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# A SPLITTING SCHEME FOR DIFFUSION AND HEAT CONDUCTION PROBLEMS

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**Abstract.** *The problem of mathematical modeling and optimization of nonstationary diffusion and heat conduction processes is considered. An approach that uses the idea of splitting and computation of the obtained difference schemes using explicit schemes of point to point computing is proposed for numerical solution of multidimensional diffusion and heat conduction initial–boundary-value problems. Construction of difference splitting schemes, approximation and stability on initial data are investigated. Differential properties of the quality functional are analyzed for the numerical solution of the optimal control problem for a parabolic equation. An iterative algorithm for finding the optimal control is proposed.*

**Keywords:** *parabolic equation, optimal control problem, numerical method, splitting methods, difference scheme, stability.*

## INTRODUCTION

Mathematical modeling is the major and most promising direction in the analysis of important ecological problems, numerous dynamic thermal and diffusion processes described by second-order parabolic equations [1–5].

Fundamentals of the computer technology of mathematical modeling of distributed-parameter processes are basic models and efficient numerical algorithms for solution of partial differential equations that are based on finite-difference, finite-volume, and finite-element approximations [5–20].

For computing practice, of considerable interest are factorization and splitting methods, which allow reducing original problems to equations of smaller dimension.

The purpose of the present study is to develop discrete mathematical models and create unconditionally stable schemes for numerical modeling and optimization of nonstationary thermal and diffusion processes on the basis of difference schemes of point to point computing with explicit computations.

In the basis of splitting schemes, passage to a new time layer involves solution of a number of simpler problems. The approach proposed to creation of discrete models uses the idea of splitting and implementation of the obtained schemes on the basis of explicit schemes of point to point computing presented in [7] for one-dimensional diffusion equation.

In the paper, for the constructed difference schemes of point to point computing, we will investigate approximation and stability under initial data. To apply the proposed difference schemes for numerical solution of the optimal control problem, we will investigate differential properties of the quality functional and present an iteration scheme for determining optimal control.

Note that implementation of the approach proposed for solution of spatial nonstationary equations on graphic processors and multiprocessor distributed-memory computing systems considerably reduces time costs as compared with serial algorithms.

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**PROBLEM STATEMENTS**

To illustrate construction and stability analysis of difference splitting schemes, we will use an example of a boundary-value problem for a second-order parabolic equation of the form

$$\frac{\partial u}{\partial t} = \text{div}\,(k\,\text{grad}\,u) + f,$$

which is basic in modeling and optimization of numerous thermophysical or diffusion processes [2, 3, 6].

Let in a Cartesian coordinate system $(x, y)$ on a time interval $0 < t \le T$ in the rectangular domain $G = \{(x, y)|, 0 < x < l_1, 0 < y < l_2\}$ with boundary $\partial G$, function $u(x, y, t)$ satisfy the two-dimensional nonstationary parabolic equation

$$\frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(k_1 \frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(k_2 \frac{\partial u}{\partial y}\right) = f(x, y, t),\ (x, y) \in G,\ t \in (0, T], \tag{1}$$

where $u(x, y, t)$ is the required function (characteristics of the processes under study), coefficients $k_\alpha = k_\alpha(x, y) > \chi > 0$, $\alpha = 1, 2$, are positive continuously differentiable functions, and $f(x, y, t)$ is function of source distribution. Equation (1) is supplemented with homogeneous Dirichlet boundary conditions

$$u(x, y, t) = 0,\ (x, y) \in \partial G,\ 0 < t \le T. \tag{2}$$

Moreover, for correct statement of the mathematical models, boundary conditions should be supplemented with the initial condition

$$u(x, y, 0) = u_0(x, y),\ (x, y) \in G. \tag{3}$$

Let us formulate the mathematical statement of the optimal control problem for the parabolic equation (1) for the case where it is required to find the characteristics of the distributed system with given properties.

For problems of control of diffusion (thermophysics) processes that take place in a bounded simply connected domain $G$ with boundary $\partial G$ on the time interval $0 < t \le T$, the state of the distributed system can be described by the parabolic equation

$$\frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(k_1 \frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(k_2 \frac{\partial u}{\partial y}\right) = f(x, y, t) + v(x, y, t),\ (x, y) \in G,\ t \in (0, T], \tag{4}$$

where $f(x, y, t)$ is a given function, $v(x, y, t)$ is control function, and $k_1(x, y,)$ and $k_2(x, y)$ are given positive functions, $k_\alpha(x, y) > \chi > 0,\ \alpha = 1, 2$.

For Eq. (4), we will consider the initial

$$u(x, y, 0) = u_0(x, y),\ (x, y) \in G, \tag{5}$$

and boundary

$$\left.\left(\frac{\partial u}{\partial N} + \beta(x, y, t)u\right)\right|_{\partial G} = \sigma(x, y, t),\ (x, y) \in \partial G,\ 0 < t \le T, \tag{6}$$

conditions, respectively, where $\partial u / \partial N$ is a conormal derivative, which is defined by

$$\frac{\partial u}{\partial N} = k_1 \frac{\partial u}{\partial x} \cos(n, x) + k_2 \frac{\partial u}{\partial y} \cos(n, y),$$

$n$ is a unit vector of outward normal to $\partial G$, $\sigma(x, y, t)$ is a given function, and $\beta(x, y, t) > 0$ is a function defined on $\partial G$.

In what follows, without loss of generality we will assume that $k_1(x, y) = k_2(x, y) = k(x, y)$, i.e., conormal derivative $\partial u / \partial N$ coincides with the expression $k \partial u / \partial n$.

Let us formulate mathematical statement of the extremum problem as minimization of some functional in order to provide minimum deviation of the characteristics of the modeled field from those given in the domain $G$. As the control, we take distribution of $v(x, y, t)$ on the right-hand side of the parabolic equation (4). Then one of the extremum problems can be formulated as follows.

Find the admissible control $v = v_0(x, y, t)$ and respective solution $u = u_0(x, y, t)$ of problem (4)–(6) such that the functional

$$J_\varepsilon(v) = \int_G (u(x, y, T) - h(x, y))^2 \, dxdy + \frac{1}{\varepsilon^2} \int_0^T dt \int_G v^2(x, y, t) dxdy \tag{7}$$

takes the least possible value. Here, $T$ is a fixed instant of time, $h(x, y)$ is a given function, $v(x, y, t)$ is a control from some convex closed set $U = \{v(x, y, t) \in L_2(Q)\}$, where $L_2(Q)$ is the space of real functions, square integrable in the domain

$$Q = \{(x, y, t)|, 0 < x < l_1, 0 < y < l_2, 0 < t \le T\}. \tag{8}$$

Scalar product and norm in $L_2(Q)$ are defined by the formulas

$$(u, v) = \int_Q u(x, y, t) v(x, y, t) dGdt, \; \| v \| = (v, v)^{1/2} = \left( \int_Q v(x, y, t)^2 \, dGdt \right)^{1/2}.$$

Note that to select a bounded solution, a stabilizing functional $\frac{1}{\varepsilon^2} \| v \|^2$ for some set $\varepsilon > 0$ is added to the quality functional (7).

Let us consider an unconstrained control problem ($U = H = L_2(Q)$), i.e., the optimization problem is to find control $w$ such that functional (7) attains its greatest lower bound

$$J_\varepsilon(w) = \inf_{v \in H} J_\varepsilon(v). \tag{9}$$

## THE DIFFERENCE SCHEME OF POINT TO POINT COMPUTING

A lot of computing algorithms, which are mostly based on splitting methods [6, 8, 16], have been developed for numerical solution of multidimentional problems of propagation of contaminations. Of considerable interest is development of difference splitting schemes with given properties, in particular, with the explicit organization of computations.

**A Two-Step Splitting Scheme.** Let us present the approach to constructing difference splitting schemes for solution of multidimentional problems on the example of the two-step splitting scheme for the initial–boundary-value problem (1)–(3). Within the framework of this approach, two-step splitting scheme at the differential level can be obtained by representing the parabolic equation (1) in operator form

$$\frac{\partial u}{\partial t} + (L_1 + L_2) u = f, \tag{10}$$

where

$$L_1 u = L_2 u = -\frac{1}{2} \frac{\partial}{\partial x} \left( k_1 \frac{\partial u}{\partial x} \right) - \frac{1}{2} \frac{\partial}{\partial y} \left( k_2 \frac{\partial u}{\partial y} \right).$$

Let solution of Eq. (10) be known for some instant of time $t$, then the value $u(x, y, \hat{t})$ for time $\hat{t} = t + \tau$ can be presented by means of the Taylor series as

$$u(x, y, \hat{t}) = u(x, y, t) + \tau \frac{\partial u(x, y, t)}{\partial t} + O(\tau^2) = [E - \tau L_1 - \tau L_2] u(x, y, t) + \tau f + O(\tau^2). \tag{11}$$

Let us consider two auxiliary problems:

$$\frac{\partial u_1}{\partial t} + L_1 u_1 = \frac{1}{2} f, \; u_1(x, y, t) = u(x, y, t), \tag{12}$$

$$\frac{\partial u_2}{\partial t} + L_2 u_2 = \frac{1}{2} f, \; u_2(x, y, t) = u_1(x, y, \hat{t}). \tag{13}$$

It can be easily seen that solutions of the considered problems (12), (13) can be written as

$$u_1(x, y, \hat{t}) = [E - \tau L_1] u_1(x, y, t) + \frac{\tau}{2} f + O(\tau^2),$$

$$u_2(x, y, \hat{t}) = [E - \tau L_2] u_2(x, y, t) + \frac{\tau}{2} f + O(\tau^2).$$

Considering that $u_2(x, y, t) = u_1(x, y, \hat{t})$, we get

$$u_2(x, y, \hat{t}) = [E - \tau L_1 - \tau L_2] u(x, y, t) + \tau f + O(\tau^2). \tag{14}$$

Putting $u(x, y, \hat{t}) = u_2(x, y, \hat{t})$ and comparing expressions (11) and (14), we can state that sequential solution of problems (12), (13) yields solution of Eq. (10) for instant of time $\hat{t}$ with error $O(\tau)^2$.

For numerical solution of the nonstationary equations (12) and (13) in the domain $\overline{G}$, let us introduce a uniform difference grid

$$\overline{\omega}_h = \omega_h \cup \gamma_h = \{(x, y) : x = x_i = ih_1,\ i = \overline{0, N_1};$$

$$y = y_j = jh_2,\ j = \overline{0, N_2};\ h_\alpha = l_\alpha / N_\alpha,\ \alpha = 1, 2\},$$

where $\omega_h$ is set of interior nodes and $\gamma_h$ is set of boundary nodes. Let us define a finite-dimensional Hilbert space $H_h$ of mesh functions defined on grid $\overline{\omega}_h$ and equal to zero on its boundary. Let us define scalar product in $H_h$ by the relation

$$(\varphi, \psi) = \sum_{(x, y \in \omega_h)} \varphi(x, y) \psi(x, y) h_1 h_2, \tag{15}$$

then the norm $\|\varphi\| = \sqrt{(\varphi, \varphi)}$. For self-adjoint and positive difference operator $D$, we can define energy space $H_D$ with scalar product $(\varphi, \psi)_D = (D\varphi, \psi)$ and norm $\|\varphi\|_D = \sqrt{(D\varphi, \varphi)}$.

Let $\omega_\tau = \{t : t = t_n = n\tau,\ n = \overline{0, N},\ N\tau = T\}$ be a uniform time grid with spacing $\tau$. In what follows, in the analysis of nonstationary problems, we will consider mesh functions $\varphi(t_n)$ of discrete argument $t_n \in \omega_\tau$ with values from finite-dimensional space $H_h$, i.e., $\varphi(t_n) \in H_h$.

We will approximate differential operators $L_1$ and $L_2$ by difference schemes with the use of integro-interpolation method; to approximate diffusion operators at time $t = t_n$, we will use mesh operators

$$\frac{\partial}{\partial x}\left(k_1 \frac{\partial u}{\partial x}\right) \cong \frac{1}{h_1}\left( k_1\Big|_{i+\frac{1}{2}, j} \frac{(\varphi^n_{i+1,j} - \varphi^n_{i,j})}{h_1} - k_1\Big|_{i-\frac{1}{2}, j} \frac{(\varphi^n_{i,j} - \varphi^n_{i-1,j})}{h_1} \right),$$

$$\frac{\partial}{\partial y}\left(k_2 \frac{\partial u}{\partial y}\right) \cong \frac{1}{h_2}\left( k_2\Big|_{i, j+\frac{1}{2}} \frac{(\varphi^n_{i,j+1} - \varphi^n_{i,j})}{h_2} - k_2\Big|_{i, j-\frac{1}{2}} \frac{(\varphi^n_{i,j} - \varphi^n_{i,j-1})}{h_2} \right).$$

Then, for example, it is possible to associate operator $L_1$ at nodes $(x_i, y_j)$ of two-dimensional grid with the difference operator

$$\Lambda_1 \varphi = -\frac{1}{2}(a_1 \varphi_{\bar{x}})_x - \frac{1}{2}(a_2 \varphi_{\bar{y}})_y,\ (x, y) \in \omega_h,$$

which approximates the differential operator with second order. Here, $\varphi$ is a mesh function defined at nodes of grid $\omega_h$ and standard notation from the theory of difference schemes is used [6, 21]

$$\varphi = \varphi(x_i, y_j, t_n) = \varphi^n_{i,j} = \varphi^n = \varphi_{i,j},$$

$$\varphi_t = (\varphi^{n+1} - \varphi^n)/\tau,\ \varphi_x = (\varphi_{i+1,j} - \varphi_{i,j})/h_1,\ \varphi_{\bar{x}} = (\varphi_{i,j} - \varphi_{i-1,j})/h_1,$$

$$(a_1\varphi_{\bar{x}})_x = \frac{1}{h_1}(a_{1i+1}\varphi_x - a_{1i}\varphi_{\bar{x}}) = \frac{1}{h_1^2}(a_{1i+1}\varphi_{i+1} - (a_{1i+1} + a_{1i})\varphi_i + a_{1i}\varphi_{i-1}),$$

$$a_1 = a_{1i} = a_{1i,j,k} = k_{1i-1/2} = k_1(x_{i-1/2}, y_j).$$

Difference operators in another coordinate direction, which are used for approximation of differential expressions $L_1$ and $L_2$ can be defined similarly:

$$\varphi_y = (\varphi_{i,j+1} - \varphi_{i,j})/h_2,\ \varphi_{\bar{y}} = (\varphi_{i,j} - \varphi_{i,j-1})/h_2,$$

$$(a_2\varphi_{\bar{y}})_y = \frac{1}{h_2}(a_{2j+1}\varphi_y - a_{2j}\varphi_{\bar{y}}) = \frac{1}{h_2^2}(a_{2j+1}\varphi_{j+1} - (a_{2j+1} + a_{2j})\varphi_j + a_{2j}\varphi_{j-1}),$$

$$a_2 = a_{2j} = a_{2i,j} = k_{2i,j-1/2} = k_2(x_i, y_{j-1/2}).$$

Since the relation

$$\Lambda_1 u_1 = L_1 u_1 + O(|h|^2),\ |h|^2 = h_1^2 + h_2^2,$$

is true on the solution of differential problem (12), one can easily see that the implicit difference scheme

$$\varphi_t - \frac{1}{2}(a_1\varphi_{\bar{x}}^{n+1})_x - \frac{1}{2}(a_2\varphi_{\bar{y}}^{n+1})_y = \frac{1}{2}f^{n+1/2} \tag{16}$$

approximates Eq. (12) with first-order accuracy with respect to time and second-order accuracy with respect to space.

If in Eq. (16) we replace operators $\varphi_x^{n+1}$ and $\varphi_y^{n+1}$ with respective operators for $t = t_n$, then we obtain double-layer scheme of point to point computing

$$\varphi_t - \frac{1}{2h_1}(a_{1i+1}\varphi_x^n - a_{1i}\varphi_{\bar{x}}^{n+1}) - \frac{1}{2h_2}(a_{2j+1}\varphi_y^n - a_{2j}\varphi_{\bar{y}}^{n+1}) = \frac{1}{2}f^{n+1/2}. \tag{17}$$

Acting similarly, we can obtain double-layer scheme of point to point computing for the solution of Eq. (13). Indeed, the implicit difference scheme is considered in this case

$$\varphi_t - \frac{1}{2}(a_1\varphi_{\bar{x}}^{n+1})_x - \frac{1}{2}(a_2\varphi_{\bar{y}}^{n+1})_y = \frac{1}{2}f^{n+1/2}.$$

Unlike the previous case, operators $\varphi_{\bar{x}}^{n+1}$ and $\varphi_{\bar{y}}^{n+1}$ in this equation should be replaced with respective operators at the previous layer $t = t_n$. As a result, we obtain the double-layer scheme of point to point computing

$$\varphi_t - \frac{1}{2h_1}(a_{1i+1}\varphi_x^{n+1} - a_{1i}\varphi_{\bar{x}}^n) - \frac{1}{2h_2}(a_{2j+1}\varphi_y^{n+1} - a_{2j}\varphi_{\bar{y}}^n) = \frac{1}{2}f^{n+1/2}. \tag{18}$$

A distinctive feature of the considered difference schemes of point to point computing (17), (18) is that they can be implemented by explicit recurrence relations. Indeed, an analysis of the template of the difference scheme (17) testifies that to determine the value of function $\varphi_i^{n+1}$, it is necessary to know the value of the function at the left-hand adjacent point on the difference grid. Therefore, using boundary conditions, it is possible to calculate sequentially the value of mesh function at the $(n+1)$th step with respect to time.

An analysis of the template of difference scheme (18) shows that to determine mesh function $\varphi_i^{n+1}$, it is necessary to know the value of function $\varphi$ at the right-hand adjacent point on the difference grid, which also makes it possible to carry out calculations using recurrence relations.

Solution of Eq. (17) at time $t = t_{n+1}$ is initial one for the difference equation (18).

It can be easily seen that numerical implementation of the splitting algorithm (17), (18) can be presented as follows. Interval $\tau$ between points $t_n$ and $t_{n+1}$ is split into two equal parts. Denote the obtained intermediate point by $t_{n+1/2}$. On the first part of the interval, the explicit difference scheme

$$\frac{(\varphi^{n+1/2} - \varphi^n)}{\tau} = \frac{1}{2}\left( \frac{1}{h_1}(a_{1i+1}\varphi_x^n - a_{1i}\varphi_{\bar{x}}^{n+1/2}) + \frac{1}{h_2}(a_{2j+1}\varphi_y^n - a_{2j}\varphi_{\bar{y}}^{n+1/2}) \right) + \frac{1}{2} f^{n+1/2} \tag{19}$$

is considered, on the second part, the second subsystem is written

$$\frac{(\varphi^{n+1} - \varphi^{n+1/2})}{\tau} = \frac{1}{2}\left( \frac{1}{h_1}(a_{1i+1}\varphi_x^{n+1} - a_{1i}\varphi_{\bar{x}}^{n+1/2}) + \frac{1}{h_2}(a_{2j+1}\varphi_y^{n+1} - a_{2j}\varphi_{\bar{y}}^{n+1/2}) \right) + \frac{1}{2} f^{n+1/2}. \tag{20}$$

Each of the difference equations (19), (20) separately does not approximate the initial differential equations (12), (13). However, in aggregate, (19) and (20) make the difference scheme of the point to point computing, which approximates the initial differential problem. Indeed, adding Eqs. (19), (20) yields

$$\frac{1}{\tau}(\varphi^{n+1} - \varphi^n) = \frac{1}{2}\left( \frac{1}{h_1}(a_{1i+1}\varphi_x^n - a_{1i}\varphi_{\bar{x}}^{n+1/2}) + \frac{1}{h_2}(a_{2j+1}\varphi_y^n - a_{2j}\varphi_{\bar{y}}^{n+1/2}) \right) + \frac{1}{2} f^{n+1/2}$$
$$+ \frac{1}{2}\left( \frac{1}{h_1}(a_{1i+1}\varphi_x^{n+1} - a_{1i}\varphi_{\bar{x}}^{n+1/2}) + \frac{1}{h_2}(a_{2j+1}\varphi_y^{n+1} - a_{2j}\varphi_{\bar{y}}^{n+1/2}) \right) + \frac{1}{2} f^{n+1/2}$$

or after transformations

$$\frac{1}{\tau}(\varphi^{n+1} - \varphi^n) = \frac{1}{h_1}(a_{1i+1}\varphi_x^{n+1/2} - a_{1i}\varphi_{\bar{x}}^{n+1/2}) + O(\tau^2 / |h|^2) + \frac{1}{h_2}(a_{2j+1}\varphi_y^{n+1/2} - a_{2j}\varphi_{\bar{y}}^{n+1/2}) + f^{n+1/2}$$
$$= (a_1\varphi_{\bar{x}})_x^{n+1/2} + (a_2\varphi_{\bar{y}})_y^{n+1/2} + f^{n+1/2} + O(\tau^2 / |h|^2).$$

From here it follows that difference scheme (19), (20) approximates differential equation (1) with error $O(|h|^2 + \tau^2 + \tau^2/|h|^2)$, where the item $\tau^2/|h|^2$ influences the approximation error. Therefore, accuracy of the results obtained in the use of the difference problem (19), (20) will depend on mesh spacing ratio.

Let us now analyze the important property of stability of difference schemes (17), (18) with respect to initial data and show uniform stability. For stability analysis of mesh problems, we will use the approach based on obtaining a priori estimates for each auxiliary problem.

To obtain a priori estimate, we will use the principle of frozen coefficients [11] and transform homogeneous equations (17) and (18) with constant diffusion coefficients $a_\alpha(x, y, z) = c_\alpha = \text{const}$, $\alpha = 1, 2$, to the canonical operator form

$$B\varphi_t + A\varphi = 0, \tag{21}$$

where the linear operators $A$ and $B$ act in the Hilbert space $H_h$, $\varphi = \varphi^n \in H_h$.

As is generally known [6, 21], the necessary and sufficient condition of stability with respect to initial data of the double-layer difference scheme (21) with self-adjoint positive operators $A$ and $B$ means that the operator inequality holds

$$B \geq 0.5\tau A, \tag{22}$$

and for the solution $\varphi^{n+1}$ estimate in energy norm $||\cdot||_A$ is true:

$$||\varphi^{n+1}||_A \leq ||\varphi^n||_A, \quad n = \overline{0, N}.$$

For definiteness, let us first consider the homogeneous equation (17) with zero right-hand side

$$\varphi_t - \frac{1}{2h_1}(a_{1i+1}\varphi_x^n - a_{1i}\varphi_{\bar{x}}^{n+1}) - \frac{1}{2h_2}(a_{2j+1}\varphi_y^n - a_{2j}\varphi_{\bar{y}}^{n+1}) = 0. \tag{23}$$

Taking into account the expressions

$$\frac{1}{h_1}(a_{1i+1}\varphi_x^n - a_{1i}\varphi_{\bar{x}}^{n+1}) = (a_1\varphi_{\bar{x}}^n)_x - \frac{\tau}{h_1}a_{1i}\varphi_{\bar{x}t}^n,$$

$$\frac{1}{h_2}(a_{2j+1}\varphi_y^n - a_{2j}\varphi_{\bar{y}}^{n+1}) = (a_2\varphi_{\bar{y}}^n)_y - \frac{\tau}{h_2}a_{2j}\varphi_{\bar{y}t}^n,$$

we can write it in the equivalent form

$$\varphi_t + \frac{c_1}{2}\Lambda_1\varphi + \frac{c_2}{2}\Lambda_2\varphi + \frac{\tau c_1}{2h_1}\Lambda_x\varphi_t + \frac{\tau c_2}{2h_2}\Lambda_y\varphi_t = 0,$$

where $\Lambda_1\varphi = -\varphi_{\bar{x}x}$, $\Lambda_2\varphi = -\varphi_{\bar{y}y}$, $\Lambda_x\varphi = \varphi_{\bar{x}}$, and $\Lambda_y\varphi = \varphi_{\bar{y}}$. From here it follows that the difference equation (23) can be written in the operator form (21), where linear operators $A$ and $B$ act in the mesh space $H_h$ and are defined by the formulas

$$A\varphi = \frac{c_1}{2}\Lambda_1\varphi + \frac{c_2}{2}\Lambda_2\varphi,\ B\varphi = E\varphi + \frac{\tau c_1}{2h_1}\Lambda_x\varphi_t + \frac{\tau c_2}{2h_2}\Lambda_y\varphi_t,$$

where $E$ is a unit operator.

Since

$$\varphi_{\bar{x}} = \varphi_{\overset{\circ}{x}} - 0.5h_1\varphi_{\bar{x}x} = \varphi_{\overset{\circ}{x}} + 0.5h_1\Lambda_1\varphi,\ \varphi_{\overset{\circ}{x}} = 0.5(\varphi_{\bar{x}} + \varphi_x),$$

$$\varphi_{\bar{y}} = \varphi_{\overset{\circ}{y}} - 0.5h_2\varphi_{\bar{y}y} = \varphi_{\overset{\circ}{y}} + 0.5h_2\Lambda_2\varphi,\ \varphi_{\overset{\circ}{y}} = 0.5(\varphi_{\bar{y}} + \varphi_y),$$

we finally obtain the expressions for operators $A$ and $B$:

$$A = \frac{c_1}{2}\Lambda_1 + \frac{c_2}{2}\Lambda_2,\ B = B_0 + B_1,\ B_0 = E + \frac{\tau c_1}{4}\Lambda_1 + \frac{\tau c_2}{4}\Lambda_2, \tag{24}$$

$$B_1\varphi = \frac{\tau c_1}{2h_1}\varphi_{\overset{\circ}{x}} + \frac{\tau c_2}{2h_2}\varphi_{\overset{\circ}{y}}. \tag{25}$$

Using Green's difference formulas [6, 21], it is possible to show self-conjugacy and positive definiteness of operators $A$ and $B_0$ in the sense of scalar product (15). Similarly, it is possible to establish that operators $B_1$ are skew-symmetric; then $(B_1\varphi, \varphi) = 0$. Therefore, stability condition (22) is equivalent to the condition $B_0 \geq 0.5\tau A$. Since

$$B_0 = E + \frac{\tau c_1}{4}\Lambda_1 + \frac{\tau c_2}{4}\Lambda_2 = E + \frac{\tau}{2}A,$$

we write the stability condition as

$$E + \frac{\tau}{2}A \geq \frac{\tau}{2}A.$$

This condition is always satisfied; therefore, the difference scheme (23) is uniformly stable with respect to initial data in the energy norm $||\cdot||_A$.

Thus, the following statement is true.

**THEOREM 1.** The double-layer difference scheme of point to point computing (21), (24), (25) is uniformly stable with respect to initial data in energy norm $||\cdot||_A$ and the a priori estimate takes place for its solution

$$||\varphi^{n+1}||_A \leq ||\varphi^n||_A,\ n = \overline{0, N}.$$

From the previous reasoning it follows that for the auxiliary problem (17) for all possible values of diffusivion coefficients $a_\alpha(x, y)$, $\alpha = 1, 2$, the operator stability condition is satisfied.

According to the principle of frozen coefficients, scheme (17) is uniformly stable with respect to initial data if condition (22) is satisfied for all possible values of diffusion coefficients.

We can similarly establish uniform stability of the auxiliary problem (18), which generally guarantees stability of computations when passing from $n$th to the $(n+1)$th time layer.

## OPTIMAL CONTROL PROBLEM

Numerical methods developed for solution of direct problems of the form (1)–(3) can be applied to solve inverse problems, optimal control problems, etc.

For optimal control problem (4)–(9), in order to obtain optimality conditions and to use gradient methods of optimization, let us analyze differential properties of the quality criterion (7). Let us show that functional (7) is differentiable at an arbitrary point $v \in U$. To this end, we will estimate the principal linear part of the increment of functional $\Delta J_\varepsilon(v) = J_\varepsilon(v+\delta v) - J_\varepsilon(v)$ depending on increment of control $v$.

Let us set some increment $\delta v = \delta v(x, y, t)$ to control $v(x, y, t)$ and denote the corresponding increment of function $u = u(x, y, t)$ by $\delta u = \delta u(x, y, t)$.

It can be easily seen that increment of solution $\delta u(x, y, t)$ satisfies the initial–boundary-value problem $(k_1 = k_2 = k)$

$$\frac{\partial \delta u}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial \delta u}{\partial x}\right) - \frac{\partial}{\partial y}\left(k\frac{\partial \delta u}{\partial y}\right) = \delta v(x, y, t),\ (x, y) \in G,\ t \in (0, T], \tag{26}$$

$$\left.\left(k\frac{\partial \delta u}{\partial n} + \beta(x, y, t)\delta u\right)\right|_{\partial G} = 0,\ (x, y) \in \partial G,\ 0 < t \le T, \tag{27}$$

$$\delta u(x, y, 0) = 0,\ (x, y) \in G. \tag{28}$$

Then we can write the expression for increment of functional (7) as

$$\Delta J_\varepsilon(v) = \int_G [\,(u(x, y, T) + \delta u(x, y, T) - h(x, y))^2 - (u(x, y, T) - h(x, y))^2\,]dxdy$$
$$+\frac{1}{\varepsilon^2}\int_0^T dt \int_G [(v(x, y, t) + \delta v(x, y, t))^2 - v^2(x, y, t)]dxdy.$$

Since

$$(u(x, y, T) + \delta u(x, y, T) - h(x, y))^2 - (u(x, y, T) - h(x, y))^2$$
$$= 2\delta u(x, y, T)[u(x, y, T) - h(x, y)] + \delta u^2(x, y, T),$$
$$(v(x, y, t) + \delta v(x, y, t))^2 - v^2(x, y, t) = 2v(x, y, t)\delta v(x, y, t) + \delta v^2(x, y, t),$$

increment of the functional becomes

$$\Delta J_\varepsilon(v) = 2\int_G [u(x, y, T) - h(x, y)]\delta u(x, y, T)dxdy + \frac{2}{\varepsilon^2}\int_0^T dt \int_G v(x, y, t)\delta v(x, y, t)dxdy$$
$$+\int_G (\delta u(x, y, T))^2 dxdy + \frac{1}{\varepsilon^2}\int_0^T dt \int_G (\delta v(x, y, t))^2 dxdy. \tag{29}$$

To finally determine the expression for the principal linear part, we introduce conjugate function $\psi(x, y, t)$ as a solution of some initial–boundary-value problem in the domain $Q$. Classical procedure of deriving the conjugate operator is as follows. Both sides of Eq. (26) are multiplied by function $\psi(x, y, t)$ and are integrated in time and space within the limits specified by the statement of initial–boundary-value problem (26)–(28)

$$\int_0^T dt \int_G \psi \left[ \frac{\partial \delta u}{\partial t} - \frac{\partial}{\partial x}\left( k \frac{\partial \delta u}{\partial x} \right) - \frac{\partial}{\partial y}\left( k \frac{\partial \delta u}{\partial y} \right) \right] dxdy = \int_0^T dt \int_G \psi \delta v \, dxdy. \tag{30}$$

Then we carry out transformations in (30) in order to introduce function $\psi(x, y, t)$ into the differential expressions instead of $\delta u$. Integrating by parts, for the first term in (30) with regard for the initial condition (28) we get

$$\int_0^T dt \int_G \psi \frac{\partial \delta u}{\partial t} dxdy = \int_G \psi \delta u \Big|_{t=0}^{T} dxdy - \int_0^T dt \int_G \delta u \frac{\partial \psi}{\partial t} dxdy = \int_G \psi \delta u \Big|_{t=T} dxdy - \int_0^T dt \int_G \delta u \frac{\partial \psi}{\partial t} dxdy. \tag{31}$$

Applying Green's first formula [22], considering boundary condition (27), and transforming the elliptic operator in (30) we sequentially obtain

$$\int_0^T dt \int_G \psi \left[ -\frac{\partial}{\partial x}\left( k \frac{\partial \delta u}{\partial x} \right) - \frac{\partial}{\partial y}\left( k \frac{\partial \delta u}{\partial y} \right) \right] dxdy = \int_0^T dt \int_G k \left[ \frac{\partial \psi}{\partial x}\frac{\partial \delta u}{\partial x} + \frac{\partial \psi}{\partial y}\frac{\partial \delta u}{\partial y} \right] dxdy$$

$$- \int_0^T dt \int_{\partial G} \psi k \frac{\partial \delta u}{\partial n} ds = \int_0^T dt \int_G k \left[ \frac{\partial \psi}{\partial x}\frac{\partial \delta u}{\partial x} + \frac{\partial \psi}{\partial y}\frac{\partial \delta u}{\partial y} \right] dxdy + \int_0^T dt \int_{\partial G} \beta \psi \delta u \, ds, \tag{32}$$

$$\int_0^T dt \int_G \delta u \left[ -\frac{\partial}{\partial x}\left( k \frac{\partial \psi}{\partial x} \right) - \frac{\partial}{\partial y}\left( k \frac{\partial \psi}{\partial y} \right) \right] dxdy = \int_0^T dt \int_G k \left[ \frac{\partial \psi}{\partial x}\frac{\partial \delta u}{\partial x} + \frac{\partial \psi}{\partial y}\frac{\partial \delta u}{\partial y} \right] dxdy - \int_0^T dt \int_{\partial G} \delta u k \frac{\partial \psi}{\partial n} ds. \tag{33}$$

Thus, the transformed expression follows from (30)–(33):

$$\int_G \psi \delta u \Big|_{t=T} dxdy + \int_0^T dt \int_G \delta u \left[ -\frac{\partial \psi}{\partial t} - \frac{\partial}{\partial x}\left( k \frac{\partial \psi}{\partial x} \right) - \frac{\partial}{\partial y}\left( k \frac{\partial \psi}{\partial y} \right) \right] dxdy + \int_0^T dt \int_{\partial G} \beta \psi \delta u \, ds$$

$$= - \int_0^T dt \int_{\partial G} \delta u k \frac{\partial \psi}{\partial n} ds + \int_0^T dt \int_G \psi \delta v \, dxdy. \tag{34}$$

From here it follows that with function $\psi(x, y, t)$ introduced as a solution of the conjugate equation

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x}\left( k \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial y}\left( k \frac{\partial \psi}{\partial y} \right) = 0, \; (x, y) \in G, \; t \in (0, T], \tag{35}$$

with boundary condition

$$\left( k \frac{\partial \psi}{\partial n} + \beta \psi \right)\Big|_{\partial G} = 0, \quad (x, y) \in \partial G, \; 0 < t \le T, \tag{36}$$

expression (34) becomes

$$\int_G \psi \delta u \big|_{t=T} dxdy = \int_0^T dt \int_G \psi \delta v \, dxdy. \tag{37}$$

If we define initial condition for the retrospective problem by the formula

$$\psi \big|_{t=T} = u(x, y, T) - h(x, y), \tag{38}$$

then from (37) it follows that

$$\int_G (u(x, y, T) - h(x, y)) \delta u \big|_{t=T} dxdy = \int_0^T dt \int_G \psi \delta v dxdy. \tag{39}$$

On the basis of (39), we can write increment of functional (29) as

$$\Delta J_\varepsilon(v) = 2\int_0^T dt \int_G \left[\psi + \frac{1}{\varepsilon^2} v\right] \delta v dx dy + o\|\delta u\| + o\|\delta v\|.$$

From here it follows that functional $J_\varepsilon(v)$ is differentiable with respect to $v$ in space $L_2(Q)$.

Thus, we have established the following theorem.

**THEOREM 2.** Functional (7) is Frechet differentiable in space $L_2(Q)$. Gradient of the functional is defined in terms of conjugate state by the expression

$$\text{grad } J_\varepsilon(v) = 2(\psi(x, y, t) + \frac{1}{\varepsilon^2} v(x, y, t)), \quad (40)$$

where $\psi$ is the solution of conjugate problem (35), (36), (38).

Optimality condition of the optimal control problem (4)–(9) grad $J_\varepsilon(v) = 0$ with regard for (40) becomes

$$\psi(x, y, t) + \frac{1}{\varepsilon^2} v(x, y, t) = 0, \ (x, y) \in G, \ t \in (0, T].$$

From the aforesaid, it follows that to find the gradient, it is necessary to obtain the solution of two boundary-value problems for fixed $v$. First, using the direct problem (4)–(6), it is necessary to determine function $u(x, y, t)$ and then to find the value of the conjugate function from (35), (36), and (38).

Approximate solution of the optimal control problem (4)–(9) can be obtained by gradient methods [6, 23, 24] and by the technique presented earlier for creating difference schemes of point to point computing for numerical solution of direct differential problem. Note that two-step difference schemes can be applied immediately for numerical solution of conjugate problems as well.

## CONCLUSIONS

In the paper, we have developed methods of mathematical modeling and optimization of processes of diffusion (heat conduction) in the form of direct and extremum problems for multidimentional parabolic equations. For numerical solution of nonstationary diffusion equations, we have proposed an approach that uses the idea of splitting and implementation of the obtained difference schemes by means of explicit schemes of point to point computing. We have considered and analyzed problems of creating the schemes of splitting, approximation, and stability of explicit difference schemes with respect to initial data. For numerical solution of the optimal control problem, we have analyzed differential properties of the quality functional and proposed an iteration scheme for determining the optimal control. Implementing the described approach to solution of spatial nonstationary diffusion equations on multiprocessor computing systems with distributed storage will considerably reduce time costs.

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