Numerical identification of the initial condition for parabolic equation

V.I. Vasil’ev, M. Kardashevsky
677000 Yakutsk, 58, Belinsky str., North-Eastern Federal University
E-mail: vasvasil@mail.ru; kardam123@gmail.com

Abstract. The authors consider a problem of reconstructing of the initial condition in a parabolic equation through the given value of the unknown function at the final moment of time. To perform a numerical solution of the retrospective inverse problem for a multidimensional parabolic equation it is suggested to use a rapidly converging conjugate gradient method, based on a sequential refinement of the initial condition and a direct problem solution at each iteration. The article provides a discussion on the results of a computational experiment conducted on model problems with exact and quasi-realistic solutions, including random errors for desired overdetermination condition.

1. INTRODUCTION

Widely represented, inverse problems for partial differential equations are the most frequently used in construction of mathematical models for various processes. A problem of mathematical model identification through determination of differential equation coefficients, of the right side, area boundary, or initial conditions based on additional observation data or experiment. These tasks belong to inverse problems of mathematical physics and play nowadays a significant role in natural sciences and their applications all over the world. An important feature of inverse problems arising from results processing of a full-scale experiment is that the initial data in these problems is known approximately. This results from the fact that devices used at measurements have a certain level of error. It follows that methods of solving inverse problems should be resistant to small changes in the input data. Besides, an issue of uniqueness of solution is also relevant, and its study, in fact, is an answer to a question on whether the available experimental data is sufficient for unambiguous definition of the desired characteristic of the object or process studied. Studies on establishment of conditional correctness of inverse problems through construction of numerical methods for their solution are summarized in monographs [1] – [7].

Tasks with inverse time (retrospective inverse problems) with given conditions at the final moment of time belong to a class of incorrect problems in classical sense [7]. However, they are correctly set in the class of bounded solutions. Numerical solutions of a retrospective inverse problem are developed, for example, in the following works: a modified boundary element method based on a minimal energy method [8]; an iterative method of the initial condition refining [9]; an iterative algorithm with the boundary element method [10]; modified Tikhonov regularization method [11]; an iterative method with reverse direction of time [12]; conjugate gradient method for initial condition refining [13]; use of the Poisson integral [14]; quasi-inversion
method [5] and optimal filtering method [4]. In most works indicated above, a regularization method is used, and in this connection we note that incorrect tasks are very sensitive to regularization parameters.

As indicated in monograph [7] iterative algorithms for solving evolutionary inverse problems have long-term prospects that take into account the specifics of problems under consideration. They iteratively refine an initial condition, i.e., a usual direct correct initial-boundary value problem for a parabolic equation is solved at each iteration [9]. In this paper we will use an iterative method of conjugate gradients, where the number of iterations is used as a regularization parameter, which is in agreement with an error of the input data. We present calculations demonstrating the possibilities of the method.

2. PROBLEM STATEMENT
In the domain \( \Omega = \{ x \mid x = (x_1, \ldots, x_p), 0 < x_\alpha < l_\alpha, \alpha = 1, \ldots, p \} \) we seek a solution of the multidimensional parabolic equation

\[
\frac{\partial u}{\partial t} = \sum_{\alpha=1}^{p} \frac{\partial}{\partial x_{\alpha}} \left( k_{\alpha}(x) \frac{\partial u}{\partial x_{\alpha}} \right), \quad x \in \Omega, \quad 0 \leq t < T
\]

with homogeneous Dirichlet boundary conditions.

We formulate a retrospective inverse problem as follows: the value of the unknown function is set at the fixed terminal time \( u(x, T) \), and the initial condition \( u(x, 0) \) is to be determined

\[
u(x, T) = \phi(x), \quad x \in \Omega.
\]

Let the coefficients \( k_{\alpha}(x), \alpha = 1, \ldots, p \) of the differential equation (1) be sufficiently smooth, positive, and bounded functions, that is, satisfy conditions

\[
0 < \kappa_1 \leq k_{\alpha}(x, t) \leq \kappa_2 < \infty.
\]

The considered non-classical initial-boundary value problem with inverse time belongs to a class of conditionally correct problems of mathematical physics [7].

It should be noted that equation (1) has an exact analytical solution in the case of constant coefficients

\[
u(x_1, x_2, \ldots, x_p, t) = \frac{1}{\sqrt{(\beta + 4t)^p}} e^{-\frac{(x-x_0)^2}{\beta+4t}}, \quad \beta > 0,
\]

where \( x_0 = (l_1/2, \ldots, l_p/2) \). This function is fairly smooth and limited, and it can be further used to establish an accuracy of the proposed iterative method.

We carry out a numerical solution for the parabolic problem (1) – (3) on a rectangular space-time grid in steps \( h_\alpha, \alpha = 1, \ldots, p \), \( \tau = T/M \) using a finite-difference scheme [16]:

\[
\frac{y^{n+1} - y^n}{\tau} + A \left( \sigma y^{n+1} + (1 - \sigma) y^n \right) = 0, \quad x \in \omega, \quad n = 0, 1, \ldots, N - 1.
\]

\[
y_M = \phi(x), \quad x \in \omega,
\]

where the weight factor is \( \sigma \in [0, 1] \).
3. SOLUTION ALGORITHM FOR INVERSE PROBLEM

For numerical implementation of the discrete analogue of retrospective inverse problem (5) – (6) we will use an iterative method of conjugate gradients, based on sequential refinement of the initial condition and on solution of the direct problem at each iteration. Let us give the problem a corresponding operator statement. From (5) – (6) for a given \( y^0 \) at the final time instant we get

\[
y^N = A y^0, \quad x \in \Omega, \quad A = S^n,
\]

where \( S \) is an operator of transition from one temporary layer to another:

\[
S = (E + \sigma \tau A)^{-1} (E + (\sigma - 1) \tau A).
\]

Thus, it is natural to put a solution of the following grid operator equation to approximate solution of the inverse problem:

\[
A v = \phi(x), \quad x \in \Omega.
\]

Due to self-adjointness of an operator \( A \) a transition operator \( S \) is self-adjoint and, therefore, the operator \( A \) is also self-adjoint in equation (7), its unique solvability will take place, for example, if the operator \( A \) is positive. This condition will be met for the positive transition operator \( S \). Taking representation (9), into consideration, we obtain \( S > 0 \) under condition of stability

\[
\sigma \geq \frac{1}{2} - \frac{1}{\tau \| A \|}.
\]

A numerical implementation of the difference scheme will be carried out through an iterative method of conjugate gradients [15], which essence is to refine an initial condition at each iteration. Moreover, at each iteration, correct problems are solved using standard two-layer difference schemes [9].

4. NUMERICAL EXPERIMENTS

To demonstrate a working efficiency of the proposed computational algorithm for solving a retrospective inverse problem for a parabolic equation, let us consider a two-dimensional model problem

\[
\frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left( k_1(x,y) \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left( k_2(x,y) \frac{\partial u}{\partial y} \right) = 0, \quad x \in (0,l) = \Omega, \quad 0 \leq t < T.
\]

Let us suppose that homogeneous first-type boundary conditions are given

\[
u(0, y, t) = u(x, 0, t) = u(l, y, t) = u(x, l, t) = 0, \quad 0 < t \leq T,
\]

and an additional condition in the form of function value at the final time instant \( t = T \) is specified:

\[
u(x, y, T) = \phi(x, y), \quad 0 < x < l, \quad 0 < y < l.
\]

The calculations were carried out on the exact solution (4) with \( \beta = 1, \quad l = 16, \quad T = 1, \quad n = 50, \quad M = 50, \quad K = 20. \) The best accuracy in solving the direct problem was shown in a scheme with a weight factor \( \sigma = 2/3. \)
In Fig.1 on the left there is a graph of the desired function at the initial time, and on the right there is an override condition (4) \( u(x, y, T) = \phi(x, y, 1) \). In Fig.2 (left) there is an error of the desired function found by the iterative method \( u(x, y, 1) = \phi(x, y) \). Number of iterations is 20. The right is a graph of the deviation of the found approximate solution at the final time from the exact condition of redefinition. The error is rather large, since at each iteration a difference scheme is implemented, which has a substantial approximation error on this “coarse” grid.

Now let us conduct a computational experiment with an initial condition which is a discontinuous function [10], then, the additional condition will be a quasi-realistic solution obtained from the direct problem (13) – (14) with the initial condition

\[
\nu(x) = \begin{cases} 
0 & \text{for } x \leq 2l/5 \text{ or } x \geq 3l/5, \\
1 & \text{otherwise}
\end{cases}
\] (14)

As a set condition for redefinition at the final time, we take the value of a direct problem solution using a difference scheme with a weighting factor \( \sigma = 1/2 - h^2/(12\tau) \):

\[
\phi(x_i) = y_i^M, \quad i = 0, ..., n,
\]

The calculations were carried out with the following \( l = 30, \ T = 2, \ n = 50, \ M = 50, \ K = 20 \).

In Fig.3, on the left there is a graph of the sought discontinuous initial condition, and in the graph on the right there is the overdetermination condition, which is the solution value (?) at the final time instant \( u(x, y, 1) = \phi(x, y) \), calculated using an implicit difference scheme with \( \sigma = 2/3 \). In Fig.4 (left) there is the deviation of the unknown function found by the iteration method \( u(x, y, 1) = \phi(x, y) \) (left). The number of iterations is 20. On the right there is a graph of the deviation of the found approximate solution at the final time point from the quasi-real override condition. The error is rather large, since at each iteration a difference scheme is implemented, which has a substantial approximation error on this “coarse” grid.
In inverse problems, the additional conditions are the results of measurements obtained by devices with specified accuracy characteristics, i.e., they should be set with some "noise". It is necessary to find out how small perturbations introduced artificially in an additional condition affect the accuracy of identification of the initial condition. Let us simulate input errors using the following function

$$\varphi_1(x) = \varphi(x_i) + \delta \gamma(-0.5, 0.5),$$

where $\delta$ is a coefficient of the defined error, $\gamma(-0.5, 0.5)$ is a generator of random numbers uniformly distributed over the interval $(-0.5, 0.5)$. 

Fig. 3. The graph of the initial condition (left), a graph of the additional condition (right). Discontinuous initial condition.

Fig. 4. The graph of the restored initial condition (left) and the error in determining the initial condition (right). Discontinuous initial condition.

Fig. 5. Condition of overdetermination with noise $\delta = 0.007$ (left), deviation from the quasi-real overdetermination condition (right).
The calculations were carried out with the same input data on the same space-time grid as the previous examples. Figure 5 shows the result of calculations for an example with an exact analytical solution (4). The artificially introduced "noise" was of the order of about 1% when specifying the overdetermination condition. Left noisy additional condition. On the right there is a graph of the deviation of the found approximate solution at the final time from the exact condition of redefinition.

The reconstructed initial condition is shown in Fig.6(left), and in the graph on the right there is its deviation from the initial condition. 5 iterations were performed. It should be noted that the accuracy of identification of the initial condition has greatly increased due to conditional correctness of the problem under consideration.

Fig.7 presents the noisy overdetermination condition $\delta = 0.005$ (left), and the deviation from the quasi-real overdetermination condition. Fig.8(left) shows the deviation of the unknown

Fig.8. The graph of the restored initial condition (left) and the error in determining the initial condition $\delta = 0.009$ (right).
function found by the iteration method $u(x, y, 1) = \phi(x, y)$. The number of iterations is 5. On the right there is a graph of the deviation of the found approximate solution at the final moment of time from the quasi-real overdetermination condition. The error is also big enough.

5. CONCLUSION
For numerical solution of the retrospective inverse problem for a parabolic equation, an iterative conjugate gradient method was used. A computational experiment conducted on model two-dimensional problems confirmed the effectiveness of the proposed iterative method for solving a retrospective inverse problem of heat conduction. The method of conjugate gradients can be used to solve other inverse problems and these studies will be further developed in subsequent works.

6. ACKNOWLEDGMENTS
The authors express their sincere gratitude to Professor Petr Nikolaevich Vabishchevich for constructive comments and fruitful discussions. The work was partially supported by the Russian National Science Foundation (project 19-11-00230).

References
[1] Aster R. C., Borchers B., Thurber C.H. Parameter estimation and inverse problems. Academic Press. 2004.
[2] Kabaniikhin S. I. Inverse and Ill-Posed Problems. Theory and Applications. De Gruyter, Germany, 2011.
[3] Lavrent’ev M. M., Romanov V. G., Shishatskii S. P. Ill-posed problems of mathematical physics and analysis. American Mathematical Society. 1986.
[4] Isakov V. Inverse Problems for Partial Differential Equations, Springer Verlag, New York, 2006.
[5] Latte’s R., Lions J. L. The Method of Quasi-Reversibility. Applications to Partial Differential Equations. American Elsevier Publishing Company. 1969
[6] Prilepko A. I., Orlovsky D. G., Vasin I. A. Methods for solving inverse problems in mathematical physics. Marcel Dekker, 2000.
[7] Samarskii A. A., Vabishchevich P. N. Numerical methods for solving inverse problems of mathematical physics. De Gruyter, 2007.
[8] Han H., Ingham D. B., Yuan Y. The boundary element method for the solution of the backward heat conduction equation // J. Comput. Phys., 116 (1995), pp. 292–299.
[9] Samarskii A. A., Vabishchevich P. N., Vasil’ev V. I. Iterative Solution of a Retrospective Inverse Problem of Heat Conduction // Matematicheskoe Modelirovanie, Volume 9, Number 5, 1997, pp. 119–127.
[10] Mera N. S., Elliott L., Ingham D. B., Lesnic D. An iterative boundary element method for solving the one-dimensional backward heat conduction problem // International Journal of Heat and Mass Transfer, Volume 44, Issue 10, May 2001, pp. 1937–1946.
[11] Zhenyu Zhao, Zehong Meng. A modified Tikhonov regularization method for a backward heat equation // Inverse Problems in Science and Engineering. Vol. 19, No. 8, December 2011, pp.1175–1182.
[12] Tspelev I. A. Iterative algorithm for solving the retrospective problem of natural thermal convection of a viscous fluid // Computational continuum mechanics 2011. . 4, No 2, pp. 119–127.
[13] Vasil’ev V. I., Kardashevsky A. M. Iterative Solution of the Retrospective Inverse Problem for a Parabolic Equation Using the Conjugate Gradient Method / LNCS, 2017, volume 10187. pp. 698–705.
[14] Vasil’ev V. I., Kardashevsky A. M. Numerical solution of the retrospective inverse problem of heat conduction with the help of the Poisson integral // Journal of Applied and Industrial Mathematics. 2018, Volume 12, Issue 3. pp. 577–586.
[15] Saad U. Iterative Methods for Sparse Linear Systems. 2-nd Edition. SIAM, 2003.
[16] Samarskii A. A. The theory of difference schemes. Marcel Dekker, 2001.
[17] Savitsky A., Golay M. Smoothing and differentiation of data by simplified least squares procedures // Anal. Chem. 1964. Vol. 36. pp. 1627–1639.