ISSN 0012-2661, Differential Equations, 2016, Vol. 52, No. 7, pp. 855–862. © Pleiades Publishing, Ltd., 2016.
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NUMERICAL METHODS

Numerical Identification of the Leading Coefficient of a Parabolic Equation

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Received January 15, 2016

Abstract—For a multidimensional parabolic equation, we study the problem of finding the leading coefficient, which is assumed to depend only on time, on the basis of additional information about the solution at an interior point of the computational domain. For the approximate solution of the nonlinear inverse problem, we construct linearized approximations in time with the use of ordinary finite-element approximations with respect to space. The numerical algorithm is based on a special decomposition of the approximate solution for which the transition to the next time level is carried out by solving two standard elliptic problems. The capabilities of the suggested numerical algorithm are illustrated by the results of numerical solution of a model inverse two-dimensional problem.

DOI: 10.1134/S0012266116070053

INTRODUCTION

Mathematical modeling of numerous applied problems in science and engineering requires numerical solution of inverse problems. Inverse problems for partial differential equations should be studied separately [1, p. 7; 2, p. 9]. Inverse problems are posed as nonclassical problems for partial differential equations; they often belong to the class of ill-posed (conditionally well-posed) problems. Theoretical studies primarily deal with the uniqueness of the solution and its stability.

Of inverse problems for partial differential equations, one can single out coefficient inverse problems, in which the coefficients and/or right-hand side of the equation should be reconstructed from additional information on the solution. When studying nonstationary problems, one singles out problems of reconstructing the dependence of the coefficients on time or on the space variables as separate problems [3, p. 25; 4, p. 255]. Only in some cases we have linear inverse problems, which are problems of identification of the right-hand side of the equation. Other coefficient inverse problems are nonlinear, which substantially complicates their study.

Much attention is paid to the problem of finding the coefficient multiplying the leading spatial derivatives in a second-order parabolic equation, in particular, for the case in which this coefficient depends only on time [5, p. 187; 6, p. 115]. The additional condition is most frequently stated as the specification of the value of the solution at some interior point or on the boundary of the computational domain. In a more general case, the overdetermination condition is posed as some integral average over the entire domain or its part at each time. The existence and uniqueness of the solution of such a inverse problem and the well-posedness of such problems in various function classes were studied. Of other papers in this direction, note, for example, the papers [7–10] and the bibliography therein.

Numerical methods for solving the problem of reconstructing the leading coefficient in a parabolic equation were considered in numerous papers. An approach in which the time-dependent leading coefficient was reconstructed on the basis of the solution of the corresponding integral equation was used in [11, 12]. The passage to a nonclassical parabolic equation in which the coefficients depend on some functionals of the solution was used in [13–15] to study inverse problems with overdetermination of the flux on the boundary.

The paper [16] deals with determining the dependence of the right-hand side of a multidimensional parabolic equation on time on the basis of additional observations of the solution at a point of the computational domain. The numerical algorithm is based on a special decomposition of the solution for which the passage to a new time level is implemented by solving two standard grid elliptic problems. The same approach was used in [17], where the problem of finding the leading coefficient depending only on time was considered for a multidimensional parabolic equation. The main specific features of the considered nonlinear inverse problem were taken into account in the choice of linearized approximations in time. A special scheme linearized with respect to time is used in the present paper for the approximate solution of the problem of reconstructing the leading coefficient of a second-order parabolic equation. As a model problem, we consider a two-dimensional problem with the standard finite-element approximation with respect to space.

STATEMENT OF THE PROBLEM

We restrict our considerations to a two-dimensional problem. The passage to more general three-dimensional problems is mainly of editorial nature. Let $\boldsymbol{x} = (x_1, x_2)$, and let Ω be a bounded polygon. The direct problem is as follows. Find a function $u(\boldsymbol{x}, t)$, $0 \le t \le T$, $T > 0$, that is a solution of the second-order parabolic equation

$$\frac{\partial u}{\partial t} - a(t)\,\mathrm{div}(k(\boldsymbol{x})\,\mathrm{grad}\,u) + c(\boldsymbol{x})u = f(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Omega, \qquad 0 < t \le T, \tag{1}$$

where $a(t) > 0$, $k(\boldsymbol{x}) > 0$, and $c(\boldsymbol{x}) \ge 0$. In addition, we have the boundary and initial conditions

$$a(t)k(\boldsymbol{x})\frac{\partial u}{\partial n} + g(\boldsymbol{x})u = 0, \qquad \boldsymbol{x} \in \partial\Omega, \qquad 0 < t \le T, \tag{2}$$

$$u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega, \tag{3}$$

where n is the normal to the boundary of Ω and $g(\boldsymbol{x}) \ge 0$. In the form (1)–(3), we pose the direct problem in which the right-hand side, the coefficients of the equation and the boundary conditions, and the initial condition are given.

Consider the inverse problem in which the coefficient $a(t)$ in Eq. (1) is unknown. The additional condition is often stated in the form

$$\int\limits_{\Omega} u(\boldsymbol{x}, t)\omega(\boldsymbol{x})\,d\boldsymbol{x} = \varphi(t), \qquad 0 < t \le T, \tag{4}$$

where $\omega(\boldsymbol{x})$ is some weight function. In particular, for $\omega(\boldsymbol{x}) = \delta(\boldsymbol{x} - \boldsymbol{x}^*)$ $(\boldsymbol{x}^* \in \Omega)$, where $\delta(\boldsymbol{x})$ is the δ-function, from condition (4), we have

$$u(\boldsymbol{x}^*, t) = \varphi(t), \qquad 0 < t \le T. \tag{5}$$

We assume that the inverse problem of finding the pair $u(\boldsymbol{x}, t)$, $a(t)$ from conditions (1)–(3) and the additional conditions (4) or (5) is well posed. The corresponding conditions for the existence and unique solvability can be found in the above-mentioned papers. In the present paper, we focus our attention on the numerical solution of the considered inverse problems rather than theoretical problems of convergence of the approximate solution to the exact one.

PURELY IMPLICIT SCHEME

The inverse problem of finding the pair $u(\boldsymbol{x}, t)$, $a(t)$ is nonlinear. The standard approach is based on the use of the simplest time approximations and an iterative solution of the corresponding nonlinear problem for finding the approximate solution at the new level. Here we aim at using time approximations that lead to an approximate solution of linear problems for finding the solution at the new time level.

For simplicity, we define a uniform time grid with increment τ,

$$\overline{\omega}_\tau = \omega_\tau \cup \{T\} = \{t^n = n\tau,\ n = 0, \ldots, N,\ \tau N = T\},$$

and set $y^n = y(t^n)$ and $t^n = n\tau$. We use a finite-element approximation with respect to space. In the polygon Ω, we make a triangulation, and on this computational grid we define the finite-dimensional space $V \subset H^1(\Omega)$ of finite elements [18, p. 75; 19, p. 71].

When using the purely implicit scheme [20, p. 302; 21, p. 39] with respect to time, one can find an approximate solution from the variational problem

$$\int\limits_\Omega \frac{u^{n+1} - u^n}{\tau} v\, d\boldsymbol{x} + a^{n+1} \int\limits_\Omega k(\boldsymbol{x}) \operatorname{grad} u^{n+1} \operatorname{grad} v\, d\boldsymbol{x} + \int\limits_\Omega c(\boldsymbol{x}) u^{n+1} v\, d\boldsymbol{x} + \int\limits_{\partial\Omega} g(\boldsymbol{x}) u^{n+1} v\, d\boldsymbol{x}$$

$$= \int\limits_\Omega f(\boldsymbol{x}, t^{n+1}) v\, d\boldsymbol{x}, \qquad v \subset V, \qquad n = 0, \ldots, N-1, \tag{6}$$

$$\int\limits_\Omega u^0 v\, d\boldsymbol{x} = \int\limits_\Omega u_0 v\, d\boldsymbol{x}. \tag{7}$$

The additional relations (4) and (5) acquire the form

$$\int\limits_\Omega u^{n+1} \omega(\boldsymbol{x})\, d\boldsymbol{x} = \varphi^{n+1}, \tag{8}$$

$$u^{n+1}(\boldsymbol{x}^*) = \varphi^{n+1}, \qquad n = 0, \ldots, N-1. \tag{9}$$

To find the approximate solution $u^{n+1}(\boldsymbol{x})$, p^{n+1} from relations (6)–(8) or (6), (7), (9) on the new time level, one should use some iterative procedures. In the solution of nonstationary problems, the solution changes weakly when passing from one time level to another. This fundamental property of nonstationary problems is actively used for the approximate solution of nonlinear problems by means of various linearizations. We use a similar approach for the numerical solution of the inverse problem of finding the leading coefficient of a parabolic equation.

LINEARIZED SCHEME

The considered nonlinear inverse problem (1)–(3), (5) is characterized by a quadratic nonlinearity. For such problems, one can construct linearized second-order schemes in which the approximate solution at the new time step is found from a linear problem. The construction is based on the approximation to the expression $a(t)b(t)$ at the point $t^{n+1/2}$,

$$a(t^{n+1/2}) b(t^{n+1/2}) = \frac{1}{2} a(t^{n+1}) b(t^n) + \frac{1}{2} a(t^n) b(t^{n+1}) + O(\tau^2).$$

The approximation to Eq. (1) with regard of the boundary conditions (2) on the basis of the Crank–Nicolson scheme leads to the linearized scheme

$$\int\limits_\Omega \frac{u^{n+1} - u^n}{\tau} v\, d\boldsymbol{x} + \frac{a^n}{2} \int\limits_\Omega k(\boldsymbol{x}) \operatorname{grad} u^{n+1} \operatorname{grad} v\, d\boldsymbol{x} + \frac{1}{2} \int\limits_{\partial\Omega} g(\boldsymbol{x}) u^{n+1} v\, d\boldsymbol{x}$$

$$+ \frac{a^{n+1}}{2} \int\limits_\Omega k(\boldsymbol{x}) \operatorname{grad} u^n \operatorname{grad} v\, d\boldsymbol{x} + \frac{1}{2} \int\limits_{\partial\Omega} g(\boldsymbol{x}) u^n v\, d\boldsymbol{x} + \frac{1}{2} \int\limits_\Omega c(\boldsymbol{x}) u^n v\, d\boldsymbol{x} + \frac{1}{2} \int\limits_\Omega c(\boldsymbol{x}) u^{n+1} v\, d\boldsymbol{x}$$

$$= \int\limits_\Omega f(\boldsymbol{x}, t^{n+1/2}) v\, d\boldsymbol{x}, \qquad v \subset V, \qquad n = 0, \ldots, N-1. \tag{10}$$

The scheme (7), (8), (10) [and the scheme (7), (9), (10)] belongs to the class of linearized schemes. Its second prospective advantage over the scheme (6)–(8) is related to the fact that it has a higher order of approximation with respect to time. A similar linearized scheme was used in [17] for the approximate solution of the inverse problem of finding a lower coefficient of a parabolic equation.

Let us state typical conditions for the absolute stability of the linearized scheme for the direct problem on the basis of general results of stability theory of operator-difference schemes [22, p. 103; 23, p. 15]. To simplify the study, we restrict our considerations to the case of a homogeneous equation, for which the right-hand side in Eq. (1) is zero, and to boundary conditions of the second kind. By $(\cdot\,,\cdot)$ and $\|\cdot\|$, we denote the inner product and the norm, respectively, on $L_2(\Omega)$.

Theorem. *Let* $f(\boldsymbol{x},t)\equiv 0$, $g(\boldsymbol{x})\equiv 0$, *and* $a'(t)\le 0$ *in Eq.* (1). *Then the linearized scheme* (7), (10) *is unconditionally stable*, *and its approximate solution satisfies the levelwise estimate*

$$\|u^{n+1}\|^2+\frac{a^{n+1}}{2}\tau\|k^{1/2}\operatorname{grad}u^{n+1}\|^2+\frac{1}{2}\tau\|c^{1/2}u^{n+1}\|^2 \le \|u^n\|^2+\frac{a^n}{2}\tau\|k^{1/2}\operatorname{grad}u^n\|^2+\frac{1}{2}\tau\|c^{1/2}u^n\|^2. \tag{11}$$

Proof. Set $v=2\tau u^{n+1}$ in the estimate (10). Under the assumptions of the theorem, we obtain the relation

$$2\|u^{n+1}\|^2+\tau a^n\|k\operatorname{grad}u^{n+1}\|^2+\tau\|cu^{n+1}\|^2 = 2(u^n,u^{n+1})+\tau a^{n+1}(k\operatorname{grad}u^n,\operatorname{grad}u^{n+1})+\tau(cu^n,u^{n+1}).$$

By taking into account the inequalities

$$2(u^n,u^{n+1})\le\|u^n\|^2+\|u^{n+1}\|^2,$$
$$2(cu^n,u^{n+1})\le\|c^{1/2}u^n\|^2+\|c^{1/2}u^{n+1}\|^2,$$
$$2(k\operatorname{grad}u^n,\operatorname{grad}u^{n+1})\le\|k^{1/2}\operatorname{grad}u^n\|^2+\|k^{1/2}\operatorname{grad}u^{n+1}\|^2,$$

and $a^n\ge a^{n+1}$, we obtain the estimate (11). The proof of the theorem is complete.

NUMERICAL ALGORITHM

Consider the solution of problem (7), (9), (10) in more detail. To find the approximate solution at a new time level, we use (see [16, 17]) the following decomposition of the approximate solution u^{n+1} on the new level with respect to time:

$$u^{n+1}(\boldsymbol{x})=y^{n+1}(\boldsymbol{x})+a^{n+1}w^{n+1}(\boldsymbol{x}). \tag{12}$$

To find $y^{n+1}(\boldsymbol{x})$, we use the equation

$$\int\limits_\Omega\frac{y^{n+1}-u^n}{\tau}v\,d\boldsymbol{x}+\frac{a^n}{2}\int\limits_\Omega k(\boldsymbol{x})\operatorname{grad}y^{n+1}\operatorname{grad}v\,d\boldsymbol{x}+\frac{1}{2}\int\limits_{\partial\Omega}g(\boldsymbol{x})y^{n+1}v\,d\boldsymbol{x}+\frac{1}{2}\int\limits_\Omega c(\boldsymbol{x})y^{n+1}v\,d\boldsymbol{x} = \int\limits_\Omega f(\boldsymbol{x},t^{n+1/2})v\,d\boldsymbol{x}-\frac{1}{2}\int\limits_{\partial\Omega}g(\boldsymbol{x})u^nv\,d\boldsymbol{x}-\frac{1}{2}\int\limits_\Omega c(\boldsymbol{x})u^nv\,d\boldsymbol{x},\qquad v\subset V, \tag{13}$$

and find the function $w^{n+1}(\boldsymbol{x})$ from the equation

$$\int\limits_\Omega\frac{w^{n+1}}{\tau}v\,d\boldsymbol{x}+\frac{a^n}{2}\int\limits_\Omega k(\boldsymbol{x})\operatorname{grad}w^{n+1}\operatorname{grad}v\,d\boldsymbol{x}+\frac{1}{2}\int\limits_{\partial\Omega}g(\boldsymbol{x})w^{n+1}v\,d\boldsymbol{x}+\frac{1}{2}\int\limits_\Omega c(\boldsymbol{x})w^{n+1}v\,d\boldsymbol{x} = -\frac{1}{2}\int\limits_\Omega k(\boldsymbol{x})\operatorname{grad}u^n\operatorname{grad}v\,d\boldsymbol{x},\qquad v\subset V. \tag{14}$$

For the decomposition (12), (13), Eq. (10) holds automatically for any a^{n+1}.

To find a^{n+1}, we use condition (9) [or (8)]. By substituting the representation (12) into condition (9), we obtain

$$a^{n+1} = \frac{1}{w^{n+1}(\boldsymbol{x}^*)}(\varphi^{n+1} - y^{n+1}(\boldsymbol{x}^*)). \tag{15}$$

The essential point permitting one to use the considered algorithm is related to the validity of the condition $w^{n+1}(\boldsymbol{x}^*) \neq 0$. The auxiliary function $w^{n+1}(\boldsymbol{x})$ is found from the grid elliptic equation (14). The sign definiteness of the function $w^{n+1}(\boldsymbol{x})$ is guaranteed, in particular, by imposing appropriate requirements on the input data of the considered inverse problem. In any case, this problem requires a special detailed analysis. In the present paper, we assume that the condition $w^{n+1}(\boldsymbol{x}^*) \neq 0$ is satisfied.

For the solution of problem (7), (8), (10), instead of the representation (15), we have

$$a^{n+1} = \left(\int\limits_\Omega w^{n+1}\omega(\boldsymbol{x})\, d\boldsymbol{x}\right)^{-1}\left(\varphi^{n+1} - \int\limits_\Omega y^{n+1}\omega(\boldsymbol{x})\, d\boldsymbol{x}\right) \tag{16}$$

provided that

$$\int\limits_\Omega w^{n+1}\omega(\boldsymbol{x})\, d\boldsymbol{x} \neq 0.$$

In this case, we state additional conditions for the function $\omega(\boldsymbol{x})$, for example, its sign definiteness in the domain Ω.

Thus, the numerical algorithm for solving the inverse problem (1)–(4) [or problem (1)–(3), (5)] with the use of the linearized scheme (7), (8), (10) [or (7), (9), (10)] is based on the solution of two standard grid elliptic equations for the auxiliary functions $y^{n+1}(\boldsymbol{x})$ [Eq. (13)] and $w^{n+1}(\boldsymbol{x})$ [Eq. (14)], the definition of a^{n+1} by (16) [or (15)], and the use of the representation (12) for $u^{n+1}(\boldsymbol{x})$.

NUMERICAL EXAMPLES

The capabilities of the considered linearization schemes for the approximate solution of the problem of reconstructing the leading coefficient of a parabolic equation are illustrated by a model two-dimensional problem, which is considered in the unit square

$$\Omega = \{\boldsymbol{x} |\ \boldsymbol{x} = (x_1, x_2),\ 0 < x_\alpha < 1,\ \alpha = 1, 2\}.$$

In the following examples, we set

$$k(\boldsymbol{x}) = 1, \quad c(\boldsymbol{x}) = 0, \quad f(\boldsymbol{x}, t) = 0, \quad \boldsymbol{x} \in \Omega, \quad g(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \partial\Omega.$$

In this case, problem (1), (2) can be represented in the form

$$\frac{\partial v}{\partial \theta} - \Delta v = 0, \qquad \boldsymbol{x} \in \Omega, \qquad 0 < \theta \leq \Theta, \tag{17}$$

$$\frac{\partial v}{\partial n} = 0, \qquad \boldsymbol{x} \in \partial\Omega, \qquad 0 < \theta \leq \Theta, \tag{18}$$

for $v(\boldsymbol{x}, \theta) = u(\boldsymbol{x}, t)$, where

$$\theta(t) = \int\limits_0^t a(s)\, ds, \qquad \Theta = \theta(T).$$

The introduction of the new variable $\theta(t)$ permits one to construct a closed-form solution of the considered model problem. We use this solution, in particular, for the generation of the data at the point $\boldsymbol{x}^*$. However, in the solution of the inverse problem we follow the lines of the above-described algorithm and do not use the variable $\theta(t)$.

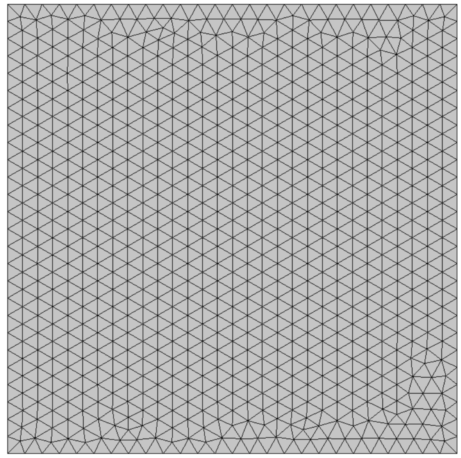

Fig. 1. Computational grid.

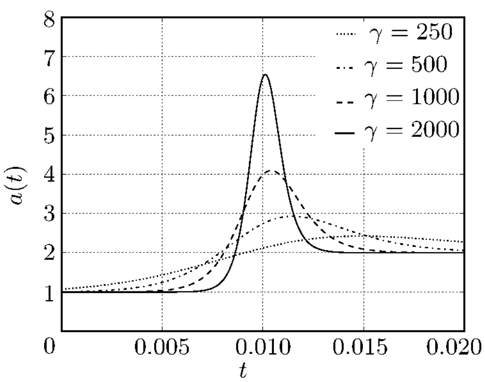

Fig. 2. Exact solution.

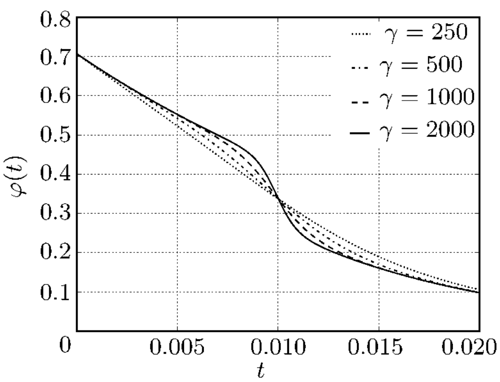

Fig. 3. Solution at the observation point.

When testing the numerical algorithm for the approximate solution of the inverse problem, we take the initial condition in the form

$$u_0(\boldsymbol{x}) = \cos(\pi x_1)\cos(2\pi x_2).$$

In this case, the solution of problem (17), (18) has the form

$$v(\boldsymbol{x}, \theta) = \exp(-\nu\theta)\cos(2\pi x_1)\cos(2\pi x_2),$$

where $\nu = 5\pi^2$.

In the considered case, the influence of the spatial computational grid is not essential. Therefore, we present the results of computations with the use of the computational grid that is shown in Fig. 1 and consists of 842 nodes (1578 triangles).

In the framework of a quasi-real numerical experiment, we first solve the direct problem and then use the obtained results for the solution of the inverse problem. Computations were carried out for $T = 0.02$. The coefficient $a(t)$ was chosen in the form

$$\begin{aligned} a(t) &= 1 + \frac{1 + (1 + \gamma t)\eta(t)}{(1 + \eta(t))^2}, \\ \eta(t) &= \exp(-\gamma(t - 0.5T)). \end{aligned} \tag{19}$$

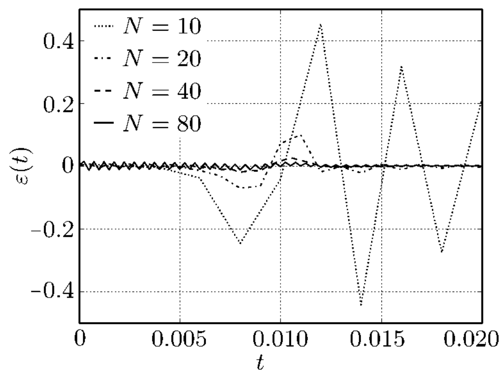

Fig. 4. The error in the solution of the inverse problem.

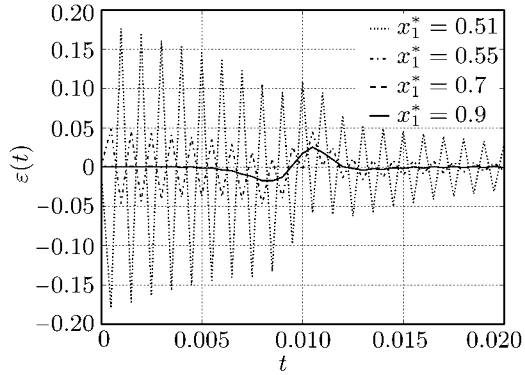

Fig. 5. The identification error for various observation points.

Therefore, for the auxiliary function $\theta(t)$ we have the representation $\theta(t) = t + \dfrac{t}{1+\eta(t)}$. The dependence of the coefficient $a(t)$ on the parameter γ is presented in Fig. 2. For large values of the parameter γ, $a(t)$ has a spike for $t = 0.5T$.

The choice of the observation point $\boldsymbol{x}^*$ should be discussed separately. By relations (14) and (15), difficulties can be caused by the sign indefiniteness of Δu. In the considered model problem, we have

$$\Delta u(\boldsymbol{x}, t) = \Delta v(\boldsymbol{x}, \theta) = -\nu \exp(-\nu\theta) \cos(2\pi x_1) \cos(2\pi x_2).$$

The sign changes for $x_1 = 0.5$. Thus, we can expect difficulties with the identification of the leading coefficient $a(t)$ if the observation point is close to the point $x_1 = 0.5$. In the following computations, the main version corresponds to the choice of $\boldsymbol{x}^* = (0.75,\ 0.5)$. The solution of the direct problem at the observation point for various values of γ is shown in Fig. 3.

The error in the approximate solution of the inverse problem is estimated at each time step,

$$\varepsilon(t) = \widetilde{a}(t) - \overline{a}(t),$$

where $\widetilde{a}(t)$ is the approximate solution of the problem and $\overline{a}(t)$ is the exact solution of the problem, which is defined by relation (19). To use the linearized scheme (10), one should determine the value of a^0. In the presented examples, we determine the exact value of a^0. In computational practice, $a(0)$ can be unknown, which requires the use of special numerical procedures. For example, to begin the computations, one can perform the computation of one time step with the use of a small time increment and the purely implicit scheme (6).

The results of the solution of the inverse problem for various time grids are shown in Fig. 4. Computations are performed for $\gamma = 1000$ with the use of Lagrangian second-order finite elements. The accuracy of the approximate solution is coordinated with the approximation error of the scheme used, and the second order with respect to τ is observed. The nonmonotonicity of the time approximations arises for a strong condensation of the grid. As expected, the error falls in the domain of a sharp change in the desired coefficient $a(t)$. The influence of the choice of the observation point is shown in Fig. 5. The accuracy of the identification of the leading coefficient $a(t)$ diminishes as the observation point $\boldsymbol{x}^* = (x_1^*,\ 0.5)$ approaches the critical point ($x_1^* = 0.5$).

ACKNOWLEDGMENTS

The work of the first author was supported by the Russian Foundation for Basic Research (project no. 14-01-00785).

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