)\| \le C\cdot\left(t^{-\gamma}\|g(0)\| + |g|_{C^\mu}\right) \ , \qquad 0 < t \le T \ , \tag{2.10}$$

with the Hölder seminorm $|g|_{C^\mu} = \sup_{0\le s<t\le T}\|g(t)-g(s)\|/|t-s|^\mu$.
(b) For every $\gamma < \mu \le 1$ and $\alpha < \mu - \gamma$, one has a continuous mapping

$$\mathcal{T} : \{g \in C^\mu(I,E); g(0) = 0\} \to C^\alpha(I,F) \ . \tag{2.11}$$

(The restriction $g(0) = 0$ can be dropped, if $\gamma = 0$.)
*(c) If $g \in C^\mu([0,\infty),E)$ with $\mu > \gamma$ is exponentially bounded *, then so is $\mathcal{T}g \in C((0,\infty),F)$. Hence Laplace transforms of both g and $\mathcal{T}g$ exist, and they satisfy*

$$\mathcal{L}(\mathcal{T}g)(\lambda) = T(\lambda)\cdot(\mathcal{L}g)(\lambda) \ . \tag{2.12}$$

Proof. (a) We split

$$g(s) = [g(s)-g(r)] + [g(r)-g(0)] + g(0) \ ,$$

and so

$$\frac{d}{dt}\int_0^t e^{\lambda(t-s)}g(s)\,ds = \lambda\int_0^t e^{\lambda(t-s)}[g(s)-g(r)]\,ds + e^{\lambda t}[g(r)-g(0)] + e^{\lambda t}g(0) \ .$$

Choosing $r = t$, it follows that for $\lambda \in L$

$$\|\frac{d}{dt}\int_0^t e^{\lambda(t-s)}g(s)\,ds\| \le C\left(|\lambda|^{-\mu} + |t^\mu e^{\lambda t}|\right)\cdot|g|_{C^\mu} + |e^{\lambda t}|\cdot\|g(0)\|$$

In view of the bound on $T(\lambda)$, this implies that $(\mathcal{T}g)(t)$ is defined by absolutely convergent integrals, and is bounded by (2.10).

(c) It is convenient to show (c) before (b). We have

$$\mathcal{L}\left(\frac{d}{dt}\int_0^t e^{\lambda(t-s)}g(s)\,ds\right)(\lambda_0) = \frac{\lambda_0}{\lambda_0-\lambda}(\mathcal{L}g)(\lambda_0) \ ,$$

*in the sense that $\|g\|_{C^\mu([0,t],E)} \le Me^{Lt}$ for all $t > 0$, for some M, L

for λ_0 with sufficiently large real part. Under the given assumptions one may interchange integrals in $\mathcal{L}(\mathcal{T}g)$ to obtain

$$\mathcal{L}(\mathcal{T}g)(\lambda_0) = \frac{1}{2\pi i}\int_L \lambda^{-1}T(\lambda)\,\frac{\lambda_0}{\lambda_0-\lambda}(\mathcal{L}g)(\lambda_0)\,d\lambda = T(\lambda_0)\mathcal{L}g(\lambda_0)\ ,$$

where the last equality holds by Cauchy's integral formula.

(b) For $0 \le \alpha < \mu - \gamma$ and $g \in C^\mu(I,E)$, we set

$$(\mathcal{T}_\alpha g)(t) = \frac{1}{2\pi i}\int_L \lambda^{-1+\alpha}T(\lambda)\frac{d}{dt}\int_0^t e^{\lambda(t-s)}g(s)\,ds\,d\lambda\ .$$

Applying the result of (a) to $\lambda^\alpha T(\lambda)$ instead of $T(\lambda)$, one gets that

$$\mathcal{T}_\alpha : \{g \in C^\mu; g(0)=0\} \to C^0 \qquad \text{is continuous,}$$

and from (c) that

$$\mathcal{L}(\mathcal{T}_\alpha g)(\lambda) = \lambda^\alpha T(\lambda)\cdot(\mathcal{L}g)(\lambda)$$

for exponentially bounded g. It follows that

$$\mathcal{L}(\mathcal{T}g)(\lambda) = \lambda^{-\alpha}\cdot\mathcal{L}(\mathcal{T}_\alpha g)(\lambda)\ ,$$

and hence $\mathcal{T}g$ is the Abel-Liouville fractional integral of order α of $\mathcal{T}_\alpha g$: $\mathcal{T} = \mathcal{I}^\alpha\mathcal{T}_\alpha$ with

$$\mathcal{I}^\alpha f(t) = \frac{1}{\Gamma(\alpha)}\int_0^t (t-s)^{\alpha-1}f(s)\,ds\ .$$

Since $\mathcal{I}^\alpha$ maps C^0 continuously into C^α, see e.g. [11], p.223, we get the desired result. □

We are now ready for the study of the single layer heat potential equation (2.1).

Theorem 2.3. *For arbitrary $\delta > \epsilon > 0$, there are continuous operators*

$$\mathcal{V} : C^\delta(I, H^{-1/2}(\Gamma)) \to C^\epsilon(I, H^{1/2}(\Gamma))$$
$$\mathcal{V}^{(-1)} : \{g \in C^{1/2+\delta}(I, H^{1/2}(\Gamma)); g(0)=0\} \to C^\epsilon(I, H^{-1/2}(\Gamma))$$

with the following properties:

(a) $\mathcal{V}\varphi$ is given by (2.2) for $\varphi \in C^\infty(\Gamma\times I)$.

(b) For $g \in C^{1/2+\delta}(I, H^{1/2}(\Gamma))$ with $g(0)=0$, the equation $\mathcal{V}\varphi = g$ has in $C^\epsilon(I, H^{-1/2}(\Gamma))$ the unique solution $\varphi = \mathcal{V}^{(-1)}g$.

The operators $\mathcal{V}$ and $\mathcal{V}^{(-1)}$ are given by formula (2.9) with $V(\lambda)$ and $V(\lambda)^{-1}$ of Theorem 2.1 in the role of $T(\lambda)$.

Proof. Let $\mathcal{V}$ and $\mathcal{V}^{(-1)}$ be constructed as in Lemma 2.2. By part (b) of that lemma, and by the estimates of Theorem 2.1, they are then continuous operators between Hölder spaces as stated.

(a) For $\varphi \in C^2(\Gamma \times I)$, we have that

$$\psi_\lambda = \frac{d}{dt} \int_0^t e^{\lambda(t-s)} \varphi(s)\, ds \in C^1(\Gamma) \ ,$$

and hence $V(\lambda)\psi_\lambda \in C^1(\Gamma)$, with $V(\lambda)\psi_\lambda(x)$ given by (2.4) for $x \in \Gamma$. Moreover,

$$\int_L \lambda^{-1} V(\lambda)\psi_\lambda \, d\lambda \in C^1(\Gamma)$$

exists as a $C^1(\Gamma)$-valued (improper Riemann) integral, and because of the continuous inclusion $C^1(\Gamma) \subset H^{1/2}(\Gamma)$ it coincides with the $H^{1/2}(\Gamma)$-valued integral. Hence we have for $x \in \Gamma$

$$[(\mathcal{V}\varphi)(t)](x) = \frac{1}{2\pi i} \int_L \lambda^{-1} \int_\Gamma K(x-y,\lambda) \frac{d}{dt} \int_0^t e^{\lambda(t-s)} \varphi(y,s)\, ds\, dy\, d\lambda \ .$$

By the Laplace inversion formula

$$k(x,t) = \frac{1}{2\pi i} \int_L K(x,\lambda) e^{\lambda t}\, d\lambda \ ,$$

and by an application of Cauchy's integral theorem:

$$\int_L \lambda^{-1} K(x,\lambda) d\lambda = 0 \ , \qquad x \neq 0 \ ,$$

we get therefore the weakly singular integral

$$[(\mathcal{V}\varphi)(t)](x) = \int_0^t \int_\Gamma k(x-y, t-s) \varphi(y,s)\, dy\, ds \ ,$$

which is (2.2).

(b) We extend g to $g \in C^{1/2+\delta}([0,\infty), H^{1/2}(\Gamma))$ with compact support, and let $\varphi = \mathcal{V}^{(-1)} g$. By Lemma 2.2(c) we then have

$$\mathcal{L}\varphi = V(\lambda)^{-1} \mathcal{L} g \ ,$$

and

$$\mathcal{L}(\mathcal{V}\varphi) = V(\lambda)\mathcal{L}\varphi = \mathcal{L} g \ .$$

It follows that $\mathcal{V}\varphi = g$ on $[0,\infty)$, and by causality *a fortiori* on $[0,\overline{t}]$.

To prove uniqueness, we have to use a different argument. Suppose $\varphi \in C^\epsilon(I, H^{-1/2}(\Gamma))$, and $\mathcal{V}\varphi = 0$ on I. Then also

$$\mathcal{I}^2 \mathcal{V}^{(-1)} \mathcal{V}\varphi = 0 \qquad \text{on } [0,\overline{t}] \ ,$$

where $\mathcal{I}$ denotes the integration operator: $\mathcal{I}f(t) = \int_0^t f(s)\,ds$, and $\mathcal{I}^2 = \mathcal{I}\cdot\mathcal{I}$. The premultiplication with $\mathcal{I}^2$ makes it possible to interchange integrals as needed. We get

$$\mathcal{I}^2\mathcal{V}^{(-1)}\mathcal{V}\varphi(t) =$$
$$\frac{1}{2\pi i}\int_L \lambda^{-1}V(\lambda)^{-1}\frac{1}{2\pi i}\int_{L'}\mu^{-1}V(\mu)\frac{1}{2\pi i}\int_{L''}\frac{1}{\nu-\lambda}\frac{1}{\nu-\mu}\int_0^t e^{\nu(t-s)}\varphi(s)\,ds\,d\nu\,d\mu\,d\lambda$$

(with L'' to the right of L' to the right of L). By Cauchy's integral formula, this reduces to

$$\mathcal{I}^2\mathcal{V}^{(-1)}\mathcal{V}\varphi(t) = \frac{1}{2\pi i}\int_{L''}\nu^{-2}\int_0^t e^{\nu(t-s)}\varphi(s)\,ds = \mathcal{I}^2\varphi(t)\ .$$

Hence $\mathcal{I}^2\varphi = 0$ on I, and this clearly implies $\varphi = 0$, proving the uniqueness of solutions. □

Remark. According to Lemma 2.2, $\mathcal{V}^{(-1)}$ can be extended to an operator $\mathcal{V}^{(-1)} : C^{1/2+\delta}(I, H^{1/2}(\Gamma)) \to C((0,\overline{t}], H^{-1/2}(\Gamma))$ satisfying for $0 < t \le \overline{t}$

$$\|(\mathcal{V}^{(-1)}g)(t)\|_{H^{-1/2}(\Gamma)} \le C\cdot(t^{-1/2}\|g(0)\|_{H^{1/2}(\Gamma)} + |g|_{C^{1/2+\delta}(I,H^{1/2}(\Gamma))})\ , \tag{2.13}$$

see formula (2.10).

3. Solution of the Dirichlet problem of the heat equation by heat potentials

In this section we consider the initial-boundary value problem for the heat equation,

$$\begin{aligned} \frac{\partial u}{\partial t} &= \Delta u && \text{in } \Omega\times(0,\overline{t}) \\ u &= g && \text{on } \Gamma\times(0,\overline{t}) \\ u &= 0 && \text{in } \Omega, \text{ at } t=0\ . \end{aligned} \tag{3.1}$$

If there exists $\varphi \in C(\Gamma\times I)$ as solution of the single layer potential equation $\mathcal{V}\varphi = g$, then it is known from classical theory, cf. Pogorzelski [21], that (3.1) is solved by

$$u(x,t) = (\mathcal{U}\varphi)(x,t) = \int_0^t\int_\Gamma k(x-y,t-s)\varphi(y,s)\,dy\,ds\ , \qquad x\in\Omega\ ,\ 0\le t\le\overline{t}\ , \tag{3.2}$$

which is in $C^\infty(\Omega\times(0,\overline{t}))\cap C(\overline{\Omega}\times[0,\overline{t}])$. For the purpose of obtaining a solution theory in terms of the Dirichlet data g, and later for the numerical analysis, we consider again the corresponding stationary operators, given for $\psi\in C(\Gamma)$ by

$$(U(\lambda)\psi)(x) = \int_\Gamma K(x-y,\lambda)\,\psi(y)\,dy\ , \qquad x\in\Omega\ . \tag{3.3}$$

We begin by studying the mapping properties of $U(\lambda)$ in appropriate Sobolev spaces.

Theorem 3.1. *Let Λ denote a sectorial region as in Theorem 2.1, and let $\lambda \in \Lambda$.*
(a) $U(\lambda)$ of (3.3) can be extended to a continuous operator $U(\lambda) : H^{-1/2}(\Gamma) \to H^1(\Omega)$ satisfying

$$\begin{aligned} \|U(\lambda)\psi\|_{H^1(\Omega)} &\le C \cdot \|\psi\|_{H^{-1/2}(\Gamma)} \\ \|U(\lambda)\psi\|_{H^{-1}(\Omega)} &\le \frac{C}{|\lambda|} \cdot \|\psi\|_{H^{-1/2}(\Gamma)} \end{aligned} \qquad \text{for all } \psi \in H^{-1/2}(\Gamma) .$$

The constants are independent of $\lambda \in \Lambda$.
(b) Let $g \in H^{1/2}(\Gamma)$, and denote $\varphi = V(\lambda)^{-1} g \in H^{-1/2}(\Gamma)$, and $u = U(\lambda)\varphi \in H^1(\Omega)$. Then u is the unique solution of the boundary value problem

$$\begin{aligned} -\Delta u + \lambda u &= 0 \qquad \text{in } \Omega \\ u &= g \qquad \text{on } \Gamma . \end{aligned} \tag{3.4}$$

Here the differential equation holds with equality in $H^{-1}(\Omega)$, and the boundary values are in the sense of traces. Moreover,

$$\begin{aligned} \|u\|_{H^1(\Omega)} &\le C\,|\lambda|^{1/2} \cdot \|g\|_{H^{1/2}(\Gamma)} \\ \|u\|_{H^{-1}(\Omega)} &\le C\,|\lambda|^{-1/2} \cdot \|g\|_{H^{1/2}(\Gamma)} \end{aligned}$$

with constants which do not depend on $\lambda \in \Lambda$.

Proof. (a) We again consider first the case $\Omega = \mathbf{R}^d_+$. Let $\psi \in C_0^\infty(\Gamma)$, and set $u = U(\lambda)\psi$, for some $\lambda \in \Lambda$. Then we have

$$(\mathcal{F}_{d-1} u)(\xi', x_d) = \tfrac{1}{2}(\lambda + |\xi'|^2)^{-1/2} \exp(-(\lambda + |\xi'|^2)^{1/2} x_d) \cdot \widehat{\psi}(\xi')$$

where $\mathcal{F}_{d-1}$ denotes the $(d-1)$-dimensional Fourier transform, with transform variables $\xi' \in \mathbf{R}^{d-1}$, and $\widehat{\psi} = \mathcal{F}_{d-1}\psi$. We define $h \in H^{1/2}(\Gamma)$ by setting

$$\widehat{h}(\xi') = (1 + |\xi'|^2)^{-1/2} \widehat{\psi}(\xi')$$

and consider h as the trace of $w \in H^1(\Omega)$, which is constructed as in the usual proof of the trace theorem, see Nečas [19], by

$$\mathcal{F}_{d-1} w(\xi', x_d) = \exp(-(1 + |\xi'|^2)^{1/2} x_d) \cdot \widehat{h}(\xi') .$$

Then

$$\|w\|_{H^1(\Omega)} = c \cdot \|h\|_{H^{1/2}(\Gamma)} = c \cdot \|\psi\|_{H^{-1/2}(\Gamma)}$$

where c is some nonzero constant.

When we extend u and w by reflection to all of $\mathbf{R}^d$: $u(x', -x_d) = u(x', x_d)$, then we obtain for $\widehat{u} = \mathcal{F}_d\, u$

$$\widehat{u}(\xi) = \frac{1 + |\xi|^2}{\lambda + |\xi|^2}\, \widehat{w}(\xi) , \qquad \xi \in \mathbf{R}^d .$$

It follows that

$$\|u\|_{H^1(\Omega)} \leq C \cdot \|w\|_{H^1(\Omega)} \ ,$$

and similarly we get

$$\|u\|_{H^{-1}(\Omega)} \leq \frac{C}{|\lambda|} \cdot \|w\|_{H^1(\Omega)} \ .$$

This gives the result for $\Omega = \mathbf{R}^d_+$.

For general smooth bounded $\Omega \subset \mathbf{R}^d$ we still have by local charts a continuous mapping

$$\psi \in H^{-1/2}(\Gamma) \mapsto w \in H^1(\Omega) \ ,$$

such that $u = U(\lambda)\psi$ is obtained from w by means of a pseudodifferential operator with principal symbol $\frac{1+|\xi|^2}{\lambda+|\xi|^2}$. As Ω is assumed to be bounded, it follows from the parameter-dependent pseudodifferential calculus, see Shubin [28], Theorem 9.1, that the mapping $w \mapsto u$ is bounded uniformly in $\lambda \in \Lambda$ (with sufficiently large R in the definition of Λ) as an operator $H^1(\Omega) \to H^1(\Omega)$, and bounded by $C \cdot |\lambda|^{-1}$ as an operator $H^1(\Omega) \to H^{-1}(\Omega)$. This gives us the first part of the theorem.

(b) Let us first recall that equation (3.4) has for $\lambda \in \Lambda$ a unique solution $u \in H^1(\Omega)$ for every $g \in H^{1/2}(\Gamma)$, which moreover depends continuously on g. Indeed, $g \in H^{1/2}(\Gamma)$ is the trace of a function $w \in H^1(\Omega)$ with $\|w\|_{H^1(\Omega)} \leq C \cdot \|g\|_{H^{1/2}(\Gamma)}$, and thus $u \in H^1(\Omega)$ is a solution of (3.4) if and only if $u_0 = u - w$ solves

$$-\Delta u_0 + \lambda u_0 = f \ , \qquad u_0 \in H^1_0(\Omega) \ ,$$

where $f = -\Delta w + \lambda w \in H^{-1}(\Omega)$ (via $\langle -\Delta w, v\rangle = (\nabla w, \nabla v)_{L^2}$ for $v \in H^1_0(\Omega)$). It follows from the spectral decomposition of $-\Delta$ with homogeneous Dirichlet boundary conditions (see e.g. [7], Ch. IX.8) that this equation has a unique solution $u_0 \in H^1_0(\Omega)$, with

$$\|u_0\|_{H^1(\Omega)} \leq C \cdot \|f\|_{H^{-1}(\Omega)} \leq C_1(\lambda) \cdot \|w\|_{H^1(\Omega)} \leq C_2(\lambda) \cdot \|g\|_{H^{1/2}(\Gamma)} \ .$$

Hence $u = u_0 + w \in H^1(\Omega)$ is the unique solution of (3.4) in the sense stated, and depends continuously on $g \in H^{1/2}(\Gamma)$.

Let now $g = V(\lambda)\psi$ with $\psi \in C^2(\Gamma)$. By Theorem 2.1, the set of all such g's is dense in $H^{1/2}(\Gamma)$. Then we have that

$$u = U(\lambda)\psi \in C^\infty(\Omega) \cap C^2(\overline{\Omega})$$

is given by (3.3), and is a classical solution of (3.4). Hence, $T(\lambda) = U(\lambda)V(\lambda)^{-1} : H^{1/2}(\Gamma) \to H^1(\Omega)$ coincides with the solution operator of (3.4) on a dense subset of $H^{1/2}(\Gamma)$, and by continuity the two operators are therefore identical.

Finally, the stated bounds for $u = T(\lambda)g$ follow directly from those given in Theorem 2.1 (formula (2.7)) and in part (a) of the present theorem. □

The solution of the Dirichlet problem of the heat equation can now be constructed as follows.

Theorem 3.2. *(a) For arbitrary $\epsilon > 0$, there is a continuous operator*

$$\mathcal{U} : C^{\epsilon}(I, H^{-1/2}(\Gamma)) \to C(I, H^1(\Omega))$$

such that $\mathcal{U}\varphi$ is given by (3.2) for $\varphi \in C^{\infty}(\Gamma \times I)$. This operator $\mathcal{U}$ is given by formula (2.9), with $U(\lambda)$ in the role of $T(\lambda)$.

(b) For arbitrary $\delta > \epsilon > 0$, let $g \in C^{1/2+\delta}(I, H^{1/2}(\Gamma))$ with $g(0) = 0$, and let $\varphi \in C^{\epsilon}(I, H^{-1/2}(\Gamma))$ be the solution of the single layer potential equation $\mathcal{V}\varphi = g$. Then

$$u = \mathcal{U}\varphi \in C(I, H^1(\Omega)) \cap C^1(I, H^{-1}(\Omega))$$

is the unique solution of the initial-boundary value problem (3.1), with equality in $H^{-1}(\Omega)$ pointwise in time in the differential equation, and with boundary values taken in the sense of traces.

Proof. Part (a) follows from Theorem 3.1(a) with the arguments used in the proof of Theorem 2.3(a). To prove (b), let us denote $\mathcal{T} = \mathcal{U}\mathcal{V}^{(-1)}$, and $T(\lambda) = U(\lambda)V(\lambda)^{-1}$. By the estimate on $T(\lambda)$ which follows from Theorems 2.1 and 3.1, and by Lemma 2.2, we thus have for $g \in C^{1/2+\delta}(I, H^{1/2}(\Gamma))$ that

$$u(t) = (\mathcal{T}g)(t) = \frac{1}{2\pi i}\int_L \lambda^{-1}T(\lambda)\frac{d}{dt}\int_0^t e^{\lambda(t-s)}g(s)\,ds\,d\lambda \ \in H^1(\Omega)$$

From Theorem 3.1(b) we know that $T(\lambda)h \in H^1(\Omega)$ solves the Dirichlet problem (3.4) for boundary values $h \in H^{1/2}(\Gamma)$. So we get, with equalities in $H^{-1}(\Omega)$, for every $t \in I$:

$$\begin{aligned}\int_0^t \Delta u(s)\,ds &= \int_0^t \frac{1}{2\pi i}\int_L \lambda^{-1}\Delta T(\lambda)\frac{d}{ds}\int_0^s e^{\lambda(s-r)}g(r)\,dr\,d\lambda\,ds \\ &= \int_0^t \frac{1}{2\pi i}\int_L \lambda^{-1}\lambda T(\lambda)\frac{d}{ds}\int_0^s e^{\lambda(s-r)}g(r)\,dr\,d\lambda\,ds \\ &= \frac{1}{2\pi i}\int_L T(\lambda)\int_0^t e^{\lambda(t-r)}g(r)\,dr\,d\lambda = \mathcal{T}g(t) = u(t)\ ,\end{aligned}$$

and similarly, with equalities in $H^{1/2}(\Gamma)$,

$$\begin{aligned}\text{trace } u(t) &= \frac{1}{2\pi i}\int_L \lambda^{-1}\ \text{trace } T(\lambda)\frac{d}{dt}\int_0^t e^{\lambda(t-s)}g(s)\,ds\,d\lambda \\ &= \frac{1}{2\pi i}\int_L \lambda^{-1}\frac{d}{dt}\int_0^t e^{\lambda(t-s)}g(s)\,ds\,d\lambda = g(t)\ .\end{aligned}$$

This gives the desired result. □

Remark. The compatibility assumption $g(0) = 0$ is not necessary for most of Theorem 3.2. According to Lemma 2.2 and part (b) of Theorem 3.1, the operator $\mathcal{T} = \mathcal{U}\mathcal{V}^{(-1)}$ can be extended, via (2.9) with $T(\lambda) = U(\lambda)V(\lambda)^{-1}$, to a linear operator

$$\mathcal{T} : C^{1/2+\delta}(I, H^{1/2}(\Gamma)) \to C((0,\bar{t}], H^1(\Omega)) \cap C(I, L^2(\Omega)) \cap C^1((0,\bar{t}], H^{-1}(\Omega))$$

so that $u = \mathcal{T}g$ is bounded pointwise in time by

$$\begin{aligned}
\|u(t)\|_{H^1(\Omega)} &\le C \cdot \Big(t^{-1/2}\|g(0)\| + |g|_{C^{1/2+\delta}(I,H^{1/2}(\Gamma))}\Big) \\
\|u(t)\|_{L^2(\Omega)} &\le C \cdot \|g\|_{C^{1/2+\delta}(I,H^{1/2}(\Gamma))} \\
\|u'(t)\|_{H^{-1}(\Omega)} &\le C \cdot \Big(t^{-1/2}\|g(0)\| + |g|_{C^{1/2+\delta}(I,H^{1/2}(\Gamma))}\Big) .
\end{aligned}$$

$\mathcal{T}$ is again the solution operator of (3.1).

4. Semidiscretization in time

The time discretization that is proposed here for the numerical treatment of evolutionary boundary integral equations is based on a linear multistep method for ordinary differential equations $y' = f(y)$, see e.g. [14], Ch. III,

$$\sum_{j=0}^{k} \alpha_j y_{n-j} = \tau \sum_{j=0}^{k} \beta_j f(y_{n-j}) \qquad (\tau > 0 \quad \text{step size}) .$$

We assume that the multistep method is A(α)-stable with positive angle α, stable in a neighbourhood of infinity, strongly zero-stable and consistent of order p. In terms of the quotient of the generating polynomials of the method,

$$\delta(\zeta) = \sum_{j=0}^{\infty} \delta_j \zeta^j = \sum_{j=0}^{k} \alpha_j \zeta^j \Big/ \sum_{j=0}^{k} \beta_j \zeta^j , \tag{4.1}$$

these conditions can be stated as follows:

$$\begin{gathered}
\delta(\zeta) \text{ has neither zeros nor poles on the closed unit disk } |\zeta| \le 1, \\
\text{with the exception of a simple zero at } \zeta = 1 ,
\end{gathered} \tag{4.2a}$$

$$|\arg \delta(\zeta)| \le \pi - \alpha , \quad |\zeta| \le 1 , \quad \text{for some } \alpha > 0 , \tag{4.2b}$$

$$\tau^{-1}\delta(e^{-\tau}) = 1 + \mathcal{O}(\tau^p) , \quad \tau \to 0 , \quad \text{for some } p \ge 1 . \tag{4.2c}$$

Well-known examples are the backward differentiation formulas of order $p \le 6$, given by $\delta(\zeta) = \sum_{j=1}^{p} (1-\zeta)^j / j$.

We turn now to the definition of *operational quadrature methods* [17], which we phrase in the abstract framework of Lemma 2.2. Let again $\Lambda = \{\lambda \in \mathbf{C} : |\arg\lambda| \le \pi - \phi, |\lambda| \ge R\}$ be a sectorial region, with the angle $\phi < \alpha$, and suppose:

$$\begin{aligned} &T(\lambda),\ \lambda \in \Lambda, \text{ is an analytic family of linear operators between} \\ &\text{Banach spaces } E \text{ and } F, \text{ whose operator norms satisfy} \\ &\|T(\lambda)\| \le c \cdot |\lambda|^{\gamma}\ , \quad \lambda \in \Lambda\ , \qquad \text{for some } \ \gamma < 1\ . \end{aligned} \tag{4.3}$$

For a (sufficiently small) positive step size τ and for $n \ge 0$, we define the "quadrature weights" $\omega_n(\tau, T) : E \to F$ as the coefficients in the expansion

$$T\left(\frac{\delta(\zeta)}{\tau}\right) = \sum_{n=0}^{\infty} \omega_n(\tau, T)\, \zeta^n\ , \qquad |\zeta| \text{ sufficiently small}\ . \tag{4.4}$$

By Theorem 5.1 of [17], the discrete convolution of these weights with the function values of $g \in C^{p+1}(I, E)$ on the grid of width τ defines an approximation of $(\mathcal{T} g)(t)$ of (2.9), whose error at $t = n\tau$ is bounded by

$$\begin{aligned} \|\sum_{j=0}^{n} \omega_{n-j}(\tau, T)\, g(j\tau) - (\mathcal{T} g)(t)\| \le C \cdot t^{-\gamma-1} \cdot \Big(&\tau \|g(0)\| + \tau^2 \|g'(0)\| + \dots \\ &+ \tau^p \big(\|g^{(p-1)}(0)\| + t \cdot \|g^{(p)}(0)\| + t^2 \max_{0 \le s \le t} \|g^{(p+1)}(s)\| \big) \Big)\ . \end{aligned} \tag{4.5}$$

The constant C is independent of $\tau \in (0, \overline{\tau}]$, $t = n\tau \in I$, and $g \in C^{p+1}(I, E)$, and is proportional to c of (4.3).

We remark that the proof of (4.5) in [17] is based on the following representation, which is a temporally discrete analogue of formula (2.9):

$$\sum_{j=0}^{n} \omega_{n-j}(\tau, T)\, g(j\tau) = \frac{1}{2\pi i} \int_L \lambda^{-1} T(\lambda) D_\tau (D_\tau - \lambda)^{-1} g(t)\, d\lambda\ , \tag{4.6}$$

with complex contour $L \subset \Lambda$ parallel to the boundary of Λ, and where, with $R_\lambda(s) = (s - \lambda)^{-1}$,

$$(D_\tau - \lambda)^{-1} g(t) = \sum_{j=0}^{n} \omega_{n-j}(\tau, R_\lambda)\, g(j\tau)$$

is a multistep approximation of $y' = \lambda y + g$, $y(0) = 0$, i.e., of $\int_0^t e^{\lambda(t-s)} g(s)\, ds$, and

$$D_\tau f(t) = \frac{1}{\tau} \sum_{j=0}^{n} \delta_{n-j}\, f(j\tau)$$

is a backward difference quotient.

By adding a suitable linear combination of a few of the first values of $g(j\tau)$ to the above approximation, such that the quadrature formula becomes exact for polynomials up to degree $p-2$ or $p-1$, the order of convergence can be improved to $O(t^{-\gamma-1}\tau^p)$ or $O(t^{-\gamma}\tau^p)$, respectively, for all $g \in C^{p+1}(I,E)$. Cf. Corollary 3.2 in [17].

On intervals bounded away from 0, the full order of convergence, p, is restored by a very simple correction: One replaces the values $g(j\tau)$ by $c_j\, g(j\tau)$, where c_j are the weights of the p-th order Newton-Gregory quadrature formula (i.e., end-point correction of the trapezoidal rule). The weights in question are:

$$c_j = 1 \quad \text{for } j \geq p-1 \ , \tag{4.7a}$$

and

$$\begin{aligned} &c_0 = \tfrac{1}{2} \qquad \text{for } p = 2 \ , \\ &c_0 = \tfrac{5}{12} \ , \ c_1 = \tfrac{13}{12} \qquad \text{for } p = 3 \ , \\ &c_0 = \tfrac{3}{8} \ , \ c_1 = \tfrac{7}{6} \ , \ c_2 = \tfrac{23}{24} \qquad \text{for } p = 4 \ . \end{aligned} \tag{4.7b}$$

Theorem 4.1. (Convergence of operational quadrature methods) *Under the assumptions (4.2) and (4.3), we have for $g \in C^{p+1}(I,E)$ the following error bound at $t = n\tau$:*

$$\| \sum_{j=0}^{n} \omega_{n-j}(\tau,T)\, c_j\, g(j\tau) - (\mathcal{T} g)(t) \| \leq C \cdot M(t,g) \cdot \tau^p \ , \tag{4.8a}$$

with

$$M(t,g) = t^{-\gamma-p} \cdot \left(\sum_{k=0}^{p} \frac{t^k}{k!} \cdot \|g^{(k)}(0)\| + \frac{t^{p+1}}{(p+1)!} \cdot \max_{0 \leq s \leq t} \|g^{(p+1)}(s)\| \right) \ . \tag{4.8b}$$

The constant C is independent of $\tau \in (0,\overline{\tau}]$, $t = n\tau \in I$, and $g \in C^{p+1}(I,E)$, and is proportional to c of (4.3).

This result is obtained as a generalization of Corollary 4.2 of [17] to the case $\mu = -\gamma < 0$, following the remark after Theorem 5.1 in [17].

We now consider the application of convolution quadrature methods to the semidiscretization in time of the single layer heat potential equation (2.1). Consider $V(\lambda) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ of Theorem 2.1 in the role of $T(\lambda)$ in Theorem 4.1. For $g \in C^{p+1}(I, H^{1/2}(\Gamma))$, let $\varphi = \mathcal{V}^{(-1)} g$ of Theorem 2.3 denote the solution of the single layer heat potential equation $\mathcal{V}\varphi = g$. For a step size $\tau > 0$, let further $\{\varphi_n\} \subset H^{-1/2}(\Gamma)$ denote the solution of the discrete Volterra convolution equation

$$\sum_{j=0}^{n} \omega_{n-j}(\tau,V)\, \varphi_j = c_n g(n\tau) \ , \qquad n\tau \in I \ , \tag{4.9}$$

which is well-defined because $\omega_0(\tau,V) = V(\delta(0)/\tau) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is an isomorphism by Theorem 2.1. As a corollary of Theorem 4.1 we get the following convergence result.

Theorem 4.2. (Convergence of semi-discrete convolution quadrature approximations of the single layer heat potential equation) *Let $\delta(\zeta)$ satisfy (4.2). For $g \in C^{p+1}(I, H^{1/2}(\Gamma))$, the error $\varphi_n - \varphi(n\tau)$ of the semi-discrete approximation (4.9) of (2.1) is bounded in $H^{-1/2}(\Gamma)$ by the right-hand side of (4.8) with $H^{1/2}(\Gamma)$ norms and $\gamma = \frac{1}{2}$.*

Proof. It follows from (4.9) and (4.4) that

$$\varphi_n = \sum_{j=0}^{n} \omega_{n-j}(\tau, V^{-1})\, c_j g(j\tau) \ . \tag{4.10}$$

The result is now obtained from Theorem 4.1 with $V^{-1}(\lambda)$ in the role of $T(\lambda)$, with $\gamma = \frac{1}{2}$ in (4.3) by (2.7). □

A semi-discrete approximation to the solution of the Dirichlet problem (3.1) of the heat equation is then given by

$$u_n = \sum_{j=0}^{n} \omega_{n-j}(\tau, U)\, \varphi_j \tag{4.11}$$

as an element in $H^1(\Omega)$ by Theorem 3.1(a). In view of (4.10) and (4.4), this equals

$$u_n = \sum_{j=0}^{n} \omega_{n-j}(\tau, UV^{-1})\, c_j g(j\tau) \ . \tag{4.12}$$

This approximate solution is now related to the semidiscretization in time of the initial-boundary value problem (3.1) by the linear multistep method:

$$\begin{aligned} \sum_{j=0}^{k} \alpha_j u_{n-j} &= \tau \sum_{j=0}^{k} \beta_j \Delta u_{n-j} && \text{in } \Omega \ , \quad \text{for } n \geq 0 \ , \\ u_n &= c_n g(n\tau) && \text{on } \Gamma \ , \quad \text{for } n \geq 0 \ , \\ u_n &= 0 && \qquad\qquad\quad \text{for } n < 0 \ , \end{aligned} \tag{4.13}$$

which we consider with equality in $H^{-1}(\Omega)$ in the differential equation and with boundary values taken in the sense of traces.

Theorem 4.3. (Equivalence of convolution quadrature and multistep method in the semi-discretization) *Let $\delta(\zeta)$ satisfy (4.2), and suppose that $g \in C^{p+1}(I, H^{1/2}(\Gamma))$. Then, the convolution quadrature approximation $u_n \in H^1(\Omega)$ given by (4.11) and (4.9) is identical to the multistep approximation (4.13) of the initial-boundary value problem. The error $u_n - u(n\tau)$ is bounded in $H^{\pm 1}(\Omega)$ by the right-hand side of (4.8) with $H^{1/2}(\Gamma)$ norms, and with $\gamma = \pm\frac{1}{2}$, respectively.*

Proof. First we note that the difference-differential equation in (4.13) is equivalent to

$$\frac{1}{\tau}\sum_{j=0}^{n}\delta_{n-j}u_j = \Delta u_n \ , \qquad n \geq 0 \ .$$

Using the representation (4.6) with $T(\lambda) = U(\lambda)V(\lambda)^{-1}$, and with $c_j g(j\tau)$ instead of $g(j\tau)$, it follows in an exactly analogous way as in the proof of Theorem 3.2 that u_n of (4.12) solves (4.13) in the sense stated. The error estimate follows from Theorem 3.1(b) and Theorem 4.1. □

5. Full discretization: Galerkin BEM in space, operational quadrature in time

In this section we combine the operational quadrature discretization in time with a standard Galerkin method in space to approximate the single layer heat potential equation (2.1). To keep to the essentials, we will not consider variational crimes such as the approximation of the boundary, which would be present in any practical computation. These could equally be treated by combining the techniques developed here with the corresponding known techniques for elliptic problems.

For a spatial discretization parameter $h > 0$, we let $X_h \subset H^{-1/2}(\Gamma)$ denote a finite dimensional approximation space of which we assume that for some $m \geq 0$

$$\inf_{\psi_h \in X_h} \|\psi_h - \psi\|_{H^{-1/2}(\Gamma)} \leq C \cdot h^{m+\frac{1}{2}} \cdot \|\psi\|_{H^m(\Gamma)} \ , \qquad \text{for all } \ \psi \in H^m(\Gamma) \ . \tag{5.1}$$

For example, approximation by piecewise constant or piecewise linear functions over a non-degenerate triangulation would give (5.1) with $m = 1$ or $m = 2$, respectively, and by interpolation also for all smaller values of m. See, e.g., Nédélec [20], §1.1.

The Galerkin approximation of the stationary equation $V(\lambda)\varphi = g$, with the single layer potential operator $V(\lambda) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ of Theorem 2.1, is then given as the solution $\varphi_h \in X_h$ of the problem

$$\langle V(\lambda)\varphi_h, \psi_h\rangle = \langle g, \psi_h\rangle \qquad \text{for all } \ \psi_h \in X_h \ . \tag{5.2}$$

Lemma 5.1. *For $\lambda \in \Lambda$ (the sectorial region of Theorem 2.1), $g \in H^{1/2}(\Gamma)$, and $h > 0$, the Galerkin scheme (5.2) has a unique solution $\varphi_h \in X_h$, which is bounded by*

$$\|\varphi_h\|_{H^{-1/2}} \leq C \cdot |\lambda|^{1/2} \cdot \|g\|_{H^{1/2}} \ . \tag{5.3}$$

For $g \in H^{m+1}(\Gamma)$, the error is bounded by

$$\|\varphi_h - \varphi\|_{H^{-1/2}} \leq C \cdot h^{m+\frac{1}{2}} \cdot |\lambda| \cdot \|g\|_{H^{m+1}} \ . \tag{5.4}$$

The constants C are independent of h, λ, and g.

Proof. The bound (5.3) is a direct consequence of Theorem 2.1 and the Lax-Milgram lemma. Céa's lemma gives

$$\|\varphi_h - \varphi\|_{H^{-1/2}} \leq C \cdot |\lambda|^{1/2} \cdot \inf_{\psi_h \in X_h} \|\psi_h - \varphi\|_{H^{-1/2}}$$

which can be further estimated using (5.1). The error bound (5.4) then follows from the regularity estimate

$$\|\varphi\|_{H^m} \leq C \cdot |\lambda|^{1/2} \cdot \|g\|_{H^{m+1}} \tag{5.5}$$

which is obtained with the help of the parameter-dependent pseudodifferential calculus as in the proof of Theorem 2.1. □

In all reasonable situations, one has actually $X_h \subset L^2(\Gamma)$, which we assume henceforth. The duality pairing between $H^{1/2}(\Gamma)$ and $H^{-1/2}(\Gamma)$ in (5.2) is then in fact the L^2 scalar product. We let $P_h : L^2(\Gamma) \to X_h$ be the $L^2(\Gamma)$-orthogonal projection defined by $(P_h\varphi, \psi_h) = (\varphi, \psi_h)$ for all $\psi_h \in X_h$, and we denote

$$V_h(\lambda) = P_h V(\lambda) P_h^* \ , \tag{5.6}$$

so that (5.2) can be rewritten as the equation $V_h(\lambda)\varphi_h = P_h g$, i.e.,

$$\varphi_h = V_h(\lambda)^{-1} P_h g \ . \tag{5.7}$$

We now turn to the time-dependent problem (2.1). In view of Theorem 2.3, a Galerkin semidiscretization in space of $\varphi(t) = (\mathcal{V}^{(-1)}g)(t)$ is given by

$$\varphi_h(t) = (\mathcal{V}_h^{(-1)} P_h g)(t) \tag{5.8}$$

where the operator $\mathcal{V}_h^{(-1)} : \{g_h \in C^{\frac{1}{2}+\delta}(I, X_h); g_h(0) = 0\} \to C^\epsilon(I, X_h)$ is defined by formula (2.9) with $V_h(\lambda)^{-1}$ in the role of $T(\lambda)$. Discretizing (5.8) in time by an operational quadrature method with step size $\tau > 0$, we get the full discretization

$$\varphi_{h,\tau}(n\tau) = \sum_{j=0}^{n} \omega_{n-j}(\tau, V_h^{-1}) P_h c_j g(j\tau) \ . \tag{5.9}$$

This can be rewritten equivalently, and in a way which is more amenable to computation, as the discrete convolution equation

$$\sum_{j=0}^{n} \omega_{n-j}(\tau, V_h)\varphi_{h,\tau}(j\tau) = P_h c_n g(n\tau) \ , \qquad n\tau \in I \ , \tag{5.10}$$

or again equivalently, in a variational setting:

$$\langle \sum_{j=0}^{n} \omega_{n-j}(\tau, V)\varphi_{h,\tau}(j\tau), \psi_h \rangle = \langle c_n g(n\tau) \ , \psi_h \rangle \qquad \text{for all } \ \psi_h \in X_h \ . \tag{5.11}$$

This equation can be solved recursively for $n = 0, 1, 2, \ldots, N$, requiring in every step the solution of a linear system with the positive definite stiffness matrix corresponding to the operator $\omega_0(\tau, V_h) = V_h(\delta(0)/\tau)$.

Theorem 5.2. (Convergence of fully discrete approximations of the single layer heat potential equation (2.1)) *Suppose that the spatial approximation is of order m as specified by (5.1), and that the temporal discretization method of order p satisfies (4.2). For $g \in C^{p+1}(I, H^{1/2}(\Gamma)) \cap C^2(I, H^{m+1}(\Gamma))$, the error of the fully discrete approximation $\varphi_{h,\tau}$ defined by either of (5.9) - (5.11), is bounded for $t = n\tau \in I$ by*

$$\|\varphi_{h,\tau}(t) - \varphi(t)\|_{H^{-1/2}(\Gamma)} \le C \cdot \|g\|_{C^2(I,H^{m+1}(\Gamma))} \cdot h^{m+\frac{1}{2}} + C \cdot M(t,g) \cdot \tau^p \ , \tag{5.12}$$

where $M(t,g)$ is defined by (4.8b), with $\gamma = \frac{1}{2}$ and $H^{1/2}(\Gamma)$ norms. The constants C are independent of $h > 0$, $\tau \in (0, \overline{\tau}]$, $t = n\tau \in I$, and g.

We remark that by a modification of the proof below, one could relax the assumption of $C^2(I, H^{m+1})$ to $C^{1+\epsilon}$ for any $\epsilon > 0$. The $C^{p+1}(I, H^{1/2})$ assumption can possibly be weakened to $C^{p+\frac{1}{2}+\epsilon}$.

Proof of Theorem 5.2. We split

$$\varphi_{h,\tau}(t) - \varphi(t) = [\varphi_{h,\tau}(t) - \varphi_h(t)] + [\varphi_h(t) - \varphi(t)] \ . \tag{5.13}$$

Since $V_h(\lambda)^{-1}P_h : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ is bounded uniformly in h by $C \cdot |\lambda|^{1/2}$ for $\lambda \in \Lambda$ because of (5.3) (and (5.7)), we get from Theorem 4.1 with $V_h(\lambda)^{-1}P_h$ in the role of $T(\lambda)$ that the first term on the right-hand side of (5.13) is bounded by the last term in (5.12). It remains to bound the last term in (5.13), which represents the error introduced by semidiscretization in space. Denoting the stationary error operator $E_h(\lambda) = V_h(\lambda)^{-1}P_h - V(\lambda)^{-1}$, we have by (5.8) and Theorem 2.3 (recall (2.9))

$$\begin{aligned}
\varphi_h(t) - \varphi(t) &= \frac{1}{2\pi i}\int_L \lambda^{-1} E_h(\lambda) \frac{d}{dt}\int_0^t e^{\lambda(t-s)} g(s)\, ds\, d\lambda \\
&= \frac{1}{2\pi i}\int_L \lambda^{-2} \int_0^t e^{\lambda(t-s)}\, E_h(\lambda) g''(t-s)\, ds\, d\lambda \\
&+ \frac{1}{2\pi i}\int_L \lambda^{-1} e^{\lambda t}\, E_h(\lambda)\left(\lambda^{-1} g'(0) + g(0)\right)\, d\lambda
\end{aligned}$$

The desired estimate now follows with the bound for $E_h(\lambda)$ as given by (5.4). □

6. Full discretization: Collocation BEM in space, operational quadrature in time

For the collocation method applied to the single layer heat equation the theory is not as complete as for the Galerkin method. We consider here the case where Γ is a smooth closed curve, the boundary of the simply connected domain $\Omega \subset \mathbf{R}^2$.

Let $s \mapsto x(s)$ be a 1-periodic parametrization of Γ. For a mesh width $h = 1/N$, we denote the grid points by $x_k = x(kh)$ for integer k. We consider approximation spaces X_h of piecewise constant or piecewise linear functions: X_h consists of all functions ψ_h on Γ such that $s \mapsto \psi_h(x(s))$ is either constant on the intervals $[(k-\frac{1}{2})h, (k+\frac{1}{2})h)$, or linear on $[kh, (k+1)h]$ and continuous. The grid points are thus midpoints in the piecewise constant case, and nodal points in the piecewise linear case.

Collocation of the stationary equation $V(\lambda)\varphi = g$ then requires to determine $\varphi_h \in X_h$ such that

$$(V(\lambda)\varphi_h)(x_k) = g(x_k) \quad \text{for all } k \ . \tag{6.1}$$

In order that the pointwise evaluation of g makes sense, one needs $g \in C(\Gamma)$, which is satisfied if $g \in H^r(\Gamma)$ with $r > \frac{1}{2}$.

In the same way as in Section 5, a full discretization of the single layer heat potential equation $\mathcal{V}\varphi = g$ is defined by

$$\Big(\sum_{j=0}^{n} \omega_{n-j}(\tau, V)\varphi_{h,\tau}(\cdot, j\tau)\Big)(x_k) = c_n g(x_k, n\tau) \quad \text{for } \ n \geq 0 \ \text{ and all } k \ , \tag{6.2}$$

where $\varphi_{h,\tau}(\cdot, n\tau) \in X_h$. Here c_n denote again the correction weights of (4.7).

For (6.1) we have the following stability and convergence result. Here Λ denotes once more the sector of Theorem 2.1, and Π_h denotes the interpolation projection which maps a continuous function on Γ to its piecewise linear interpolant on the grid $\{x_k\}$.

Theorem 6.1. *For $\lambda \in \Lambda$ with sufficiently large absolute value, and for sufficiently small mesh width h one has the stability bound*

$$\|\Pi_h V(\lambda)\psi_h\|_{H^{1/2}} \geq c \cdot |\lambda|^{-1/2} \cdot \|\psi_h\|_{H^{-1/2}} \quad \textit{for all } \ \psi_h \in X_h \ . \tag{6.3}$$

For $g \in H^{m+1}(\Gamma)$, the error of the collocation scheme (6.1) is bounded by

$$\|\varphi_h - \varphi\|_{H^{-1/2}} \leq C \cdot h^{m+\frac{1}{2}} \cdot |\lambda| \cdot \|g\|_{H^{m+1}} \ . \tag{6.4}$$

Here $m \leq 1$ or 2 for piecewise constant or piecewise linear collocation, respectively. The constants $c > 0$ and C are independent of h, λ, and g.

It is clear that with Theorem 6.1, one gets the convergence estimate of Theorem 5.2 also for the collocation/operational quadrature approximation (6.2) of the single layer heat potential equation.

To prove Theorem 6.1, we have to use a parameter-dependent version of the theory of collocation of elliptic pseudodifferential equations. This will be outlined in the remainder of this section.

The fact that the underlying operator $V(\lambda)$ is a parameter-dependent pseudodifferential operator, allows us to apply the local principle presented in [22],[24] with some minor modifications. The lower order perturbation terms decrease faster than the principal symbol for large $|\lambda|$ and can be handled as in the proof of Theorem 2.1. Moreover, it is possible to adapt Agranovich's theorem [3], [25] to the parameter dependent situation. From these observations it turns out that it is sufficient to study the operator, again denoted by $V(\lambda)$, which for 1-periodic smooth functions ψ is given via the formula (cf. the proof of Theorem 2.1)

$$(\mathcal{F}V(\lambda)\psi)(\xi) = \left(\lambda + |\xi|^2\right)^{-1/2} \mathcal{F}\psi(\xi) \ , \quad \xi \in \mathbf{Z} \ , \tag{6.5}$$

where $\mathcal{F}$ denotes the Fourier transform:

$$\mathcal{F}\psi(\xi) = \int_0^1 e^{-2\pi i \xi x} \psi(x)\, dx \ , \quad \xi \in \mathbf{Z} \ .$$

The collocation scheme for this operator gives rise to circulant matrices. These are diagonalized by the discrete Fourier transform, so that their eigenvalues can be calculated explicitly.

Lemma 6.2. *The eigenvalues $\alpha_k(\lambda)$ $(0 \le kh < 1 \ , \ h = 1/N)$ of the matrices arising from the collocation scheme are $\alpha_0(\lambda) = \lambda^{-1/2}$ and*

$$\alpha_k(\lambda) = \sum_{\xi = k + \ell N : \ell \in \mathbf{Z}} \left(\lambda + |\xi|^2\right)^{-1/2} \cdot \left(\frac{\sin \pi h \xi}{\pi h \xi}\right)^m \ , \tag{6.6}$$

with $m = 1$ or 2 for piecewise constant or piecewise linear collocation, respectively.

Proof. The eigenvalues are given by the formula (cf. e.g. [23])

$$\alpha_k(\lambda) = \sum_{n=0}^{N-1} e^{-2\pi i k n h} \sum_{\xi \in \mathbf{Z}} e^{2\pi i \xi n h} \left(\lambda + |\xi|^2\right)^{-1/2} \cdot \widehat{\phi}(\xi)$$

where $\widehat{\phi}(\xi) = h \cdot \left(\frac{\sin \pi h \xi}{\pi h \xi}\right)^m$ are the Fourier coefficients of the basis function $\phi(x)$, which for $m = 1$ is the box function (the 1-periodic extension of the characterisic function of the interval $(-\frac{h}{2}, \frac{h}{2})$), and for $m = 2$ the hat function (piecewise linear, continuous, taking the value 1 at the integers, and 0 at all gridpoints kh in between). Interchanging the order of summation and using the discrete orthogonality of the exponentials gives the result. □

As in [27],[23], the key to the local stability estimate is a comparison of the collocation eigenvalues $\alpha_k(\lambda)$ with those of a Galerkin approximation, whose stability is known *a priori*.

Lemma 6.3. *Let $\alpha_k(\lambda)$ denote the collocation eigenvalues of Lemma 6.2, and let β_k denote the eigenvalues of the circulant matrix coming from the Galerkin scheme on the same approximation space for the equation with $\lambda = 1$. Then there is a $c > 0$ such that*

$$\mathrm{Re}\ \alpha_k(\lambda) \geq c \cdot |\lambda|^{-1/2} \cdot \beta_k \qquad \textit{uniformly for} \ \ 0 \leq kh < 1\ ,\ \lambda \in \Lambda\ .$$

Proof. A calculation as in the proof of Lemma 6.2 gives

$$\beta_k = \sum_{\xi = k + \ell N : \ell \in \mathbf{Z}} \left(1 + |\xi|^2\right)^{-1/2} \cdot \left(\frac{\sin \pi h \xi}{\pi h \xi}\right)^{2m} . \tag{6.7}$$

For $m = 2$ (piecewise linear approximation) the result follows by a comparison of each term in the sums (6.6) and (6.7), using once more the symbol estimate (2.6). The proof for $m = 1$ (piecewise constant approximation) is a bit more subtle and can be obtained similarly to [26],[9]. □

We are now ready for the final stages in the proof of Theorem 6.1: With the aid of the local principle [22],[24] one concludes from Lemma 6.3 the desired stability estimate (6.3). The stability implies the error bound

$$\|\varphi_h - \varphi\|_{H^{-1/2}} \leq \|\varphi - P_h\varphi\|_{H^{-1/2}} + C \cdot |\lambda|^{1/2} \left(\|\Pi_h V(\lambda) P_h \varphi - V(\lambda)\varphi\|_{H^{1/2}} + \|\Pi_h g - g\|_{H^{1/2}}\right)$$

where $P_h : H^{-1/2}(\Gamma) \to X_h$ denotes the orthogonal projection in $H^{-1/2}(\Gamma)$. Using well-known approximation and inverse properties, the uniform boundedness of $V(\lambda)$ and the regularity estimate (5.5), we obtain the desired estimate (6.4). Cf. [24],[23].

Remark. A result analogous to Theorem 6.1 holds for more general trial functions: higher-order splines, and prewavelets [10]. The result can also be extended to the case where Γ is diffeomorphic to an n-dimensional torus [23].

7. Implementation and numerical experiments

In this section we describe in some detail how to implement a full discretization of the single layer heat potential equation based on operational quadrature in time, and on piecewise linear collocation in space. We illustrate the procedure by a numerical example in which heat flow through the boundary is computed from the surface temperature.

Consider again first the stationary, parameter-dependent single layer potential equation over a boundary curve Γ:

$$V(\lambda)\varphi = g \quad \text{on } \Gamma \ ,$$

viz.,

$$\int_\Gamma \frac{1}{2\pi} K_0(\sqrt{\lambda}\cdot|x-y|)\,\varphi(y)\,dy = g(x) \ , \qquad x \in \Gamma \ , \tag{7.1}$$

where K_0 is the modified Bessel function of order 0. For grid points $x_1, \ldots, x_M$ on Γ, let ϕ_j denote the piecewise linear basis function which assumes the value 1 at x_j, and 0 at all other grid points. The collocation matrix for (7.1) is then

$$V_C(\lambda) = ((V(\lambda)\phi_j)(x_i))_{i,j=1}^M \ .$$

For the actual computation it is convenient to approximate this matrix by $V_A(\lambda)$, whose entries are defined by

$$\begin{aligned}(V_A(\lambda))_{ij} = d_{j-1,j} &\int_0^1 \frac{1}{2\pi} K_0\left(\sqrt{\lambda}\cdot(d_{i,j-1} + \theta(d_{i,j} - d_{i,j-1}))\right)\cdot\theta\cdot d\theta \\ + d_{j,j+1} &\int_0^1 \frac{1}{2\pi} K_0\left(\sqrt{\lambda}\cdot(d_{i,j} + \theta(d_{i,j+1} - d_{i,j}))\right)\cdot(1-\theta)\cdot d\theta\end{aligned} \tag{7.2}$$

where $d_{k,l} = |x_k - x_l|$. Since $\int zK_0(z)\,dz = -zK_1(z) + C$, this only requires the evaluation of $K_1(z)$ and integrals of $K_0(z)$, which can be computed efficiently (cf. e.g. formulas (11.1.9) and (11.1.18) in [1]).

The single layer heat potential equation (2.1),

$$\mathcal{V}\varphi = g \quad \text{on } \Gamma \times [0, \overline{t}] \ ,$$

is then discretized by

$$\sum_{j=0}^n V_{n-j}\varphi_j = (c_n g(x_k, n\tau))_{k=1}^M \ , \qquad n = 0, 1, \ldots, N \ . \tag{7.3}$$

Here $\tau = \overline{t}/N$ is the temporal step size, φ_n is to approximate $(\varphi(x_k, n\tau))_{k=1}^M$, and $V_n = \omega_n(\tau, V_A)$ are the coefficients of the generating function

$$\sum_{n=0}^\infty V_n\zeta^n = V_A\left(\frac{\delta(\zeta)}{\tau}\right) \ , \qquad |\zeta| < 1 \ ,$$

where, e.g., $\delta(\zeta) = \sum_{\ell=1}^p (1-\zeta)^\ell/\ell$ is a BDF method of order $p \le 6$. The correction weights c_n are defined in (4.7).

By Cauchy's integral formula,

$$V_n = \frac{1}{2\pi i} \int_{|\zeta|=\rho} V_A\left(\frac{\delta(\zeta)}{\tau}\right) \zeta^{-n-1}\, d\zeta \ .$$

This integral is approximated with high accuracy by the trapezoidal rule,

$$V_n \approx \frac{\rho^{-n}}{L} \sum_{\ell=0}^{L-1} V_A\left(\frac{\delta(\zeta_\ell)}{\tau}\right) e^{-2\pi i n \ell/L} \ , \qquad n = 0, 1, \ldots, N \ , \tag{7.4}$$

where $\zeta_\ell = \rho e^{2\pi i \ell/L}$. Suppose now that $V_A(\lambda)$ is computed with precision ϵ (in some norm). Choosing $L = 2N$ and $\rho^N = \sqrt{\epsilon}$, one gets that the error in V_n is $O(\sqrt{\epsilon})$, cf. [17], Section 7. Using fast Fourier transforms, the evaluation of (7.4) requires $O(N \log N)$ operations.

The solution of the discrete convolution equation (7.3) requires a matrix factorization only of V_0. The recursion (7.3) can be solved in $O(N(\log N)^2)$ $M \times M$-matrix multiplications by using a technique of [13]: One computes the first $r = 32$ values $\varphi_0, \ldots, \varphi_{r-1}$ by direct recursion. For $n = r, \ldots, 2r-1$ the convolution sums $\sum_{j=0}^{r-1} V_{n-j}\varphi_j$, which use only the previously computed solution values, are computed simultaneously using FFT. These sums are then used in the recursive computation of $\varphi_r, \ldots, \varphi_{2r-1}$. Then the sums $\sum_{j=0}^{2r-1} V_{n-j}\varphi_j$ are computed by FFT for $n = 2r, \ldots, 4r-1$ and are later used in the computation of the corresponding solution values φ_n. For the computation of φ_n for $n = 3r, \ldots, 4r-1$ one uses also the convolution sums $\sum_{j=2r}^{3r-1} V_{n-j}\varphi_j$, again computed by FFT. Continuing this procedure up to N requires $O(N(\log N)^2)$ operations, so that the computational complexity is almost linear in time. We remark that recent techniques have made it possible to achieve almost linear complexity also in space, using panel clustering [12] or wavelet basis functions [6],[10].

As a numerical example, we consider the problem of computing the Neumann data $\varphi = \frac{\partial u}{\partial n}$ from given Dirichlet data $u = g$ on the boundary, for the heat equation over the unit disk. This is done by solving the equation (see e.g. [8])

$$\mathcal{V}\varphi = \tfrac{1}{2} g + \mathcal{K} g \qquad \text{on } \Gamma \times (0, \bar{t}]$$

where $\mathcal{V}$ and $\mathcal{K}$ denote the single and double layer heat potential operators, respectively. We note that $\mathcal{K}$ is the integral operator whose kernel has the Laplace transform $(\partial/\partial n_y)\frac{1}{2\pi} K_0(\sqrt{\lambda} \cdot |x-y|)$. The integral operator $\mathcal{K}$ has been discretized in a way analogous to that of $\mathcal{V}$ described above. We give numerical results for two examples, with the following data: $M = 32$ equidistant grid points x_k on the unit circle, time step $\tau = 1/32$, over a time interval of length $\bar{t} = 1$.

As a first example we chose Dirichlet data $g(x,t) = 25 \cdot \exp(-|x - x^*|^2/4t)/(4\pi t)$ with $x^* = (3, 0)$. The exact solution is here $\varphi(x,t) = \frac{\partial}{\partial n} g(x,t)$, which is plotted in Fig. 1 as the function $(\theta, t) \mapsto \varphi((\cos\theta, \sin\theta), t)$. Figure 2 shows the error obtained with the second order BDF method in the above discretization. The numerically observed pointwise order of convergence was 2 in both space and time.

In our second example we took $g(x,t) = \cos(\theta - \pi t)$ for $x = (\cos\theta, \sin\theta)$. This is an example with a heat shock, where the exact heat flow $\varphi(x,t)$ is singular at $t = 0$, bounded by $O(t^{-1/2})$ (cf. (2.13)). The numerical solution obtained with the second order BDF method is shown in Figure 3. Here we have plotted the solution curves $t \mapsto \varphi(x_k, t)$ for all k. The height of the "numerical singularity" at $t = 0$ was observed to be proportional to $\tau^{-1/2}$. In accordance with Theorem 5.2 (or rather its collocation analogue), the numerical method gives accurate approximations away from the origin. Since the exact solution is not available for this example, we have plotted in Figure 4 the difference of the second and third order BDF discretizations, as a numerically accessible estimate of the temporal error. One notices that a reasonable approximation is obtained after ca. 5 time steps. This phenomenon (which is in agreement with Theorem 5.2) has been observed to be almost independent of the time step size: For $\tau = 1/320$ and $\tau = 1/3200$ we obtained plots which were very similar to Figure 4, where $\tau = 1/32$. If desired, the singular solution behaviour on an interval near 0 can thus be resolved to high accuracy with small computational effort, by solving the equation with a fixed number of time steps (e.g., 16) on shorter and shorter time intervals.

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