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On the numerical solution of direct and inverse problems for the heat equation in a semi-infinite region

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Abstract

We consider the initial boundary value problem for the heat equation in a region with infinite and finite boundaries (direct problem) and the related problem to reconstruct the finite boundary from Cauchy data on the infinite boundary (inverse problem). The numerical solution of the direct problem is realized by a boundary integral equation method. For an approximate solution of the inverse problem we use a regularized Newton method based on numerical approach for the direct problem. Numerical examples illustrating our results are presented. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

The numerical solution of the initial boundary value problems for the linear parabolic equation is of considerable significance for a number of applied sciences [11]. These problems are of particular interest for the case of unbounded domains. Then almost all numerical methods are based on boundary integral equations [3,4,7,13,20]. Since the unknown solution has to be found according to the known boundary and boundary data, these linear problems are referred to as the direct problems. The inverse problems for a parabolic equation can be divided into the following principal groups [21]: (1) the problems of the estimation of the heat flux history along a boundary part of a domain from a known temperature measurements on the rest of the boundary and at interior locations; (2) the problems of determining the initial condition if the temperature distributions inside a domain are known at some time; (3) the problems on recovering the diffusion coefficient from boundary

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measurements of the solution of a parabolic equation; (4) the problems in determining a boundary part for the bounded domain from a knowledge of the rest of the boundary, the heat and the heat flux on it (see [1,2,5,8]).

In this paper we consider the direct and the related inverse problems from the fourth group for the heat equation in the case of a specific unbounded domain. Primarily we are interested in the aspects of the numerical solution of these problems.

Let $D_2 := \{x \in \mathbb{R}^2: x_2 > 0\}$ be the upper half-plane in \mathbb{R}^2 and D_1 a simply connected bounded domain in \mathbb{R}^2 with the boundary Γ_1 of the class C^2 such that $\bar{D}_1 \subset D_2$. Let $T > 0$, $I := (0, T]$, $\Gamma_2 := \{x: x_2 = 0, -\infty < x_1 < \infty\}$, $D := D_2 \setminus \bar{D}_1$ and let φ be a given function on $\partial D \times I$. Further denote by φ_1 and φ_2 the restrictions of φ on $\Gamma_1 \times I$ and $\Gamma_2 \times I$, respectively. We shall consider the following direct initial boundary value problem for the heat equation: Find a bounded function $u(x, t)$ satisfying

$$\frac{\partial u}{\partial t} = \Delta u \quad \text{in } D \times I, \quad (1.1)$$

$$u(\cdot, 0) = 0 \quad \text{in } D, \quad (1.2)$$

$$u = \varphi \quad \text{on } \partial D \times I. \quad (1.3)$$

We shall also consider the following related inverse boundary value problem. Under the assumption that $\varphi_1 = 0$, $\varphi_2 \neq 0$, to determine the boundary Γ_1 from a knowledge of the heat flux

$$\frac{\partial u}{\partial \nu}(x, t) \quad \text{on } \Sigma,$$

where $\Sigma := \{x: x_2 = 0, \sigma_0 \leq x_1 \leq \sigma_1\} \times [T_0, T_1]$, $[\sigma_0, \sigma_1] \subset (-\infty, \infty)$ with $\sigma_0 < \sigma_1$, $[T_0, T_1] \subseteq [0, T]$ with $T_0 < T_1$ and ν is the outward unit normal on Γ_2 . The existence and uniqueness of classical or weak solutions for the initial boundary value problem (1.1)–(1.3) are well established [12,18]. For our inverse problem analogous to [8] we have the following uniqueness result.

Theorem 1.1. *Let $D_{1,1}$ and $D_{1,2}$ be two bounded domains in the upper half-plane with the boundaries $\Gamma_{1,1}$ and $\Gamma_{1,2}$, respectively. Let u_1 and u_2 be the classical solutions to the initial boundary value problems (1.1) – (1.3) in the domains $D_2 \setminus D_{1,1}$ and $D_2 \setminus D_{1,2}$, respectively, for $\varphi_1 = 0$ and $\varphi_2 \neq 0$. Let us assume that the heat fluxes of both solutions coincide:*

$$\partial u_1 / \partial \nu = \partial u_2 / \partial \nu \quad \text{on } \Sigma.$$

Then $\Gamma_{1,1} = \Gamma_{1,2}$.

In the case of the direct problem (1.1)–(1.3) we shall seek the solution of a linear problem in a semi-infinite region with the boundary conditions on the finite and infinite boundaries, and in the case of the inverse problem we have to solve a nonlinear and ill-posed problem. The idea for the numerical solution of (1.1)–(1.3) consists in the application of the integral approach based on the special fundamental solution satisfying the boundary condition on the infinite boundary [4]. Following [8,9] we use the Newton method for the numerical solution of the inverse problem and for every Newton step solve the direct problem (1.1)–(1.3) with special boundary conditions.

The outline of the paper is as follows. In Section 2 we will describe the numerical solution of the initial boundary value problem (1.1)–(1.3) via boundary integral equations of the first kind. For the integral representation of the solution we use the single-layer potential with the Green's function for the half-plane. Some aspects of using the Newton method for the numerical solution of our inverse problem are described in Section 3. Finally, in Section 4, we present the results of some numerical experiments.

2. Numerical solution of the direct problem

The special features of the domain D determine the numerical method for the solution of the direct problem (1.1)–(1.3). Since D is an unbounded domain, clearly most efficient numerical method is the application of boundary integral equations. To avoid the determination of a density on the infinite boundary we use the single-layer approach with a Green's function as a special fundamental solution. The Green's function for the heat equation in the upper half-plane has the form

$$G_{\infty}(x - y, t) := G(x_1 - y_1, x_2 - y_2, t) - G(x_1 - y_1, x_2 + y_2, t),$$

where

$$G(x_1, x_2, t) = \frac{e^{-|x_1^2 + x_2^2|^2/4t}}{t}, \quad t > 0, \quad x_1^2 + x_2^2 > 0 \quad (2.1)$$

is the fundamental solution of the heat equation in \mathbb{R}^2 . Then we can seek the solution of the problem (1.1)–(1.3) in the form

$$\begin{aligned} u(x, t) = & \frac{1}{4\pi} \int_0^t \int_{\Gamma_1} q(y, \tau) G_{\infty}(x - y, t - \tau) ds(y) d\tau \\ & - \frac{1}{4\pi} \int_0^t \int_{\Gamma_2} \varphi_2(y, \tau) \frac{\partial G_{\infty}}{\partial \nu(y)}(x - y, t - \tau) ds(y) d\tau, \quad (x, t) \in D \times I, \end{aligned} \quad (2.2)$$

with a density q on $\Gamma_1 \times I$ and the outward unit normal ν on Γ_2 . The heat potential (2.2) satisfies the heat equation (1.1), the homogeneous initial condition (1.2) and the boundary condition on the infinite curve Γ_2 . By the classical results on the continuity of the single-layer potential [12] and by the properties of Green's functions [14] the problem (1.1)–(1.3) is reduced to the integral equation of the first kind:

$$\frac{1}{4\pi} \int_0^t \int_{\Gamma_1} q(y, \tau) G_{\infty}(x - y, t - \tau) ds(y) d\tau = f(x, t), \quad (x, t) \in \Gamma_1 \times I, \quad (2.3)$$

where

$$f(x, t) = \varphi_1(x, t) + \frac{1}{4\pi} \int_0^t \int_{\Gamma_2} \varphi_2(y, \tau) \frac{\partial G_{\infty}}{\partial \nu(y)}(x - y, t - \tau) ds(y) d\tau. \quad (2.4)$$

For this equation we can apply the existence result from [10,15] for the integral equation of the general form in anisotropic Sobolev spaces.

Theorem 2.1. For any given function $\varphi_1 \in H_{00}^{1/2,1/4}(\Gamma_1 \times I)$ and $\varphi_2 \in L^2(\Gamma_2 \times I)$ the integral equation (2.3) possesses a unique solution $q \in H_{00}^{-1/2,-1/4}(\Gamma_1 \times I)$.

We assume that the boundary curve is given through a parametric representation

$$\Gamma_1 = \{x(s) = (x_1(s), x_2(s)): 0 \leq s \leq 2\pi\},$$

where $x: \mathbb{R} \rightarrow \mathbb{R}^2$ is twice continuously differentiable and 2π -periodic with $|x'(s)| > 0$ and $x_2(s) > 0$ for all s . Then we transform (2.3) and (2.4) into the parametric form

$$\frac{1}{4\pi} \int_0^t \int_0^{2\pi} \mu(\sigma, \tau) K^{(1)}(s, \sigma; t, \tau) d\sigma d\tau = F(s, t), \quad (s, t) \in [0, 2\pi] \times I \quad (2.5)$$

and

$$F(s, t) = 2g_1(s, t) + \frac{1}{2\pi} \int_0^t \int_{-\infty}^{\infty} g_2(\sigma, \tau) K^{(2)}(s, \sigma; t, \tau) d\sigma d\tau, \quad (2.6)$$

where we have set $\mu(s, t) := q(x(s), t)|x'(s)|$, $g_1(s, t) := \varphi_1(x(s), t)$, and $g_2(s, t) := \varphi_2(s, 0, t)$, and where the kernels are given by

$$K^{(1)}(s, \sigma; t, \tau) := G_{\infty}(x(s) - x(\sigma), t - \tau)$$

and

$$K^{(2)}(s, \sigma; t, \tau) := -\frac{x_2(s)}{(t - \tau)^2} \exp \left\{ -\frac{(x_1(s) - \sigma)^2 + x_2^2(s)}{4(t - \tau)} \right\}$$

for $s \neq \sigma$. For the semi-discretization of the integral equation (2.5) we use a collocation method with respect to the time-variable [3,4,20]. We choose an equidistant mesh on I by

$$t_n = nh_t, \quad n = 0, \dots, N, h_t = T/N,$$

and use the constant-time interpolation for the unknown density μ and for the given boundary function g_2 . Then for $t = t_n$ from (2.5) and (2.6) we obtain for approximations $\mu_n(s) \approx \mu(s, t_n)$ the following system of Fredholm integral equations of the first kind:

$$\frac{1}{2\pi} \int_0^{2\pi} \mu_n(\sigma) K_0^{(1)}(x(s), \sigma) d\sigma = F_n(s) - \frac{1}{2\pi} \sum_{m=1}^{n-1} \int_0^{2\pi} \mu_m(\sigma) K_{n-m}^{(1)}(x(s), \sigma) d\sigma \quad (2.7)$$

for $s \in [0, 2\pi]$, $n = 1, \dots, N$. Here we have set

$$F_n(s) = 2g_{1,n}(s) - \frac{1}{2\pi} \sum_{m=1}^n \int_{-\infty}^{\infty} g_{2,m}(\sigma) K_{n-m}^{(2)}(x(s), \sigma) d\sigma, \quad (2.8)$$

where $g_{i,n}(s) := g_i(s, t_n)$, $i = 1, 2$, and where the functions $K_p^{(i)}$ are given by

$$K_{n-m}^{(i)}(x(s), \sigma) := \int_{t_{m-1}}^{t_m} K_i(s, \sigma; t_n, \tau) d\tau.$$

After some elementary calculations we find

$$K_p^{(1)}(x(s), \sigma) = K_{1,p}^{(1)}(x(s), \sigma) - K_{2,p}^{(1)}(x(s), \sigma), \quad (2.9)$$

where

$$K_{i,p}^{(1)}(x(s), \sigma) = E_1 \left(\frac{r_i^2(x(s), \sigma)}{4h_i(p+1)} \right) - E_1 \left(\frac{r_i^2(x(s), \sigma)}{4h_i p} \right),$$

for $i = 1, 2$ and

$$K_p^{(2)}(x(s), \sigma) = -\frac{4x_2(s)}{\tilde{r}^2(x(s), \sigma)} \left[\exp \left(-\frac{\tilde{r}^2(x(s), \sigma)}{4h_i(p+1)} \right) - \exp \left(-\frac{\tilde{r}^2(x(s), \sigma)}{4h_i p} \right) \right]$$

for $p = 0, \dots, N-1$ (for $p = 0$ the second terms on the right-hand sides in the two last formulas have to be set equal to zero). Here we introduced the functions

$$r_1(x(s), \sigma) := |x(s) - x(\sigma)|, \quad r_2(x(s), \sigma) := ([x_1(s) - x_1(\sigma)]^2 + [x_2(s) - x_2(\sigma)]^2)^{1/2}$$

and

$$\tilde{r}(x(s), \sigma) := ([x_1(s) - \sigma]^2 + x_2^2(s))^{1/2},$$

and E_1 denotes the exponential integral function (see [19]). Since the function E_1 has the expansion

$$E_1(z) = -\gamma - \ln z - \sum_{n=1}^{\infty} \frac{(-1)^n z^n}{n! n}, \quad \gamma = 0.57721 \dots,$$

we can write the kernel $K_{1,0}^{(1)}$ in the form

$$K_{1,0}^{(1)}(x(s), \sigma) = -\ln \left(\frac{4}{e} \sin^2 \frac{s - \sigma}{2} \right) + K_{1,0}^{(1,0)}(s, \sigma), \quad s \neq \sigma,$$

where

$$K_{1,0}^{(1,0)}(s, \sigma) = K_{1,0}^{(1)}(x(s), \sigma) + \ln \left(\frac{4}{e} \sin^2 \frac{s - \sigma}{2} \right).$$

The functions $K_{1,0}^{(1,0)}$ and $K_{1,p}^{(1)}$, $p = 1, \dots, N-1$, can be shown to be continuous with the diagonal terms

$$K_{1,0}^{(1,0)}(s, s) = -\gamma - \ln \frac{e|x'(s)|^2}{4h_i}, \quad K_{1,p}^{(1)}(x(s), s) = \ln \frac{p+1}{p}.$$

The kernels $K_{2,p}^{(1)}$ and $K_p^{(2)}$ are trivially continuous for $p = 0, 1, \dots, N-1$.

Thus we have to solve a system of integral equations of the first kind with a logarithmic singularity. For a full discretization of this system we combine a quadrature method and a collocation method based on trigonometric interpolation. For this we choose an equidistant mesh by setting

$$s_j := j\pi/M, \quad j = 0, \dots, 2M-1,$$

and use the following two quadrature rules:

$$\frac{1}{2\pi} \int_0^{2\pi} g(\sigma) \ln \left(\frac{4}{e} \sin^2 \frac{s_j - \sigma}{2} \right) d\sigma \approx \sum_{k=0}^{2M-1} R_{|j-k|} g(s_k), \quad (2.10)$$

$$\frac{1}{2\pi} \int_0^{2\pi} g(\sigma) d\sigma \approx \frac{1}{2M} \sum_{k=0}^{2M-1} g(s_k) \quad (2.11)$$

with the weights

$$R_j := -\frac{1}{2M} \left\{ 1 + 2 \sum_{m=1}^{M-1} \frac{1}{m} \cos ms_j + \frac{(-1)^j}{M} \right\}.$$

For the numerical calculation of the integrals on an infinite interval in (2.8) we use the quadrature rule

$$\frac{1}{\pi} \int_{-\infty}^{\infty} g(\sigma) d\sigma \approx h_{\infty} \sum_{j=-M_1}^{M_1} g(jh_{\infty}), \quad h_{\infty} = \frac{c}{\sqrt{M_1}}, \quad c > 0. \quad (2.12)$$

These quadrature formulas are obtained by replacing g by its trigonometric interpolation polynomial in the case of (2.10) and (2.11) (see [16]) and by sinc approximation in the case of (2.12) (see [22]) and then integrating exactly. For the rules (2.10) and (2.11) in the case of periodic analytic functions g and for the rule (2.12) in the case of analytic functions g satisfying $g(s) = O(e^{-\kappa|s|})$ for $|s| \rightarrow \infty$ and some positive constant κ we obtain exponential convergence.

Now we apply the quadrature rules (2.10) and (2.11) in the integral equations (2.7) and the rule (2.12) in (2.8) and then discretize the corresponding approximate equations by a trigonometric collocation. As a result we obtain a sequence of linear systems

$$\begin{aligned} & \sum_{j=0}^{2M-1} \tilde{\mu}_n(s_j) \left\{ -R_{|i-j|} + \frac{1}{2M} [K_{1,0}^{(1,0)}(s_i, s_j) - K_{2,0}^{(1)}(x(s_i), s_j)] \right\} \\ & = F_n(s_i) - \frac{1}{2M} \sum_{m=1}^{n-1} \sum_{j=0}^{2M-1} \tilde{\mu}_m(s_j) K_{n-m}^{(1)}(x(s_i), s_j) \end{aligned} \quad (2.13)$$

with

$$F_n(s_i) = 2g_{1,n}(s_i) + \frac{h_{\infty}}{2\pi} \sum_{m=1}^n \sum_{j=-M_1}^{M_1} g_{2,m}(jh_{\infty}) K_{n-m}^{(2)}(x(s_i), jh_{\infty})$$

for $i = 0, \dots, 2M - 1$, $n = 1, \dots, N$. This numerical method was suggested and analyzed for one integral equation of the type (2.7) in [6] in a Hölder space and in [17] in a Sobolev space setting. In the case of an analytic boundary and boundary data as shown by the error analysis in [6,17], we obtain the exponential convergence for the numerical solution of the integral equations (2.7) with respect to the number M of the space discretization. The numerical experiments (see Section 4) confirm this and show also the linear convergence with respect to the number N of the time discretization for the used numerical method.

Thus for the solution of the initial boundary value problem (1.1)–(1.3) we have the following approach:

$$u(x, t_n) \approx \sum_{m=1}^n \left\{ \frac{1}{4M} \sum_{j=0}^{2M-1} \tilde{\mu}_m(s_j) K_{n-m}^{(1)}(x, s_j) - \frac{h_{\infty}}{4\pi} \sum_{j=-M_1}^{M_1} g_{2,m}(jh_{\infty}) K_{n-m}^{(2)}(x, jh_{\infty}) \right\} \quad (2.14)$$

for $x \in D$, $n = 1, \dots, N$. Clearly, the function $K_0^{(1)}$ has no singularity and is calculated by (2.9).

For the numerical implementation of the inverse problem we need the approximations for the normal derivative of the solution (2.2) on the boundaries. From the jump relations for the normal derivative of a single-layer potential [12] and from the continuity for the normal derivative of a double-layer potential [10,15] we have

$$\begin{aligned} \frac{\partial u}{\partial \nu}(x, t) = & -\frac{1}{2} q(x, t) + \frac{1}{4\pi} \int_0^t \int_{\Gamma_1} q(y, \tau) \frac{\partial}{\partial \nu(x)} G_\infty(x - y, t - \tau) ds(y) d\tau \\ & - \frac{1}{4\pi} \int_0^t \int_{\Gamma_2} \varphi_2(y, \tau) \frac{\partial^2}{\partial \nu(x) \partial \nu(y)} G_\infty(x - y, t - \tau) ds(y) d\tau, \quad (x, t) \in \Gamma_1 \times I \end{aligned} \quad (2.15)$$

and

$$\begin{aligned} \frac{\partial u}{\partial \nu}(x, t) = & \frac{1}{4\pi} \int_0^t \int_{\Gamma_1} q(y, \tau) \frac{\partial}{\partial \nu(x)} G_\infty(x - y, t - \tau) ds(y) d\tau \\ & - \frac{1}{4\pi} \frac{\partial}{\partial \nu(x)} \int_0^t \int_{\Gamma_2} \varphi_2(y, \tau) \frac{\partial}{\partial \nu(y)} G_\infty(x - y, t - \tau) ds(y) d\tau, \quad (x, t) \in \Gamma_2 \times I. \end{aligned} \quad (2.16)$$

Then connecting formula (2.15) with the numerical solution of integral equation (2.3) we have the following approximation for the flux on Γ_1 :

$$\begin{aligned} \frac{\partial u}{\partial \nu}(x(s_i), t_n) \approx & -\frac{\tilde{\mu}_n(s_i)}{2|x'(s_i)|} + \frac{1}{4M} \sum_{m=1}^n \sum_{k=1}^2 \left\{ \frac{1}{4M} \sum_{j=0}^{2M-1} \tilde{\mu}_m(s_j) \eta_k^{(1)}(s_i, s_j) L_{n-m}^{(1,k)}(s_i, s_j) \right. \\ & \left. - \frac{h_\infty}{4\pi} \sum_{j=-M_1}^{M_1} g_{2,m}(jh_\infty) \eta_k^{(2)}(s_i, jh_\infty) L_{n-m}^{(2,k)}(s_i, jh_\infty) \right\} \end{aligned} \quad (2.17)$$

for $i = 0, 1, \dots, 2M - 1$, $n = 1, \dots, N$, where

$$L_p^{(1,k)}(s, \sigma) = \exp\left(-\frac{r_k^2(x(s), \sigma)}{4h_t(p+1)}\right) - \exp\left(-\frac{r_k^2(x(s), \sigma)}{4h_t p}\right)$$

for $k = 1, 2$,

$$\begin{aligned} L_p^{(2,1)}(s, \sigma) = & \left[\frac{1}{2h_t(p+1)} + \frac{2}{\tilde{r}^2(x(s), \sigma)} \right] \exp\left(-\frac{\tilde{r}^2(x(s), \sigma)}{4h_t(p+1)}\right) \\ & - \left[\frac{1}{2h_t p} + \frac{2}{\tilde{r}^2(x(s), \sigma)} \right] \exp\left(-\frac{\tilde{r}^2(x(s), \sigma)}{4h_t p}\right) \end{aligned}$$

and

$$L_p^{(2,2)}(s, \sigma) = \exp\left(-\frac{\tilde{r}^2(x(s), \sigma)}{4h_t(p+1)}\right) - \exp\left(-\frac{\tilde{r}^2(x(s), \sigma)}{4h_t p}\right)$$

for $p = 0, \dots, N-1$ (for $p = 0$ the second terms on the right-hand sides have to be set equal to zero). The functions $\eta_i^{(k)}$ have the form

$$\eta_1^{(1)}(s, \sigma) = \begin{cases} \frac{x_2'(s)x_1''(s) - x_1'(s)x_2''(s)}{|x'(s)|^3}, & s = \sigma, \\ -2 \frac{[x_1(s) - x_1(\sigma)]x_2'(s) - [x_2(s) - x_2(\sigma)]x_1'(s)}{|x'(s)|r_1^2(x(s), \sigma)}, & \text{otherwise,} \end{cases}$$

$$\eta_2^{(1)}(s, \sigma) = 2 \frac{[x_1(s) - x_1(\sigma)]x_2'(s) - [x_2(s) - x_2(\sigma)]x_1'(s)}{|x'(s)|r_2^2(x(s), \sigma)},$$

$$\eta_1^{(2)}(s, \sigma) = 4 \frac{x_1'(s)x_2^2(s) - x_2(s)(x_1(s) - \sigma)}{|x'(s)|\tilde{r}^2(x(s), \sigma)} \quad \text{and} \quad \eta_2^{(2)}(s, \sigma) = -4 \frac{x_1'(s)}{|x'(s)|\tilde{r}^2(x(s), \sigma)}.$$

We note here that for $h_t \rightarrow 0$ ($N \rightarrow \infty$) the kernels $L_0^{(2,1)}$ and $K_{i,0}^{(1)}$ have a pronounced delta function like behavior. A similar problem is arising also in another numerical method for the parabolic problems [7,20]. For the numerical experiments in Section 4 we choose the time discretization parameter not very large and co-ordinated it with the spatial discretization parameter, i.e. we increase the number M of quadrature points when the number N of collocation points with respect to the time is increased. This reflects the general requirement to balance spatial and time discretization in the numerical solution of the nonstationary problems.

The numerical calculation of the flux (2.16) causes additional difficulties because of a strong singularity in the kernel of the second term. We shall consider this case in more detail. Let

$$P(x, t) := \frac{1}{4\pi} \frac{\partial}{\partial v(x)} \int_0^t \int_{\Gamma_2} \varphi_2(y, \tau) \frac{\partial}{\partial v(y)} G_\infty(x - y, t - \tau) ds(y) d\tau, \quad (x, t) \in \Gamma_2 \times I.$$

After the parametrization of Γ_2 and the constant-time interpolation for φ_2 we have

$$P(s, t_n) \approx \frac{1}{4\pi} \sum_{m=1}^n \int_{-\infty}^{\infty} g_{2,m}(\sigma) H_{n-m}^{(2)}(s, \sigma) d\sigma, \quad -\infty < s < \infty, \quad n = 1, \dots, N,$$

where

$$H_p^{(2)}(s, \sigma) = \frac{4}{(s - \sigma)^2} \left\{ \exp\left(-\frac{(s - \sigma)^2}{4h_t(p+1)}\right) - \exp\left(-\frac{(s - \sigma)^2}{4h_t p}\right) \right\}$$

for $p = 0, \dots, N-1$ (for $p = 0$ the second term on the figured brackets has to be set equal to zero). Since

$$H_p^{(2)}(s, s) = \frac{1}{h_t p} - \frac{1}{h_t(p+1)} \quad \text{for } p = 1, \dots, N-1,$$

we consider only the integral with the integrand $H_0^{(2)}(s, \sigma)$ as a *finite part integral*, that is, as Hadamard's hypersingular integral. By partial integration we obtain

$$\int_{-\infty}^{\infty} g_{2,n}(\sigma) H_0^{(2)}(s, \sigma) d\sigma = 4 \int_{-\infty}^{\infty} \frac{g_{2,n}'(\sigma)}{\sigma - s} \exp\left(-\frac{(s - \sigma)^2}{4h_t}\right) d\sigma$$

$$- \frac{2}{h_t} \int_{-\infty}^{\infty} g_{2,n}(\sigma) \exp\left(-\frac{(s - \sigma)^2}{4h_t}\right) d\sigma, \quad -\infty < s < \infty.$$

Here the first integral is considered as a Cauchy singular integral. For the numerical integration of this integral we use the sinc quadrature rule [22]

$$\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{g(\sigma)}{s - \sigma} d\sigma \approx \sum_{j=-M_1}^{M_1} g(jh_{\infty}) \tilde{R}_j(s),$$

where

$$\tilde{R}_j(s) := \frac{\cos[(\pi/h_{\infty})(s - jh_{\infty})]}{(\pi/h_{\infty})(s - jh_{\infty})}.$$

Thus, finally, the approximate heat flux on Γ_2 is given by

$$\begin{aligned} \frac{\partial u}{\partial v}(s, t_n) \approx & \frac{1}{4M} \sum_{m=1}^n \sum_{j=0}^{2M-1} \tilde{\mu}_m(s_j) H_{n-m}^{(1)}(s, s_j) - \frac{h_{\infty}}{4\pi} \sum_{m=1}^{n-1} \sum_{j=-M_1}^{M_1} g_{2,m}(jh_{\infty}) H_{n-m}^{(2)}(s, jh_{\infty}) \\ & + \sum_{j=-M_1}^{M_1} \left\{ \frac{h_{\infty}}{2\pi h_t} g_{2,n}(jh_{\infty}) - g'_{2,n}(jh_{\infty}) \tilde{R}_j(s) \right\} \exp\left(-\frac{(s - jh_{\infty})^2}{4h_t}\right), \end{aligned} \quad (2.18)$$

where

$$H_p^{(1)}(s, \sigma) = -\frac{4x_2(\sigma)}{\tilde{r}^2(x(\sigma), s)} \left\{ \exp\left(-\frac{\tilde{r}^2(x(\sigma), s)}{4h_t(p+1)}\right) - \exp\left(-\frac{\tilde{r}^2(x(\sigma), s)}{4h_t p}\right) \right\}$$

for $p = 0, \dots, N-1$ (for $p=0$ the second term on the figured brackets has to be set equal to zero).

3. The numerical solution of the inverse problem

The solution of the direct initial boundary value problem (1.1)–(1.3) defines a nonlinear operator

$$\mathcal{F} : \Gamma_1 \rightarrow \frac{\partial u}{\partial v}(x, t), \quad (x, t) \in \Sigma,$$

which maps the curve Γ_1 onto the flux $\partial u / \partial v$ on the line Γ_2 . In this sense the solution of our inverse problem consists in the solution of the nonlinear equation

$$\mathcal{F}(\Gamma_1) = \psi, \quad (3.1)$$

where $\psi(x, t) := \partial u / \partial v(x, t)$, $(x, t) \in \Sigma$. Let us assume that Γ_1 is starlike, i.e.

$$x(s) = (r(s) \cos s, r(s) \sin s + d), \quad 0 \leq s \leq 2\pi \quad (3.2)$$

with a positive function $r(s) \in C^2(\Gamma_1)$ and a positive constant d , such that $x_2(s) > 0$ for all s . Clearly $r(s)$ is to be found. We transform Eq. (3.1) into the parametric form

$$\mathcal{F}(r) = \gamma(s, t), \quad (s, t) \in \Sigma^*, \quad (3.3)$$

where $\gamma(s, t) := \psi(s, 0, t)$ and $\Sigma^* := [\sigma_0, \sigma_1] \times [T_0, T_1]$.

Assume that the curve $\tilde{\Gamma}_1$, with the parametric representation $z(s)$ is an approximation for the curve Γ_1 and let $h(s)$ be the unknown correction such that $\tilde{z}(s) = z(s) + h(s)$ is a new approximation. We look for $h(s)$ in the form

$$h(s) = (q(s)\cos s, q(s)\sin s + d), \quad (3.4)$$

where $q(s)$ is the unknown. After the linearization of Eq. (3.3) we get the following approximating linear equation with respect to $h(s)$:

$$\mathcal{F}(r) + \mathcal{F}'(r; h) = \gamma(s, t), \quad (s, t) \in \Sigma^*. \quad (3.5)$$

We approximate $q(s)$ in the form

$$q(s) = \sum_{j=1}^K a_j q_j(s) \quad (3.6)$$

with basis functions $q_j(s)$. The collocation method for (3.5) with respect to the collocation points $(\tilde{s}_k, \tilde{t}_i) \in \Sigma^*$, $k = 1, \dots, M_{\text{inv}}$, $i = 1, \dots, N_{\text{inv}}$, yields the system of linear equations

$$\sum_{j=1}^K a_j \mathcal{F}'(r; h_j)(\tilde{s}_k, \tilde{t}_i) = \gamma(\tilde{s}_k, \tilde{t}_i) - \mathcal{F}(r)(\tilde{s}_k, \tilde{t}_i), \quad (3.7)$$

where $h_j(s) := (q_j(s)\cos s, q_j(s)\sin s + d)$ and $M_{\text{inv}}N_{\text{inv}} > K$. Analogous to the case of the inverse problems for the heat equation in a bounded domain [8] for the derivative $\mathcal{F}'(r, h)$ we have the following result:

Theorem 3.1. *Let \tilde{D}_1 be a bounded domain with the boundary $\tilde{\Gamma}_1$ and $\tilde{D} := D_2 \setminus \tilde{D}_1$. Let $\varphi_2 \in L^2(\Gamma_2 \times I)$, $h \in C^2(\tilde{\Gamma}_1; \mathbb{R}^2)$ and u be a weak solution of the initial boundary value problem (1.1) – (1.3) in $\tilde{D} \times I$ with $\varphi_1 = 0$. Then the domain derivative $\mathcal{F}'(r; h)$ exists and is given by*

$$\mathcal{F}'(r; h) = \left. \frac{\partial u'}{\partial \nu} \right|_{\Sigma},$$

where u' solves the heat equation

$$\frac{\partial u'}{\partial t} = \Delta u' \quad \text{in } \tilde{D} \times I \quad (3.8)$$

in the weak sense and satisfies the boundary condition

$$u' = -h \cdot \nu \frac{\partial u}{\partial \nu} \quad \text{on } \tilde{\Gamma}_1 \times I \quad \text{and} \quad u' = 0 \quad \text{on } \Gamma_2 \times I. \quad (3.9)$$

Here ν is the outward unit normal on $\tilde{\Gamma}_1$.

Due to the linear equation (3.5) being an ill-posed equation, we have to incorporate some regularization to stabilize our problem, for example a Tikhonov regularization. Hence, we replace (3.7) by the following least-squares problem to minimize the penalized residual

$$T := \alpha \sum_{k=1}^K w_k a_k^2 + \sum_{i=1}^{M_{\text{inv}}} \sum_{j=1}^{N_{\text{inv}}} \left| \sum_{k=1}^K a_k \mathcal{F}'(r; h_k)(\tilde{s}_i, \tilde{t}_j) - \gamma(\tilde{s}_i, \tilde{t}_j) + \mathcal{F}(r)(\tilde{s}_i, \tilde{t}_j) \right|^2$$

with some regularization parameter $\alpha > 0$ and some positive weights w_1, \dots, w_K . Minimizing of T with respect to a_1, \dots, a_K is equivalent to solving the following linear system:

$$\begin{aligned} \alpha w_p a_p + \sum_{k=1}^K a_k \sum_{i=1}^{M_{\text{inv}}} \sum_{j=1}^{N_{\text{inv}}} \mathcal{F}'(r; h_k)(\tilde{s}_i, \tilde{t}_j) \mathcal{F}'(r; h_p)(\tilde{s}_i, \tilde{t}_j) \\ = \sum_{i=1}^{M_{\text{inv}}} \sum_{j=1}^{N_{\text{inv}}} \{\gamma(\tilde{s}_i, \tilde{t}_j) - \mathcal{F}(r)(\tilde{s}_i, \tilde{t}_j)\} \mathcal{F}'(r; h_p)(\tilde{s}_i, \tilde{t}_j), \quad p = 1, \dots, K. \end{aligned} \quad (3.10)$$

We choose the weights w_p as in the Levenberg–Marquardt algorithm:

$$w_p = \sum_{i=1}^{M_{\text{inv}}} \sum_{j=1}^{N_{\text{inv}}} \mathcal{F}'(r; q_p)(\tilde{s}_i, \tilde{t}_j) \mathcal{F}'(r; q_p)(\tilde{s}_i, \tilde{t}_j), \quad p = 1, \dots, K.$$

Finally, we summarize the description of one step of the Newton method as follows:

1. Given the initial approximation z_0 for Γ_1 (the circle as an example), solve the direct problem (1.1)–(1.3) by the method in Section 2 and compute $\partial u / \partial v$ on Γ_2 via (2.18).
2. Compute the numerical solutions for the sequence of direct initial boundary value problems (1.1)–(1.3) with the corresponding boundary conditions.
3. Solve the system of linear equations (3.10).
4. Compute the correction h via (3.4) and (3.6) and find the new approximation $z_{i+1} = z_i + h$ for the boundary Γ_1 .

As a stopping rule for the number of iterations we use the condition

$$\|q\|_{L^2} / \|r_i\|_{L^2} < \delta,$$

where δ is a given precision.

4. Numerical experiments

At first we consider the numerical solution of the direct problem (1.1)–(1.3). The finite boundary Γ_1 is a bean-shaped curve given by (3.2) with the radial function

$$r(s) = \frac{1.0 + 0.9 \cos s + 0.1 \sin 2s}{2.0 + 1.5 \cos s}, \quad 0 \leq s \leq 2\pi, \quad (4.11)$$

and $d = 1.5$. The boundary conditions are given by the restriction of the fundamental solution (2.1) on the boundaries

$$\varphi_i(x, t) = G(x_1, x_2 - 1.5, t), \quad (x, t) \in \Gamma_i \times I, \quad i = 1, 2. \quad (4.12)$$

For the length of the time interval we assume $T = 2$ and the parameters are chosen as $M = 32$, $M_1 = 100$ and $h_\infty = 0.2$. Fig. 1 illustrates the relative errors $E_r(x, t) := |u_{\text{num}}(x, t) - u_{\text{ex}}(x, t)| / |u_{\text{ex}}(x, t)|$ at spatial point $x = (1, 1.5)$ for the various time discretization parameter N .

For the second numerical example in the case of the direct problem the boundary Γ_1 is given by (4.11) and the boundary conditions are

$$\varphi_1(x, t) = 0, \quad (x, t) \in \Gamma_1 \times I \quad (4.13)$$

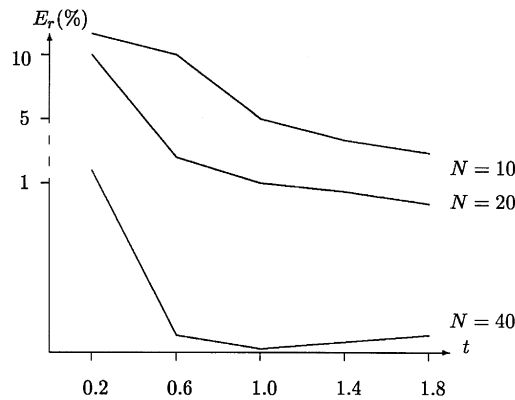
Fig. 1. Relative errors for the various time discretization parameters N .

Table 1
Numerical results for the boundary conditions (4.13) and (4.14)

t	M	$x = (0, 0.5)$			$x = (1, 1.5)$		
		$N = 10$	$N = 20$	$N = 40$	$N = 10$	$N = 20$	$N = 40$
0.2	16	0.029736	0.024630	0.021749	0.000095	0.000063	0.000045
	32	0.029736	0.024630	0.021749	0.000095	0.000060	0.000044
0.4	16	0.067445	0.064590	0.062842	0.001019	0.000903	0.000832
	32	0.067445	0.064590	0.062842	0.001019	0.000898	0.000830
0.6	16	0.078015	0.078292	0.078370	0.002488	0.002386	0.002320
	32	0.078015	0.078292	0.078370	0.002488	0.002384	0.002319
0.8	16	0.068023	0.069772	0.070752	0.003476	0.003441	0.003416
	32	0.068023	0.069772	0.070752	0.003476	0.003442	0.003416
1.0	16	0.050837	0.052784	0.053912	0.003671	0.003692	0.003703
	32	0.050837	0.052784	0.053912	0.003671	0.003694	0.003704

and

$$\varphi_2(x, t) = t^2 \exp(-4(t + |x|^2) + 2), \quad (x, t) \in \Gamma_2 \times I. \quad (4.14)$$

Table 1 gives some values for the numerical solution of the initial boundary value problem (1.1)–(1.3) at the two space points for the time interval with the length $T = 1$.

Now we turn to the numerical solution of the inverse problem to reconstruct the boundary Γ_1 given by (4.11). The boundary conditions are given by (4.13) and (4.14). For the solution of the forward problem generating the flux $\psi = \partial u / \partial v$ on Γ_2 we used the numerical method of Section 2. For an approximating subspace for the radial function we choose trigonometric polynomials of degree less than or equal to K , i.e.,

$$q(s) = \sum_{k=0}^K a_k \cos ks + \sum_{k=K+1}^{2K} a_k \sin(k - K)s.$$

Table 2

Numerical results for various space intervals

	$[\sigma_0, \sigma_1]$	M_{inv}	L	E	F	α
a	$[-1, 0]$	6	13	0.040389	0.000013	0
b	$[-0.4, 0]$	3	9	0.091784	0.000010	10^{-4}
c	$[0, 0.4]$	3	11	0.085335	0.000017	10^{-5}
d	$[-0.4, 0.4]$	6	9	0.093867	0.000007	10^{-5}

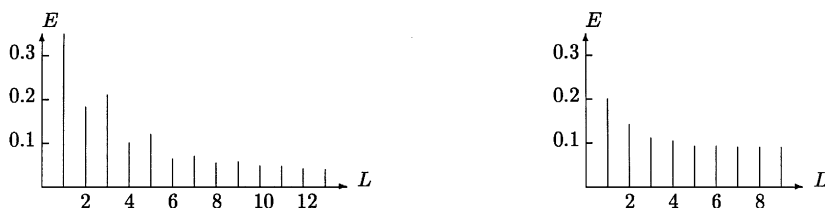
Fig. 2. Relative error of the Newton iteration for cases a and b .

Table 2 shows the relative error

$$E := \frac{\|r_L - r\|_{L^2[0, 2\pi]}}{\|r\|_{L^2[0, 2\pi]}}$$

and the relative residual

$$F := \frac{\|\partial u_L / \partial \nu - \psi\|_{L^2(\Sigma)}}{\|\psi\|_{L^2(\Sigma)}}$$

for various space intervals $[\sigma_0, \sigma_1] \subseteq [-1, 1]$ and fixed time interval $[T_0, T_1] = [0, 3]$. The number L counts the iteration steps required for the tolerance $\delta = 0.005$.

The relative errors in every Newton step for the case a and b in Table 2 are illustrated in Fig. 2. The reconstructions of the boundary Γ_1 corresponding to Table 2 are presented in Fig. 3. The full part of the straight line corresponds to the measurement interval $[\sigma_0, \sigma_1]$ on the infinite curve Γ_2 . For all examples the discretization parameters are $M = 32$, $N = 20$, $N_{\text{inv}} = N$ and $M_1 = 100$.

The finite closed boundary Γ_1 to be reconstructed is a peanut-shaped curve given by (3.2) with

$$r(s) = \sqrt{\cos^2 s + 0.26 \sin^2(s + 0.5)}, \quad 0 \leq s \leq 2\pi.$$

The boundary conditions are $\varphi_1 = 0$ and

$$\varphi_2(x, t) = t^2 \exp(-4t + 2), \quad (x, t) \in \Gamma_2 \times I$$

with $T = 2$. Table 3 gives some numerical results for this inverse problem. The reconstructions illustrated in Fig. 4 correspond to the first and third row of Table 3. In all our numerical experiments for the inverse problem we observe that the reconstruction is strongly dependent on the length of the space interval $[\sigma_0, \sigma_1]$ on the infinite line Γ_2 and on the distance between the reconstructed boundary and the measurement interval.

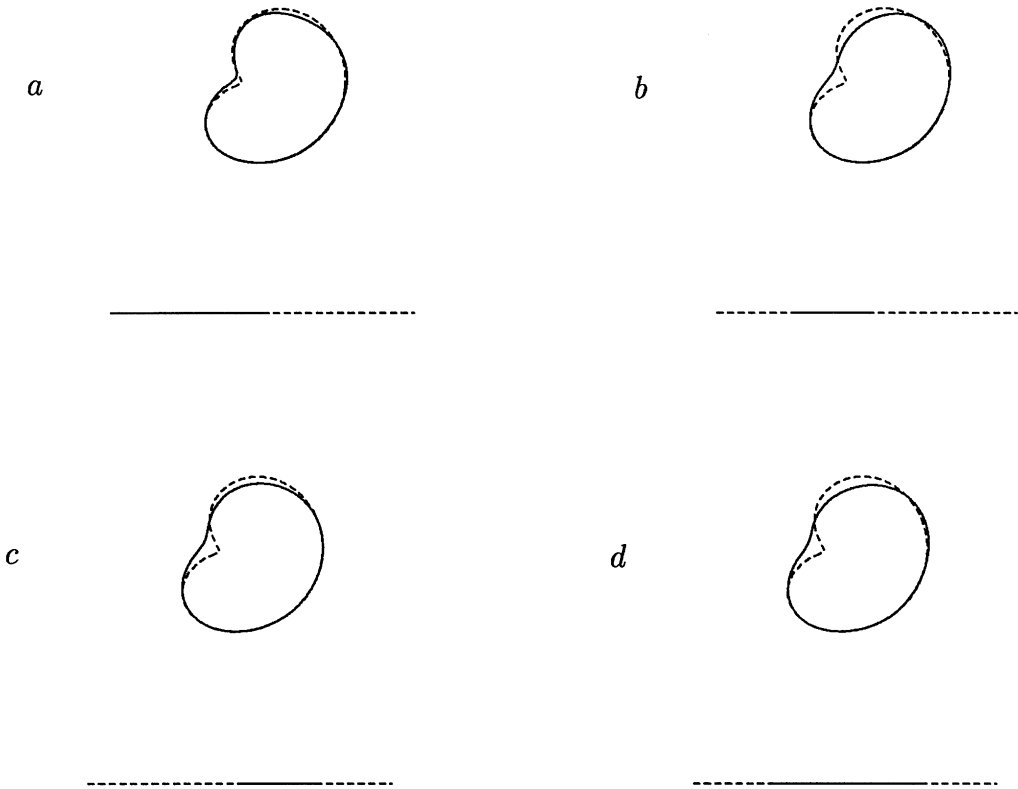


Fig. 3. Reconstruction of a bean-shaped figure with $K = 4$.



Fig. 4. Reconstruction of a peanut-shaped figure with $K = 4$.

Table 3
Numerical results for a peanut-shaped figure

$[\sigma_0, \sigma_1]$	d	M_{inv}	N_{inv}	L	E	F	α
$[-2, 2]$	1	21	12	26	0.075709	0.000469	10^{-4}
	2	21	12	6	0.187662	0.000462	10^{-3}
$[-1, 1]$	1	11	20	15	0.125483	0.000393	10^{-4}
	2	11	20	7	0.197161	0.000241	10^{-3}

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