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ROTHE'S METHOD FOR THE HEAT EQUATION AND BOUNDARY INTEGRAL EQUATIONS

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Dedicated to E. Martensen on the occasion of this 70th birthday

ABSTRACT. Rothe's method for parabolic initial boundary value problems, also known as the horizontal line method, consists of a time discretization by finite differences and leads to a sequence of boundary value problems for an inhomogeneous elliptic equation. Whereas in the traditional approach in the solution of this sequence of boundary value problems volume potentials are incorporated, in order to preserve the advantages of the boundary integral equation method we present an approach involving only boundary integrals.

1. Introduction. For boundary value problems for elliptic differential equations with constant coefficients the use of boundary integral equations has a long history both for establishing existence of solutions and for numerical approximations. Similarly, integral equations have also been successfully applied to initial boundary value problems for parabolic equations. These integral equations, in general, are of Fredholm type with respect to the space variable and of Volterra type with respect to the time variable. Due to the simplicity of the Fredholm alternative and the use of successive approximations, integral equations of the second kind for the heat equation have been considered already for almost a century. Following earlier work of Holmgren [**11, 12**] and Gevrey [**10**], a rigorous existence proof for the initial boundary value problem with Dirichlet boundary condition via an integral equation of the second kind obtained through a double-layer heat potential approach was given by Müntz [**20**] already in 1934 (see also [**14**]). On the other hand, a corresponding theory for the integral equation of the first kind arising from a single-layer heat potential approach has been developed only very recently by Arnold and Noon [**1**], by Costabel [**6**] and by Hsiao and Saranen [**13**].

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Semi-discrete approximation methods for the heat equation can be obtained by a discretization of these integral equations with respect to the time variable, that is, by discretization of the Volterra part of the integral equations. This leads to a system of boundary integral equations for the approximate solution on each of the consecutive time levels. Using any of the well established methods for the approximate solution of boundary integral equations, the semi-discrete methods can be turned into fully discrete methods. For details we refer to Brebbia, Telles, and Wroblel [**2**] and Lubich and Schneider [**17**], and the literature therein.

In this paper we shall present a slightly different approach for obtaining semi-discrete methods in terms of systems of boundary integral equations without using heat potentials and Volterra integral equations. This is achieved through applying the time discretization directly to the differential equation as suggested by Rothe [**23**] in 1930. This method where only the time derivative in the heat equation is approximated by finite differences and which is also known as horizontal line method has been analyzed by many authors [**2, 9, 22**] and has also been extended to hyperbolic problems [**19**]. The Rothe method reduces the initial boundary value problem to a sequence of boundary value problems for inhomogeneous elliptic equations with a positive definite operator. As mentioned above, for these boundary value problems the boundary integral equation approach can be used both for establishing existence of solutions and for numerical approximations. In particular for exterior problems, the reformulation of the boundary value problem in terms of a boundary integral equation not only reduces the dimensionality of the problem, but also replaces a problem over an unbounded domain by one over a bounded domain.

For Rothe's method, a difficulty arises through the fact that the resulting sequence of elliptic equations consists of inhomogeneous equations with the inhomogeneities given in terms of the solutions on the previous time levels. The classical approach to deal with such a boundary value problem for an inhomogeneous elliptic equation is to reduce it to a problem for the homogeneous equation by incorporating a volume potential as a particular solution to the inhomogeneous equation. This approach also has been suggested in the literature for the Rothe method [**2, 9**]. However, using volume potentials has the drawback of destroying the two main advantages of the boundary integral equation

method mentioned above. In this paper we therefore will describe a solution method which only uses boundary integrals for the solution of the Rothe system. The basic tool for achieving this goal is the construction of single- and double-layer potentials for the sequence of elliptic equations arising in the Rothe method. In contrast, the classical approach via volume potentials uses only single- and double-layer potentials for the homogeneous part which remains invariant on each time level.

In order to explain the basic ideas of our approach we confine ourselves to the initial boundary value problem for the two-dimensional heat equation in an exterior domain with Dirichlet boundary condition and to the use of the backward Euler method for the time discretization. The extensions to interior problems and other boundary conditions are obvious. The analysis can also be carried over to higher order finite difference approximations for the time discretization and also to the case of three dimensions. In the latter case, of course, one is faced with the more delicate problem to discretize surface integral equations for the fully discrete version.

The plan of this paper is as follows. In Section 2 we will describe the basic features of the Rothe method. The following Section 3 is the main part of our paper since it presents the idea of reducing the sequence of boundary value problems resulting from the time discretization into integral equations merely involving boundary integrals. In Section 4 we will briefly describe how well established numerical methods can be applied to numerically solve these boundary integral equations. Then we proceed with some convergence and error analysis in Section 5, and in Section 6 we will demonstrate the feasibility of our method through some numerical examples. Finally, in Section 7 we conclude with some observations on similarities of our method with the method of the Laguerre transformation [**4, 8**].

As we will describe in more detail in Section 3, our method is closely related to the method proposed by Lubich and Schneider [**17**] based on the operational quadrature method. However, we feel that the approach of the present paper is more easily accessible. In addition, we will provide a more explicit procedure for the computation of the kernels involved in the sequence of boundary integral equations.

2. Rothe's method. Let $D \subset \mathbf{R}^2$ be an unbounded domain such

that its complement is bounded and simply connected, assume that the boundary Γ of D is of class C^2 and let $T > 0$. We consider the initial boundary value problem for the heat equation

$$\frac{1}{c}\frac{\partial u}{\partial t} = \Delta u \quad \text{in } D \times (0,T] \tag{2.1}$$

with heat conduction coefficient $c > 0$. We are looking for a classical solution $u \in C(\bar{D} \times [0,T])$ of (2.1) which is twice continuously differentiable with respect to the space variable and continuously differentiable with respect to the time variable on $D \times (0,T]$ and satisfies the homogeneous initial condition

$$u(x,0) = 0, \quad x \in D, \tag{2.2}$$

and the boundary condition

$$u = F \quad \text{on } \Gamma \times [0,T] \tag{2.3}$$

where F is a given function satisfying the compatibility condition

$$F(x,0) = 0, \quad x \in \Gamma.$$

At infinity we assume that

$$u(x,t) \longrightarrow 0, \quad |x| \to \infty, \tag{2.4}$$

uniformly with respect to all directions $x/|x|$ and all $t \in [0,T]$. Existence and uniqueness of a solution to this initial boundary value problem is well established (see [**7, 14**]). The homogeneity of the initial condition (2.2) is not a severe restriction since inhomogeneous initial conditions can be reduced to the homogeneous case through the use of an appropriate volume heat potential (see [**7, 14**]).

Now Rothe's method consists of discretizing the time derivative in the heat equation (2.1) by a finite difference approximation. For the sake of simplicity here we only consider the backward Euler difference approximation. We choose $N \in \mathbf{N}$ and with the stepsize $h = T/N$ we consider the grid points $t_n = (n+1)h$, $n = 0, 1, \ldots, N-1$. Then we replace the initial boundary value problem for the heat equation by the sequence of N Dirichlet boundary value problems

$$\Delta u_n - \gamma^2 u_n = -\gamma^2 u_{n-1} \quad \text{in } D \tag{2.5}$$

with the boundary condition

$$u_n = f_n \quad \text{on } \Gamma \tag{2.6}$$

where we have set $f_n = F(\cdot, (n+1)h)$ and $\gamma^2 = 1/(ch)$. At infinity we have to require

$$u_n(x) \longrightarrow 0, \quad |x| \to \infty, \tag{2.7}$$

uniformly for all directions. With the initial condition $u_{-1} = 0$ in D for $n = 0, 1, \ldots, N-1$, we need to recursively find solutions $u_n \in C^2(D) \cap C(\bar{D})$ of (2.5)–(2.7).

We proceed by noting the following results on uniqueness and stability.

Theorem 2.1. *The system* (2.5)–(2.7) *has at most one solution.*

Proof. By the maximum-minimum principle (see [**21**]) any solution $v \in C^2(D) \cap C(\bar{D})$ of $\Delta v - \gamma^2 v = 0$ in D which has vanishing boundary values $v = 0$ on Γ and vanishes at infinity uniformly for all directions must vanish identically in D. Then the statement of the theorem follows by induction. □

Theorem 2.2. *Let $g \in C(\bar{D})$ be bounded and $f \in C(\Gamma)$. Then for the unique solution $v \in C^2(D) \cap C(\bar{D})$ of the Dirichlet problem*

$$\Delta v - \gamma^2 v = -g \quad \textit{in } D \tag{2.8}$$

with boundary condition

$$v = f \quad \textit{on } \Gamma \tag{2.9}$$

and $v(x) \to 0$, $|x| \to \infty$, uniformly for all directions we have the estimate

$$\|v\|_{\infty,D} \leq \|f\|_{\infty,\Gamma} + \frac{1}{\gamma^2} \|g\|_{\infty,D} \tag{2.10}$$

Proof. We follow Gerdes [**9**] and split $v = v_1 + v_2$, where $\Delta v_1 - \gamma^2 v_1 = 0$ in D, $v_1 = f$ on Γ, and $\Delta v_2 - \gamma^2 v_2 = -g$ in D, $v_2 = 0$ on Γ. Then for v_1, by the maximum-minimum principle, we have

$$\|v_1\|_{\infty,D} \leq \|f\|_{\infty,\Gamma}. \tag{2.11}$$

For v_2 we can write

$$v_2(x) = \int_D G(x,y)g(y)\,dy, \quad x \in D,$$

where G denotes the Green's function for the boundary value problem (2.8)–(2.9). By the maximum-minimum principle it can be seen that the Green's function satisfies

$$0 \leq G(x,y) \leq \frac{1}{2\pi}\,\Phi_0(x,y), \quad x \neq y \in D,$$

where

$$\Phi_0(x,y) = K_0(\gamma|x-y|) \tag{2.12}$$

denotes the fundamental solution of (2.8) in terms of the modified Hankel function K_0 which is also known as Basset function or as Macdonald function. Then we can estimate

$$\begin{aligned} |v_2(x)| &\leq \frac{1}{2\pi}\|g\|_{\infty,D} \int_D \Phi_0(x,y)\,dy \\ &\leq \frac{1}{2\pi}\|g\|_{\infty,D} \int_{\mathbf{R}^2} K_0(\gamma|y|)\,dy, \quad x \in D, \end{aligned}$$

and use the integral (see [**16**])

$$\int_{\mathbf{R}^2} K_0(\gamma|y|)\,dy = \frac{2\pi}{\gamma^2}\int_0^\infty K_0(s)s\,ds = \frac{2\pi}{\gamma^2}$$

to obtain that

$$\|v_2\|_{\infty,D} \leq \frac{1}{\gamma^2}\,\|g\|_{\infty,D}. \tag{2.13}$$

Now the statement (2.10) follows by piecing (2.11) and (2.13) together. □

3. Boundary integral equation method. The solution of the sequence of boundary value problems (2.5)–(2.7), in principle, can be obtained by the boundary integral equation approach involving volume potentials for the inhomogeneity in (2.5) (see [**2, 9**]). For this, the solution u_n is decomposed $u_n = u_{n,1} + u_{n,2}$ where the volume potential

$$u_{n,1}(x) = \frac{\gamma^2}{2\pi} \int_D \Phi_0(x,y) u_{n-1}(y)\, dy, \quad x \in D,$$

satisfies the inhomogeneous differential equation, and where the double-layer potential

$$u_{n,2}(x) = \frac{1}{\pi} \int_\Gamma \frac{\partial \Phi_0(x,y)}{\partial \nu(y)}\, \varphi_n(y)\, ds(y), \quad x \in D,$$

with density $\varphi_n \in C(\Gamma)$ is used to deal with the boundary condition. By ν we denote the outward unit normal to the boundary curve Γ. The boundary condition (2.6) is fulfilled if φ_n is a solution to the boundary integral equation

$$\varphi_n(x) + \frac{1}{\pi} \int_\Gamma \frac{\partial \Phi_0(x,y)}{\partial \nu(y)}\, \varphi_n(y)\, ds(y) = f_n(x) - u_{n,1}(x), \quad x \in \Gamma. \tag{3.1}$$

However, as already mentioned in the introduction, the numerical evaluation of the volume potential, in particular for unbounded exterior domains, poses difficulties. Hence, an approach avoiding volume potentials altogether is highly desirable.

This can be achieved by constructing a singular solution Φ_n to the sequence of equations (2.5) of the form

$$\Phi_n(x,y) = \ln \frac{1}{|x-y|} + \Psi_n(x,y) \tag{3.2}$$

where the Ψ_n are continuously differentiable in $\mathbf{R}^2 \times \mathbf{R}^2$. The fundamental solution (2.12) and the modified Bessel differential equation

$$z^2 K_0''(z) + z K_0'(z) - z^2 K_0(z) = 0 \tag{3.3}$$

suggest to try to find Φ_n in the form

$$\begin{aligned} \Phi_n(x,y) = {} & K_0(\gamma|x-y|)\, v_n(|x-y|) \\ & - K_0'(\gamma|x-y|)\, w_n(|x-y|), \quad x \neq y, \end{aligned} \tag{3.4}$$

where v_n and w_n are polynomials with $v_0 = 1$ and $w_0 = 0$. Using (3.3), straightforward calculations show that the Φ_n satisfy (2.5) if and only if the polynomials v_n and w_n solve the sequence of systems of ordinary differential equations

$$\begin{aligned} v_n'' + \frac{1}{r}\, v_n' - 2\gamma w_n' &= -\gamma^2 v_{n-1}, \\ -2\gamma v_n' + w_n'' - \frac{1}{r}\, w_n' + \frac{1}{r^2}\, w_n &= -\gamma^2 w_{n-1} \end{aligned} \tag{3.5}$$

for $n = 1, 2, \ldots, N-1$. In view of $v_0 = 1$ and $w_0 = 0$, obviously the v_n must be even and the w_n must be odd polynomials. Therefore, for $n = 0, 1, 2, \ldots, N-1$ we write

$$v_n(r) = \sum_{k=0}^{[n/2]} a_{n,2k} r^{2k}, \qquad w_n(r) = \sum_{k=0}^{[(n-1)/2]} a_{n,2k+1} r^{2k+1} \tag{3.6}$$

where by the square bracket $[\cdot]$ we denote the integer part of a real number. Inserting (3.6) into (3.5), straightforward equating of powers of r shows that the polynomials v_n and w_n solve the system (3.5) if and only if the coefficients $a_{n,k}$ satisfy the recurrence relation

$$\begin{aligned} a_{n,n} &= \frac{\gamma}{2n}\, a_{n-1,n-1}, \\ a_{n,k} &= \frac{1}{2\gamma k}\left\{ 4\left[\frac{k+1}{2}\right]^2 a_{n,k+1} + \gamma^2 a_{n-1,k-1} \right\}, \\ & \qquad k = n-1, \ldots, 1, \end{aligned} \tag{3.7}$$

for $n = 1, 2, \ldots, N-1$.

Clearly, by (3.7) the coefficients are uniquely determined with the exception of the coefficient $a_{n,0}$ of the constant term in v_n. (This reflects the possibility to add an arbitrary solution to the homogeneous equation.) To ensure the form (3.2) and keep in line with [**4, 8**] we choose

$$a_{n,0} = 1, \quad n = 1, 2, \ldots, N-1. \tag{3.8}$$

Before we proceed, at this stage we wish to discuss the relation of our method to the method presented by Lubich and Schneider based

on the method of operational quadratures. For the special case of the backward Euler method in [**17**] the sequence $\tilde{\Phi}_n$ of kernels is defined through the power series expansion of the holomorphic function

$$K_0(\gamma\sqrt{(1-z)}\,|x-y|) = \sum_{n=0}^{\infty} \tilde{\Phi}_n(x,y)\, z^n, \quad |z|<1. \tag{3.9}$$

From

$$\Delta K_0(\gamma\sqrt{(1-z)}\,|x-y|) - \gamma^2(1-z)K_0(\gamma\sqrt{(1-z)}\,|x-y|) = 0,$$

by applying the Laplacian to (3.9) and equating powers of z, it readily follows that the coefficients $\tilde{\Phi}_n$ solve (2.5). By induction, it can be seen that

$$\begin{aligned}&\frac{1}{n!}\frac{d^n}{dz^n}\, K_0(\gamma\sqrt{(1-z)}\,|x-y|)\\ &\quad = \sum_{k=1}^{n} \alpha_{n,k}\gamma^k|x-y|^k\,\sqrt{1-z}^{\,k-2n} K_0^{(k)}(\gamma\sqrt{(1-z)}\,|x-y|)\end{aligned}$$

with real coefficients $\alpha_{n,k}$. Hence, for the coefficients

$$\tilde{\Phi}_n(x,y) = \frac{1}{n!}\frac{d^n}{dz^n} K_0(\gamma\sqrt{(1-z)}\,|x-y|)\Big|_{z=0} \tag{3.10}$$

in the Taylor series (3.9), it follows that

$$\tilde{\Phi}_n(x,y) = \sum_{k=1}^{n} \alpha_{n,k}\gamma^k|x-y|^k K_0^{(k)}(\gamma|x-y|). \tag{3.11}$$

In view of the modified Bessel differential equation (3.3), this implies that

$$\begin{aligned}\tilde{\Phi}_n(x,y) = {}& K_0(\gamma|x-y|)\tilde{v}_n(|x-y|)\\ &- K_0'(\gamma|x-y|)\,\tilde{w}_n(|x-y|), \quad x\neq y,\end{aligned} \tag{3.12}$$

where the $\tilde{v}_n$ are even polynomials of degree $2[n/2]$ and the $\tilde{w}_n$ are odd polynomials of degree $2[(n-1)/2]+1$. From our above analysis on system (3.5), it now can be concluded that the coefficients in

$$\begin{aligned}\tilde{v}_n(r) &= \sum_{k=0}^{[n/2]} \tilde{a}_{n,2k} r^{2k},\\ \tilde{w}_n(r) &= \sum_{k=0}^{(n-1)/2} \tilde{a}_{n,2k+1} r^{2k+1}\end{aligned}$$

must satisfy the recurrence relation (3.7). Only the coefficient for the constant term in $\tilde{v}_n$ is different from the one in v_n since $\tilde{a}_{0,0} = 1$ and $\tilde{a}_{n,0} = 0$ for $n = 1, 2, \ldots$. Comparing this to the solution $\Phi_n - \Phi_{n-1}$ of (2.5), this implies the relations $\tilde{\Phi}_0 = \Phi_0$ and

$$\tilde{\Phi}_n = \Phi_n - \Phi_{n-1}, \quad n = 1, 2, \ldots, \tag{3.13}$$

between the kernels in our method and in the method of Lubich and Schneider.

This coincidence (3.13) is not surprising since the operational quadrature method coincides with time discretization in the differential equation as pointed out in Theorem 4.3 of [**17**]. However, as a simplification obtained through our approach, we wish to point out that we are working with the explicit recurrence formulas (3.7) for the construction of the kernels whereas Lubich and Schneider rely on evaluating (3.10) by the Cauchy integral formula and numerical integration in the complex plane.

Now we consider the single-layer potential

$$U_n(x) = -\frac{1}{\pi} \sum_{m=0}^{n} \int_\Gamma q_m(y) \Phi_{n-m}(x, y)\, ds(y), \quad x \in \mathbf{R}^2 \setminus \Gamma, \tag{3.14}$$

and the double-layer potential

$$V_n(x) = \frac{1}{\pi} \sum_{m=0}^{n} \int_\Gamma q_m(y) \frac{\partial}{\partial \nu(y)} \Phi_{n-m}(x, y)\, ds(y), \quad x \in \mathbf{R}^2 \setminus \Gamma, \tag{3.15}$$

with continuous densities q_n for $n = 0, 1, 2, \ldots, N-1$. Then both the single- and the double-layer potential solve (2.5). The asymptotic behavior of the modified Hankel function $K_0(z)$ as $z \to \infty$ (see [**16**]) implies that both potentials tend to zero for $|x| \to \infty$ uniformly for all directions. From the power series expansions for K_0 (see [**16**]) we conclude that Φ_n indeed is of the form (3.2). Hence, by the classical jump- and regularity properties of the logarithmic potentials (see [**14**]), we have the following transformations into sequences of boundary integral equations.

Theorem 3.1. *The single-layer potential U_n given by* (3.14) *solves the sequence of boundary value problems* (2.5)–(2.7) *provided the den-*

sities solve the sequence of integral equations of the first kind

$$
\begin{aligned}
&-\frac{1}{\pi}\int_\Gamma q_n(y)\Phi_0(x,y)\,ds(y)\\
&\qquad = f_n(x)+\frac{1}{\pi}\sum_{m=0}^{n-1}\int_\Gamma q_m(y)\Phi_{n-m}(x,y)\,ds(y), \quad x\in\Gamma,
\end{aligned}
\tag{3.16}
$$

for $n = 0, 1, 2, \dots, N-1$. *The double-layer potential* V_n *given by* (3.15) *solves the sequence of boundary value problems* (2.5)–(2.7) *provided the densities solve the sequence of integral equations of the second kind*

$$
\begin{aligned}
&q_n(x)+\frac{1}{\pi}\int_\Gamma q_n(y)\frac{\partial}{\partial\nu(y)}\,\Phi_0(x,y)\,ds(y)\\
&\qquad = f_n(x)-\sum_{m=0}^{n-1} q_m(x)\\
&\qquad\quad -\frac{1}{\pi}\sum_{m=0}^{n-1}\int_\Gamma q_m(y)\frac{\partial}{\partial\nu(y)}\Phi_{n-m}(x,y)\,ds(y), \quad x\in\Gamma,
\end{aligned}
\tag{3.17}
$$

for $n = 0, 1, 2, \dots, N-1$.

As in the approach using volume potentials, on each time level we have to solve an integral equation where the integral operator remains the same and only the righthand side changes. However, as opposed to (3.1), the righthand sides of (3.16) and (3.17) contain only boundary integrals.

By standard potential theoretic arguments (see [**14**] for the corresponding case of Laplace's equation) and the Riesz-Fredholm theory, the following existence results can be established (through induction).

Theorem 3.2. *For any given righthand sides* f_n, $n = 0, \dots, N-1$, *from the Hölder space* $C^{1,\alpha}(\Gamma)$ *the sequence* (3.16) *of integral equations of the first kind possesses a unique solution* q_n, $n = 0, \dots, N-1$, *in* $C^{0,\alpha}(\Gamma)$. *For any given righthand sides* f_n, $n = 0, \dots, N-1$, *in* $C(\Gamma)$ *the sequence* (3.17) *of integral equations of the second kind possesses a unique solution* q_n, $n = 0, \dots, N-1$, in $C(\Gamma)$.

These existence results for the boundary integral equations of course imply the following existence result for the Rothe sequence of boundary value problems.

Theorem 3.3. *The system* (2.5)–(2.7) *has a unique solution.*

4. Numerical solution of the integral equations. We assume that the boundary curve Γ is given through a parametric representation

$$\Gamma = \{x(s) : 0 \le s \le 2\pi\}$$

where $x : \mathbf{R} \to \mathbf{R}^2$ is C^2 and 2π-periodic with $|x'(s)| > 0$ for all s. Then we transform (3.16) into the parametric form

$$\begin{aligned} &\frac{1}{2\pi}\int_0^{2\pi} H_0(s,\sigma)\psi_n(\sigma)\,d\sigma \\ &\quad = g_n(s) - \frac{1}{2\pi}\sum_{m=0}^{n-1}\int_0^{2\pi} H_{n-m}(s,\sigma)\varphi_m(\sigma)\,d\sigma, \quad 0 \le s \le 2\pi, \end{aligned} \tag{4.1}$$

where we have set

$$\begin{aligned} \varphi_n(s) &:= |x'(s)|\, q_n(x(s)), \\ \psi_n(s) &:= \sum_{m=0}^{n} \varphi_m(s), \\ g_n(s) &:= f_n(x(s)) \end{aligned}$$

and where the kernels are given by

$$\begin{aligned} H_0(s,\sigma) &:= -2\Phi_0(x(s),x(\sigma)), \\ H_n(s,\sigma) &:= -2[\Phi_n(x(s),x(\sigma)) - \Phi_0(x(s),x(\sigma))] \end{aligned}$$

for $s \ne \sigma$ and $n = 1, 2, \ldots, N-1$.

Taking into account the logarithmic singularity of K_0, we can write

$$H_0(s,\sigma) = \ln\left(\frac{4}{e}\sin^2\frac{s-\sigma}{2}\right)\left\{1 + H_0^1(s,\sigma)\sin^2\frac{s-\sigma}{2}\right\} + H_0^2(s,\sigma)$$

and

$$H_n(s,\sigma) = \ln\left(\frac{4}{e}\sin^2\frac{s-\sigma}{2}\right)H_n^1(s,\sigma) + H_n^2(s,\sigma)$$

for $n = 1, 2, \dots, N-1$, with appropriately chosen smooth kernels H_n^1 and H_n^2. In particular, the kernels H_n^1 are defined analogously to the kernels H_n in terms of the modified Bessel function I_0 instead of K_0, that is,

$$H_0^1(s,\sigma) = \frac{I_0(\gamma|x(s) - x(\sigma)|) - 1}{\sin^2(s-\sigma)/2},$$

and

$$\begin{aligned} H_n^1(s,\sigma) = {} & I_0(\gamma|x(s) - x(\sigma)|)\{v_n(|x(s) - x(\sigma)|) - 1\} \\ & - I_0'(\gamma|x(s) - x(\sigma)|)w_n(|x(s) - x(\sigma)|), \end{aligned}$$

for $n = 1, 2, \dots, N-1$. Hence, we have to solve a sequence of integral equation of the first kind of the form

$$\begin{aligned} \frac{1}{2\pi}\int_0^{2\pi} \left[\ln\left(\frac{4}{e}\sin^2\frac{s-\sigma}{2}\right)\left\{1 + H_0^1(s,\sigma)\sin^2\frac{s-\sigma}{2}\right\} \right. \\ \left. + H_0^2(s,\sigma)\right]\psi_n(\sigma)\,d\sigma = G_n(s) \end{aligned} \tag{4.2}$$

for $0 \le s \le 2\pi$ with righthand sides

$$\begin{aligned} G_n(s) := g_n(s) - \frac{1}{2\pi}\sum_{m=0}^{n-1}\int_0^{2\pi} \left[\ln\left(\frac{4}{e}\sin^2\frac{s-\sigma}{2}\right) H_{n-m}^1(s,\sigma) \right. \\ \left. + H_{n-m}^2(s,\sigma)\right]\varphi_m(\sigma)\,d\sigma. \end{aligned}$$

For integral equations of the form (4.2), a combined quadrature and collocation method based on trigonometric interpolation with equidistant grid points has been suggested and analyzed by Chapko and Kress [**3**] and by Kress and Sloan [**15**], including an error and convergence analysis.

For this method, we choose $M \in \mathbf{N}$ and an equidistant mesh by setting

$$s_k := k\pi/M, \quad k = 0, \dots, 2M-1,$$

and use the following quadrature rules

$$\frac{1}{2\pi}\int_0^{2\pi} g(\sigma)\ln\left(\frac{4}{e}\sin^2\frac{s_j-\sigma}{2}\right)d\sigma \approx \sum_{k=0}^{2M-1} R_{|j-k|}\,g(s_k), \tag{4.3}$$

(4.4)
$$\frac{1}{2\pi}\int_0^{2\pi} g(\sigma)\sin^2\frac{s_j-\sigma}{2}\ln\left(\frac{4}{e}\sin^2\frac{s_j-\sigma}{2}\right)d\sigma \approx \sum_{k=0}^{2M-1} F_{|j-k|}\, g(s_k),$$

(4.5)
$$\frac{1}{2\pi}\int_0^{2\pi} g(\sigma)\,d\sigma \approx \frac{1}{2M}\sum_{k=0}^{2M-1} g(s_k)$$

with the weights

$$R_j := \frac{1}{2M}\left\{c_0 + 2\sum_{m=1}^{M-1} c_m \cos\frac{mj\pi}{M} + (-1)^j c_M\right\},$$
$$F_j := \frac{1}{2M}\left\{\gamma_0 + 2\sum_{m=1}^{M-1} \gamma_m \cos\frac{mj\pi}{M} + (-1)^j \gamma_M\right\}$$

where

$$c_m := -\frac{1}{\max(1,|m|)},$$
$$\gamma_m := \frac{1}{4}\,(2c_m - c_{m+1} - c_{m-1})$$

for $m = 0, \pm 1 \pm 2, \ldots$. These quadratures are obtained by replacing the integrand g by its trigonometric interpolation polynomial of degree M with respect to the grid points s_k, $k = 0, \ldots, 2M-1$.

We collocate the integral equation (4.2) at the nodal points and use the quadrature rules (4.3)–(4.5) to approximate the three types of integrals to obtain the linear system

$$\sum_{k=0}^{2M-1} \psi_{n,M}(s_k)\left\{R_{|j-k|} + F_{|j-k|}H_0^1(s_j,s_k) + \frac{1}{2M}H_0^2(s_j,s_k)\right\}$$
$$= G_{n,M}(s_j), \quad j = 0, \ldots, 2M-1,$$

which we have to solve for the nodal values $\psi_{n,M}(s_j)$ of the approximating trigonometric polynomial $\psi_{n,M}$. Of course, the approximate values $G_{n,M}(s_j)$ for the righthand side are also obtained through using

(4.3) and (4.5) by

$$G_{n,M}(s_j) = g_n(s_j) - \sum_{m=0}^{n-1} \sum_{k=0}^{2M-1} \left\{ R_{|j-k|} H^1_{n-m}(s_j, s_k) + \frac{1}{2M} H^2_{n-m}(s_j, s_k) \right\} \varphi_{m,M}(s_k) \tag{4.6}$$

(where $\varphi_{0,M}(s_k) = \psi_{0,M}(s_k)$ and $\varphi_{n,M}(s_k) = \psi_{n,M}(s_k) - \psi_{n-1,M}(s_k)$ for $n = 1, 2, \ldots, N-1$).

The sequence of integral equation (3.17) of the second kind can be solved numerically by a similar approach using a Nyström method (see [**4, 5, 14**]).

5. Error analysis. For the semi-discrete Rothe method, we have the following convergence result.

Theorem 5.1. *Assume that the boundary values F are three times continuously differentiable with respect to the time variable (with vanishing derivatives for $t = 0$). Then we have the error estimate*

$$\sup_{n=0,1,\ldots,N-1} \|u(\cdot, (n+1)h) - u_n\|_{\infty,D} \leq \frac{1}{2} h \left\| \frac{\partial^2 F}{\partial t^2} \right\|_{\infty,\Gamma\times[0,T]}. \tag{5.1}$$

Proof. We first note that by the regularity results on the initial boundary value problem (see [**7**]) our assumption on F implies that the solution u to (2.1)–(2.3) is three times continuously differentiable with respect to t and the second derivate $\partial^2 u/\partial t^2$ also satisfies the heat equation. From the representation of the solution in terms of a heat potential with density on $\Gamma \times [0, T]$, it can be seen that $\partial^2 u/\partial t^2$ tends to zero for $|x| \to \infty$ uniformly for all directions and all $t \in [0, T]$. Therefore, from the maximum-minimum principle for the heat equation (see **7**) it follows that

$$\left\| \frac{\partial^2 u}{\partial t^2} \right\|_{\infty,D\times[0,T]} = \left\| \frac{\partial^2 F}{\partial t^2} \right\|_{\infty,\Gamma\times[0,T]}. \tag{5.2}$$

We now define $e_n := u(\cdot, (n+1)h) - u_n$, $n = 0, 1, \ldots, N-1$, and using (2.1) for u we have that

$$\Delta e_n - \gamma^2 e_n = -\gamma^2 e_{n-1} + r_n \quad \text{in } D$$

with homogeneous boundary condition

$$e_n = 0 \quad \text{on } \Gamma$$

and $e_n(x) \to 0$, $|x| \to \infty$, for $n = 0, 1, \ldots, N-1$. Here we have set $e_{-1} = 0$ and

$$r_n := \frac{1}{c}\left\{ \frac{\partial u}{\partial t}(\cdot, (n+1)h) - \frac{1}{h}[u(\cdot, (n+1)h) - u(\cdot, nh)] \right\},$$
$$n = 0, 1, \ldots, N-1.$$

The classical error estimate for the approximation of the derivative by finite differences yields that

$$\|r_n\|_{\infty,D} \le \frac{h}{2c} \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{\infty, D\times[0,T]}, \quad n = 0, 1, \ldots, N-1. \tag{5.3}$$

Now we apply Theorem 2.2 and use (5.2) and (5.3) to obtain

$$\|e_n\|_{\infty,D} \le \|e_{n-1}\|_{\infty,D} + \frac{1}{2}\, h^2 \left\| \frac{\partial^2 F}{\partial t^2} \right\|_{\infty, \Gamma\times[0,T]},$$
$$n = 0, 1, \ldots, N-1,$$

whence

$$\|e_n\|_{\infty,D} \le \frac{n+1}{2}\, h^2 \left\| \frac{\partial^2 F}{\partial t^2} \right\|_{\infty, \Gamma\times[0,T]},$$
$$n = 0, 1, \ldots, N-1,$$

and therefore the error estimate (5.1) follows. □

Now let $u_{n,M}$, $n = 0, 1, \ldots, N-1$, denote the approximate solution to (2.5)–(2.7) corresponding to the approximate solution $\varphi_{n,M}$, $n = 0, 1, \ldots, N-1$, of the integral equation (3.16) obtained via the method described in Section 4. Here we can base a discussion of the error on the

results of Chapko and Kress [**3**] and of Kress and Sloan [**15**]. The error analysis in [**15**] is carried out in a Sobolev space setting and implies that

$$\|u_n - u_{n,M}\|_{\infty,D} \leq C_1 \frac{1}{M^q} \tag{5.4}$$

for some constant C_1 provided Γ is analytic and the boundary function F is $(q+1)$-times continuously differentiable with respect to the space variable. The error analysis in [**3**] is carried out in a Hölder space setting and implies that

$$\|u_n - u_{n,M}\|_{\infty,D} \leq C_2 e^{-aM} \tag{5.5}$$

for some constants C_2 and a provided Γ and the boundary values F are analytic. Of course, here the constants C_1, C_2 and a depend on the integral operator, that is, they depend on the stepsize h of the time discretization since it enters the integral equation through the parameter γ in the kernel. Since $\gamma \to \infty$ for $h \to 0$, the fundamental solution given in terms of $K_0(\gamma|x-y|)$ will have a pronounced delta function like behavior which requires a sufficiently large number M of quadrature points for sufficient accuracy. This need for an increase of the number M of spatial grid points when the number N of time grid points is increased, of course, is in agreement with the general requirement to balance spatial and time discretization in the numerical solution of the heat equation.

6. Numerical examples. For a first numerical example we consider the boundary curve

$$\Gamma = \{x(s) = (0.2\cos s,\, 0.4\sin s - 0.3\sin^2 s)\}, \quad 0 \leq s \leq 2\pi, \tag{6.1}$$

which is illustrated in Figure 1. The boundary function is given by the restriction of the fundamental solution

$$u(x,t) = \frac{1}{4\pi t} \exp\left(-\frac{|x|^2}{4t}\right), \quad |x| > 0,\ t > 0, \tag{6.2}$$

on the boundary Γ. Obviously, the heat coefficient is chosen $c = 1$. For the length of the time interval we assume $T = 1$.

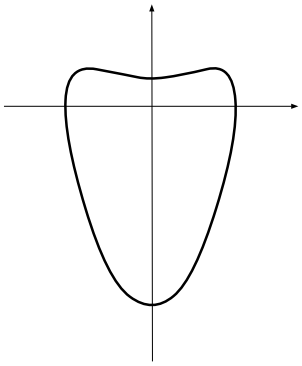

FIGURE 1. Boundary curve (6.1).

Table 1 gives the error between the exact solution u and the numerical solution obtained via the integral equations of the first kind at the two points $x = (0.3, 0)$ and $x = (0.6, 0)$ and for the time steps $t = 0.2, 0.4, 0.6, 0.8, 1.0$. The exponential convergence with respect to the number M of quadrature points and the linear convergence with respect to the time stepsize h as described in Section 5 is clearly exhibited.

TABLE 1. Numerical results for the boundary condition (6.2).

		$x = (0.3, 0)$			$x = (0.6, 0)$		
t	M	$N = 10$	$N = 20$	$N = 40$	$N = 10$	$N = 20$	$N = 40$
0.2	16	0.037041	0.016590	0.006758	0.090398	0.047760	0.021026
	32	0.037042	0.016591	0.006758	0.090398	0.047760	0.021026
0.4	16	0.009531	0.004943	0.002157	0.029354	0.015252	0.006741
	32	0.009532	0.004945	0.002160	0.029354	0.015252	0.006741
0.6	16	0.004840	0.002620	0.001112	0.014893	0.007966	0.003568
	32	0.004841	0.002620	0.001171	0.014893	0.007966	0.003568
0.8	16	0.003088	0.001701	0.000237	0.009408	0.005121	0.002312
	32	0.003089	0.001701	0.000768	0.009408	0.005121	0.002312
1.0	16	0.002057	0.001225	0.016353	0.006675	0.003671	0.001657
	32	0.002058	0.001225	0.000557	0.006675	0.003671	0.001665

For the second numerical example the boundary curve is again given by (6.1) and the boundary function now is

$$F(x,t) = 4t^2 \exp(-4t+2). \tag{6.3}$$

Table 2 gives some values for the numerical solution obtained via the integral equations of the first kind at the two points $x = (0.6, 0)$ and $x = (0.9, 0)$. Again our theoretical results on the convergence order are confirmed.

TABLE 2. Numerical results for the boundary condition (6.3).

	$x = (0.6, 0)$			$x = (0.9, 0)$			
t	M	$N = 10$	$N = 20$	$N = 40$	$N = 10$	$N = 20$	$N = 40$
0.2	16	0.138605	0.125782	0.119124	0.053948	0.043383	0.037730
	32	0.138605	0.125782	0.119124	0.053948	0.043383	0.037730
0.4	16	0.358963	0.356059	0.354857	0.176034	0.169198	0.165712
	32	0.358963	0.356059	0.354857	0.176034	0.169198	0.165712
0.6	16	0.471362	0.475889	0.478338	0.274481	0.275544	0.276246
	32	0.471362	0.475889	0.478338	0.274481	0.275544	0.276246
0.8	16	0.466251	0.472258	0.475306	0.311024	0.315963	0.318569
	32	0.466251	0.472258	0.475306	0.311024	0.315963	0.318569
1.0	16	0.397980	0.402688	0.405013	0.297807	0.303078	0.305762
	32	0.397980	0.402688	0.405013	0.297807	0.303078	0.305762

7. Laguerre transformation. In passing we wish to mention the close connection of the above analysis to using the Laguerre transformation for the numerical solution of the initial boundary value problem (2.1)–(2.3). To this end, let by

$$L_n(z) := \frac{1}{n!} e^z \frac{d^n}{dz^n} z^n e^{-z}, \quad z \in \mathbf{R}, \quad n = 0, 1, 2, \ldots . \tag{7.1}$$

denote the normalized Laguerre polynomials. They form a complete orthonormal system with respect to the scalar product

$$(f, g) := \int_0^\infty e^{-z} f(z) g(z)\, dz$$

in the space $L^2([0,\infty);\omega)$ of real valued functions with the weight function $\omega(z) = e^{-z}$. Choosing a fixed parameter $\kappa > 0$ we can scale the Fourier expansion with respect to the Laguerre polynomials into

$$u(x,t) = \kappa \sum_{n=0}^{\infty} \tilde{u}_n(x) L_n(\kappa t) \tag{7.2}$$

where

$$\tilde{u}_n(x) := \int_0^{\infty} e^{-\kappa t} L_n(\kappa t) u(x,t)\, dt, \quad n = 0, 1, 2, \ldots . \tag{7.3}$$

For these Laguerre-Fourier coefficients, by using the recurrence relations for the Laguerre polynomials, it can be shown that they solve the sequence of boundary value problems

$$\Delta \tilde{u}_n - \beta \tilde{u}_n = \beta \sum_{m=0}^{n-1} \tilde{u}_m \quad \text{in } D, \tag{7.4}$$

with boundary condition

$$\tilde{u}_n = \tilde{f}_n \quad \text{on } \Gamma \tag{7.5}$$

and

$$\tilde{u}_n(x) \to 0, \quad |x| \to \infty, \tag{7.6}$$

uniformly for all directions. Here,

$$\tilde{f}_n(x) := \int_0^{\infty} e^{-\kappa t} L_n(\kappa t) F(x,t)\, dt, \quad n = 0, 1, 2, \ldots ,$$

are the Laguerre-Fourier coefficients of the given boundary values and $\beta = \kappa/c$. The sequence (7.4)–(7.6) can be treated analogously to our analysis for (2.5)–(2.7). For details we refer to [**4, 8**].

In order to illustrate that both methods yield comparable results, we conclude with Table 3 which gives the numerical results for the boundary curve (6.1) with boundary values (6.3) obtained via the method of Laguerre transformation with scaling coefficient $\kappa = 4$. By

$\tilde{N}$ we denote the number of terms in the finite truncation of the series (7.2).

TABLE 3. Numerical results for Laguerre transformation.

		$x = (0.6, 0)$			$x = (0.9, 0)$		
t	M	$\tilde{N} = 30$	$\tilde{N} = 35$	$\tilde{N} = 40$	$\tilde{N} = 30$	$\tilde{N} = 35$	$\tilde{N} = 40$
0.0	16	0.000119	-0.000026	-0.000080	-0.000295	-0.000172	-0.000095
	32	0.000119	-0.000026	-0.000080	-0.000295	-0.000172	-0.000095
0.2	16	0.112226	0.112278	0.112292	0.031782	0.031738	0.031720
	32	0.112226	0.112278	0.112292	0.031782	0.031738	0.031720
0.4	16	0.353852	0.353827	0.353841	0.162233	0.162253	0.162231
	32	0.353852	0.353827	0.353841	0.162233	0.162253	0.162231
0.6	16	0.480926	0.480952	0.480926	0.277068	0.277051	0.277089
	32	0.480926	0.480952	0.480926	0.277068	0.277051	0.277089
0.8	16	0.478417	0.478341	0.478371	0.321280	0.321338	0.321293
	32	0.478417	0.478341	0.478371	0.321280	0.321338	0.321293
1.0	16	0.407189	0.407347	0.407335	0.308569	0.308437	0.308461
	32	0.407189	0.407347	0.407335	0.308569	0.308437	0.308461

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