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A Finite Difference Scheme with Improved Boundary Approximation for the Heat Conduction Equation with Third-Type Boundary Conditions

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Abstract

Introduction. The development, analysis, and modification of finite difference schemes tailored to the specific features of the considered problem can significantly enhance the accuracy of modeling complex systems. In simulations of various processes, including hydrodynamic phenomena in shallow water bodies, it has been observed that for problems with third-type (Robin) boundary conditions, the theoretical error order of spatial discretization drops from second-order to first-order accuracy, which in turn decreases the overall accuracy of the numerical solution. The present study addresses the relevant issue of how the approximation of third-type boundary conditions affects the accuracy of the numerical solution to the heat conduction problem. It also proposes a finite difference scheme with improved boundary approximation for the heat conduction equation with third-type boundary conditions and compares the accuracy of the numerical solutions obtained by the authors with known benchmark solutions.

Materials and Methods. The paper considers the one-dimensional heat conduction equation with third-type boundary conditions, for which an analytical solution is available. The problem is discretized, and it is shown that under standard boundary approximation, the theoretical order of approximation error for the second-order differential operator in the diffusion equation is $O(h)$. To improve the accuracy of the numerical solution under specific third-type boundary conditions, a finite difference scheme is proposed. This scheme achieves second-order accuracy $O(h^2)$, for the differential operator not only at interior nodes but also at the boundary nodes of the computational domain.

Results. Test problems were used to compare the accuracy of numerical solutions obtained using the proposed scheme and those based on the standard boundary approximation.

Discussion and Conclusion. Numerical experiments demonstrate that the proposed scheme with enhanced boundary approximation for the heat conduction equation under specific third-type boundary conditions exhibits an effective accuracy order close to 2, which corresponds to the theoretical prediction. It is noteworthy that the scheme with standard boundary approximation also demonstrates an effective accuracy order close to 2, despite the lower theoretical order of boundary approximation. Importantly, the numerical error of the proposed scheme decreases significantly faster compared to the scheme with standard boundary treatment.

Keywords: heat conduction equation, third-type boundary conditions, numerical solution, approximation error

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Оригинальное теоретическое исследование

Разностная схема с улучшенной аппроксимацией на границе для уравнения теплопроводности с граничными условиями третьего рода

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Аннотация
Введение. Построение разностных схем, их исследование и модификация с учетом специфики рассматриваемой задачи позволяет повысить точность моделирования сложных систем. При моделировании различных процессов, включая гидродинамические процессы в мелководных водоемах, было отмечено, что при решении задач с граничными условиями третьего рода теоретическая оценка порядка погрешности аппроксимации падает со второго порядка погрешности относительно пространственных шагов расчетной сетки до первого порядка, а, следовательно, падает и точность численного решения задачи. Настоящая работа посвящена актуальной проблеме исследования влияния аппроксимации граничных условий третьего рода на точность численного решения задачи теплопроводности, а также построению разностной схемы с улучшенной аппроксимацией граничных условий для уравнения теплопроводности с граничными условиями третьего рода и сравнению точности численных решений, полученных авторами, с известными решениями.
Материалы и методы. Рассматривается уравнение теплопроводности с граничными условиями третьего рода, для которого получено аналитическое решение. Проведена аппроксимация рассмотренной задачи и показано, что при стандартной аппроксимации задачи на границе расчетной области теоретическая оценка порядка погрешности аппроксимации дифференциального оператора второго порядка в уравнении диффузии составляет $O(h)$. Для повышения точности численного решения в случае граничных условий третьего рода специального вида предложена разностная схема, имеющая погрешность аппроксимации дифференциального оператора второго порядка $O(h^2)$, как во внутренних, так и в граничных узлах расчетной области.
Результаты исследования. На тестовых задачах проведено сравнение точности численных решений, полученных на основе предлагаемой схемы и схемы со стандартной аппроксимацией границы.
Обсуждение и заключение. Из проведенных численных экспериментов видно, что предложенная схема с улучшенной аппроксимацией на границе расчетной области для уравнения теплопроводности при граничных условиях третьего рода специального вида имеет эффективный порядок точности около 2, что соответствует полученной теоретической оценке. При этом стоит отметить, что разностная схема со стандартной аппроксимацией на границе расчетной области также имеет эффективный порядок точности, близкий к 2, несмотря на полученную теоретическую оценку порядка погрешности аппроксимации для граничных узлов. Важно отметить, что для предложенной схемы расчетная погрешность численного решения падает существенно быстрее, чем для решения на основе схемы со стандартной аппроксимацией на границе.

Ключевые слова: уравнение теплопроводности, граничные условия третьего рода, численное решение, погрешность аппроксимации

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Introduction. The heat conduction equation is widely used to describe a broad class of problems related to the modeling of three-dimensional diffusion processes [1]. This diffusion equation has been extensively studied, and its solutions are broadly applied in practice to describe many physical phenomena. Analytical approaches to solving this equation are presented in [2, 3], while numerical methods for solving the heat conduction equation with first- and second-type boundary conditions are discussed in [4, 5].

When designing complex engineering structures, it is necessary to account for the impact of ambient temperature regimes. In many cases, heat propagation in such systems is described using the heat conduction equation with third-type (Robin) boundary conditions [6]. Therefore, the goal of this study is to develop a finite difference scheme with improved boundary condition approximation and to evaluate the performance of the proposed scheme on benchmark problems. This approach allows for a comparison of the accuracy of numerical solutions obtained from various finite difference schemes under different initial and boundary conditions. In [7, 8], the Burgers equation is used as a test case; in [9, 10], the transport equation; and in [11, 12], the convection-diffusion equation.

The problem of improving the accuracy of numerical solutions has been addressed by many prominent Russian and international researchers. Notably, P.N. Vabishchevich [13, 14] studied finite difference schemes for solving second-order parabolic-type equations involving specially structured non-self-adjoint operators. B.N. Chetverushkin has contributed significantly to the development, analysis, and parameter tuning of difference schemes for applied problems, particularly in the context of high-performance computing architectures [15, 16]. V.F. Tishkin explored the modification of discontinuous Galerkin methods for gas and hydrodynamic modeling [17, 18]. The use of a regularized finite difference scheme for hydrodynamic problems was discussed in [19], with its accuracy analyzed in [20]. Methods to improve the order of accuracy in the grid-characteristic method for two-dimensional linear elasticity problems are addressed in [21], and extended to three dimensions in [22]. A numerical approach for heat and mass transfer in two-phase fluids is presented in [23], while [24] proposes a finite difference scheme for single-phase filtration in fractured media, and [25] investigates two-phase filtration in complex environments.

Developing finite difference schemes and modifying existing ones with consideration of problem-specific features enables improved modeling accuracy of complex systems [26]. In simulations of various processes, including hydrodynamic flows in shallow water bodies, it has been observed that, for problems with third-type boundary conditions, the theoretical order of approximation error for spatial discretization drops from second order to first order. Consequently, the accuracy of the numerical solution is reduced. A.I. Sukhinov [27] recommended a more detailed study of the approximation of problems with third-type boundary conditions. Accordingly, this work is devoted to examining the impact of third-type boundary condition approximation on the accuracy of the numerical solution to the heat conduction problem. It also presents the construction of a finite difference scheme with improved boundary approximation and compares the accuracy of solutions obtained with the proposed scheme against those derived using a standard boundary approximation scheme on benchmark problems.

Materials and Methods

1. Analytical Solution of the Heat Conduction Equation

Let us consider the homogeneous heat conduction equation

$$\frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2},\ 0 < x < l,\ 0 < t < T, \tag{1}$$

subject to the initial condition

$$u(x,t)\big|_{t=0} = u_0(x) \tag{2}$$

and third-kind (Robin) boundary conditions

$$\left(\frac{\partial}{\partial x}u(x,t) - \alpha u(x,t)\right)\Bigg|_{x=0} = \beta,\ \left(\frac{\partial}{\partial x}u(x,t) + \alpha u(x,t)\right)\Bigg|_{x=l} = -\beta. \tag{3}$$

To find the analytical solution of the boundary value problem (1)–(3), we introduce a transformation $u(x,t) = v(x,t) - \beta/\alpha$, which reduces the problem to one with homogeneous third-kind boundary conditions:

$$\begin{gathered}\frac{\partial v}{\partial t} = a\frac{\partial^2 v}{\partial x^2},\ 0 < x < l,\ 0 < t < T,\ v(x,t)\big|_{t=0} = u_0(x) + \frac{\beta}{\alpha},\\ \left(\frac{\partial}{\partial x}v(x,t) - \alpha v(x,t)\right)\Bigg|_{x=0} = 0,\ \left(\frac{\partial}{\partial x}v(x,t) + \alpha v(x,t)\right)\Bigg|_{x=l} = 0.\end{gathered} \tag{4}$$

We seek the solution of (4) in the form:

$$v(x,t) = X(x)T(t). \tag{5}$$

Substituting (5) into the differential equation (4) and separating variables yields:

$$\frac{1}{a}\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} = -\lambda^2. \tag{6}$$

The boundary conditions in (4) transform into:

$$\left(X'(0) - \alpha X(0)\right)T(t) = 0,\ \left(X'(l) + \alpha X(l)\right)T(t) = 0. \tag{7}$$

Thus, taking (7) into account and assuming that $v(x,t) \neq 0$ we arrive at the Sturm–Liouville problem for the function $X(x)$:

$$\begin{gathered}X'' + \lambda^2 X = 0,\ 0 < x < l,\\ X'(0) - \alpha X(0) = 0,\ X'(l) + \alpha X(l) = 0.\end{gathered} \tag{8}$$

The general solution to (8) is:

$$X(x) = C_1 \cos\lambda x + C_2 \sin\lambda x. \tag{9}$$

Considering the boundary conditions in (8) and the general form (9), the eigenfunctions $X_k(x)$ are written as:

$$X_k(x) = \lambda_k \cos\lambda_k x + \alpha \sin\lambda_k x,\ k = 1,\ 2,\ldots\ , \tag{10}$$

where λ_k, $k = 1, 2,\ldots$ are the eigenvalues of the problem (8), which are the positive roots of the transcendental equation

$$2\ \mathrm{ctg}\ \lambda l = \frac{\lambda}{\alpha} - \frac{\alpha}{\lambda}. \tag{11}$$

For the function $T(t)$ based on equation (6) and under the condition $\lambda = \lambda_k$ we arrive at the following problem:

$$T'(t) + a\lambda_k T(t) = 0,$$

the general solution of which is given by

$$T_k(t) = C_k \exp\left(-a\lambda_k^2 t\right),\ k = 1,\ 2,\ldots\ . \tag{12}$$

Then, taking into account equations (5), (10), and (12), the solution to problem (4) can be written in the form:

$$v(x,t) = \sum_{k=1}^{\infty} C_k \left(\lambda_k \cos\lambda_k x + \alpha \sin\lambda_k x\right) \exp\left(-a\lambda_k^2 t\right), \tag{13}$$

where λ_k, $k = 1, 2,\ldots$ are the positive roots of equation (11).

To determine the coefficients C_k we use the initial condition of problem (4):

$$\sum_{k=1}^{\infty} C_k \left(\lambda_k \cos\lambda_k x + \alpha \sin\lambda_k x\right) = u_0(x) + \beta/\alpha,$$

i. e., this represents the expansion of a function $f(x) = u_0(x) + \beta/\alpha$ for $0 \le x \le l$ into a Fourier series in terms of the eigenfunctions of the Sturm–Liouville problem (8). Then, assuming the eigenfunctions $X_k(x)$, $k = 1, 2,\ldots$ are orthogonal on the interval $0 \le x \le l$ the coefficients C_k are given by:

$$C_k = \frac{1}{\|X_k\|^2} \int_0^l f(x)\left(\lambda_k \cos\lambda_k x + \alpha \sin\lambda_k x\right) dx, \tag{14}$$

where $f(x) = u_0(x) + \beta/\alpha$,

$$\|X_k\|^2 = \int_0^l \left(\lambda_k \cos\lambda_k x + \alpha \sin\lambda_k x\right)^2 dx = \frac{\lambda_k^2 + \alpha^2}{2} + \frac{\lambda_k^2 - \alpha^2}{4\lambda_k} \sin 2\lambda_k l - \frac{\alpha}{2} \cos 2\lambda_k l + \frac{\alpha}{2}. \tag{15}$$

Taking into account the condition (11) for $\lambda = \lambda_k$, $k = 1, 2,\ldots$ and the trigonometric identities

$$\sin 2x = \frac{2\ \mathrm{tg}\ x}{1 + \mathrm{tg}^2 x},\ \cos 2x = \frac{1 - \mathrm{tg}^2 x}{1 + \mathrm{tg}^2 x}$$

the expression for the norm squared of the eigenfunctions $X_k(x)$ in (15) becomes:

$$\|X_k\|^2 = \frac{\left(\lambda_k^2 + \alpha^2\right) l + 2\alpha}{2}. \tag{16}$$

Thus, expression (14) for the coefficients C_k, $k = 1, 2,\ldots$ can be rewritten in the form:

$$C_k = \frac{2}{\left(\lambda_k^2 + \alpha^2\right) l + 2\alpha} \int_0^l \left(u_0(x) - \frac{\beta}{\alpha}\right)\left(\lambda_k \cos\lambda_k x + \alpha \sin\lambda_k x\right) dx = C_k^{(1)} + C_k^{(2)}, \tag{17}$$

where

$$C_k^{(1)} = \frac{2}{\left(\lambda_k^2 + \alpha^2\right) l + 2\alpha} \int_0^l u_0(x)\left(\lambda_k \cos\lambda_k x + \alpha \sin\lambda_k x\right) dx,$$

$$C_k^{(2)} = \frac{2\beta}{\left(\lambda_k^2 + \alpha^2\right)\alpha l + 2\alpha^2} \int_0^l \left(\lambda_k \cos\lambda_k x + \alpha \sin\lambda_k x\right) dx = \frac{2\beta}{\left(\lambda_k^2 + \alpha^2\right)\alpha l + 2\alpha^2} \left(\sin\lambda_k l - \frac{\alpha}{\lambda_k}\left(\cos\lambda_k l - 1\right)\right) = \tag{18}$$

$$=\frac{2\beta}{\left(\lambda_k^2+\alpha^2\right)\alpha l+2\alpha^2}\left(\frac{\alpha}{\lambda_k}+\sin\lambda_k l\left(1-\frac{\alpha}{\lambda_k}\mathrm{ctg}\lambda_k l\right)\right)=\frac{2\beta}{\left(\lambda_k^2+\alpha^2\right)\alpha l+2\alpha^2}\left(\frac{\alpha}{\lambda_k}+\frac{\lambda_k^2+\alpha^2}{2\lambda_k^2}\frac{(-1)^{k+1}}{\sqrt{1+\mathrm{ctg}^2\lambda_k l}}\right)=$$

$$=\frac{2\beta}{\lambda_k\left(\lambda_k^2+\alpha^2\right)l+2\lambda_k\alpha}\left(1+(-1)^{k+1}\right),$$

Thus, for $k = 2n$ the coefficients $C_k^{(2)} = 0$. Then the expression for the coefficients $C_k^{(2)}$ will be written as:

$$C_{2n}^{(2)}=0,\ C_{2n+1}^{(2)}=\frac{4\beta}{\lambda_{2n+1}\left(\lambda_{2n+1}^2+\alpha^2\right)l+2\lambda_{2n+1}\alpha},\ n=1,\ 2,\dots\ . \tag{19}$$

Then, the analytical solution of the original problem (1)–(3), taking into account the substitution and expressions (13), (18), and (19), can be written as:

$$u(x,t)=-\frac{\beta}{\alpha}+\sum_{k=1}^{\infty}C_k\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right)\exp\left(-a\lambda_k^2 t\right), \tag{20}$$

where $C_k=C_k^{(1)}+C_k^{(2)}$, the coefficients $C_k^{(1)}$ and $C_k^{(2)}$ are defined by expressions (18) and (19), respectively, and λ_k, $k = 1, 2,\dots$ are the positive roots of equation (11).

In the case of solving the nonhomogeneous analog of the heat conduction equation (1):

$$\frac{\partial u}{\partial t}=a\frac{\partial^2 u}{\partial x^2}+f(x,t),\ 0<x<l,\ 0<t<T \tag{21}$$

with the initial and boundary conditions (2)–(3), the solution will be sought in the form $u(x,t)=v(x,t)+w(x,t)-\beta/\alpha$, where $v(x,t)$ is the solution to problem (4), defined by formula (13) with coefficients (18)–(19), and $w(x,t)$ is the solution to the following problem:

$$\begin{gathered}\frac{\partial w}{\partial t}=a\frac{\partial^2 w}{\partial x^2}+f,\ 0<x<l,\ 0<t<T,\ w(x,t)\big|_{t=0}=0,\\ \left(\frac{\partial}{\partial x}w(x,t)-\alpha w(x,t)\right)\Bigg|_{x=0}=0,\ \left(\frac{\partial}{\partial x}w(x,t)+\alpha w(x,t)\right)\Bigg|_{x=l}=0.\end{gathered} \tag{22}$$

The function $w(x,t)$ is sought as an expansion in terms of the eigenfunctions of the corresponding homogeneous Sturm–Liouville problem:

$$w(x,t)=\sum_{k=1}^{\infty}C_k^{(w)}(t)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right). \tag{23}$$

We also expand the function $f(x,t)$ over the considered interval as $0 \le x \le l$:

$$f(x,t)=\sum_{k=1}^{\infty}C_k^{(f)}(t)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right), \tag{24}$$

where

$$C_k^{(f)}(t)=\frac{1}{\|X_k\|^2}\int_0^l f(x,t)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right)dx, \tag{25}$$

where $\|X_k\|^2$ is defined by formula (16).

Substituting (23) and (24) into (22), we obtain:

$$\sum_{k=1}^{\infty}\left(\left(C_k^{(w)}(t)\right)'+a\lambda_k^2C_k^{(w)}(t)\right)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right)=\sum_{k=1}^{\infty}C_k^{(f)}(t)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right). \tag{26}$$

Due to the completeness of the orthogonal system of eigenfunctions $X_k(x)$, $k = 1, 2,\dots$, equality (26) holds if and only if:

$$\left(C_k^{(w)}(t)\right)'+a\lambda_k^2C_k^{(w)}(t)=C_k^{(f)}(t). \tag{27}$$

Given (23) and the homogeneous initial conditions in (22), we have:

$$C_k^{(w)}(0)=0. \tag{28}$$

Thus, we obtain a Cauchy problem for an ordinary differential equation (27) with the initial condition (28). The solution to this problem can be found, for example, by the method of variation of arbitrary constant (Lagrange method):

$$C_k^{(w)}(t)=\int_0^t C_k^{(f)}(\tau)\exp\left(a\lambda_k^2(\tau-t)\right)d\tau, \qquad (29)$$

where $C_k^{(f)}(\tau)$ is defined by formula (25).

Thus, the solution to the nonhomogeneous heat equation (21) with third-kind boundary conditions (3) can be written as:

$$u(x,t)=-\frac{\beta}{\alpha}+\sum_{k=1}^{\infty}C_k\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right)\exp\left(-a\lambda_k^2 t\right)+\sum_{k=1}^{\infty}C_k^{(w)}(t)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right), \qquad (30)$$

where $C_k=C_k^{(1)}+C_k^{(2)}$, the coefficients $C_k^{(1)}$, $C_k^{(2)}$ and $C_k^{(w)}(t)$ are defined by formulas (18), (19), and (29), respectively, and λ_k, $k=1,2,...$ are the positive roots of equation (11).

2. Approximation of the Second-Order Differential Operator in the Diffusion Equation

Assume we need to consider the approximation of the nonhomogeneous heat conduction (diffusion) equation:

$$\frac{\partial u}{\partial t}=a\frac{\partial^2 u}{\partial x^2}+f(x,t),\ 0<x<l,\ 0<t<T, \qquad (31)$$

with the following initial condition:

$$u(x,t)\big|_{t=0}=u_0(x) \qquad (32)$$

and third-kind (Robin) boundary conditions:

$$\left.\left(\frac{\partial}{\partial x}u(x,t)-\alpha u(x,t)\right)\right|_{x=0}=0,\ \left.\left(\frac{\partial}{\partial x}u(x,t)+\alpha u(x,t)\right)\right|_{x=l}=0. \qquad (33)$$

To obtain a numerical solution to the problem (31)–(33), we divide the computational domain using a uniform grid $\overline{\omega}=\overline{\omega}_t\times\overline{\omega}_h$, where

$$\overline{\omega}_t=\left\{t^n=n\tau,\ n=\overline{0..N_t},\ N_t\tau=T\right\},\ \ \overline{\omega}_h=\left\{x_i=ih,\ i=\overline{0..N_x},\ N_x h=l\right\}, \qquad (34)$$

where τ is the time step size; N_t is the number of time steps; h is the spatial step size; N_x is the number of spatial nodes.

The analytical solution of the problem (31)–(33), according to equation (30), can be written as:

$$u(x,t)=\sum_{k=1}^{\infty}\left(C_k^{(1)}\exp\left(-a\lambda_k^2 t\right)+C_k^{(w)}(t)\right)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right), \qquad (35)$$

where the coefficients $C_k^{(1)}$ and $C_k^{(w)}(t)$ are defined by expressions (18) and (29), respectively, and λ_k, $k=1,2,...$ are the positive roots of equation (11).

To simplify further calculations, let us introduce the following notation:

$$C_k^{(u)}(t)=C_k^{(1)}\exp\left(-a\lambda_k^2 t\right)+C_k^{(w)}(t). \qquad (36)$$

We now write the approximation of equation (31) at the interior nodes of the computational grid (34) as:

$$\frac{u_i^{n+1}-u_i^n}{\tau}=a\frac{u_{i+1}^n-2u_i^n+u_{i-1}^n}{h^2}+f_i^n, \qquad (37)$$

where $u_{i\pm1}^n=u(t^n,x_{i\pm1}),\ u_i^n=u(t^n,x_i)$.

Then, taking into account expressions (24), (35), and (36), the approximation (37) can be written in the form:

$$\frac{1}{\tau}\sum_{k=1}^{N-1}\left(C_k^{(u)}(t^{n+1})-C_k^{(u)}(t^n)\right)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right)=$$
$$=\frac{a}{h^2}\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\left(\lambda_k\cos\left(\lambda_k(x_i+h)\right)+\alpha\sin\left(\lambda_k(x_i+h)\right)-2\lambda_k\cos\lambda_k x_i-2\alpha\sin\lambda_k x_i+\right. \qquad (38)$$
$$\left.+\lambda_k\cos\left(\lambda_k(x_i-h)\right)+\alpha\sin\left(\lambda_k(x_i-h)\right)\right)+\sum_{k=1}^{N-1}C_k^{(f)}(t^n)\left(\lambda_k\cos\lambda_k x_i+\alpha\sin\lambda_k x_i\right).$$

Using the transformations

$$\lambda_k\cos\left(\lambda_k(x_i+h)\right)+\lambda_k\cos\left(\lambda_k(x_i-h)\right)=2\lambda_k\cos\lambda_k x_i\cos\lambda_k h,$$
$$\alpha\sin\left(\lambda_k(x_i+h)\right)+\alpha\sin\left(\lambda_k(x_i-h)\right)=2\alpha\sin\lambda_k x_i\cos\lambda_k h,$$

expression (38) becomes:

$$\frac{1}{\tau}\sum_{k=1}^{N-1}\left(C_k^{(u)}(t^{n+1})-C_k^{(u)}(t^n)\right)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right)=a\frac{2}{h^2}\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\left(\cos\lambda_k h-1\right)\left(\lambda_k\cos\lambda_k x_i+\alpha\sin\lambda_k x_i\right)+$$
$$+\sum_{k=1}^{N-1}C_k^{(f)}(t^n)\left(\lambda_k\cos\lambda_k x_i+\alpha\sin\lambda_k x_i\right).$$

Taking into account the orthogonality of the basis functions $X_k(x)$, $k = 1, 2,...,$ defined in (10), the final expression can be written as:

$$\frac{C_k^{(u)}(t^{n+1})-C_k^{(u)}(t^n)}{\tau}=a\frac{2\left(\cos\lambda_k h-1\right)}{h^2}C_k^{(u)}(t^n)+C_k^{(f)}(t^n). \tag{39}$$

Let us find the second derivative of the function $u(x,t)$ with respect to the spatial variable:

$$\frac{\partial^2 u}{\partial x^2}=\frac{\partial^2}{\partial x^2}\left(\sum_{k=1}^{\infty}C_k^{(u)}(t)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right)\right)=\frac{\partial}{\partial x}\left(\sum_{k=1}^{\infty}C_k^{(u)}(t)\left(-\lambda_k^2\sin\lambda_k x+\alpha\lambda_k\cos\lambda_k x\right)\right)=$$
$$=-\sum_{k=1}^{\infty}\lambda_k^2C_k^{(u)}(t)\left(\lambda_k\cos\lambda_k x+\alpha\sin\lambda_k x\right). \tag{40}$$

From formulas (39) and (40), it follows that in the approximation of problem (31)–(33) on the computational grid (34) using scheme (37), the obtained solution for each harmonic deviates from the exact value by the quantity $\alpha^*=1-2\left(1-\cos\lambda_k h\right)/\left(\lambda_k h\right)^2$.

Let's consider the resulting value separately α^*:

$$\alpha^*=1-\frac{2\left(1-\cos\lambda_k h\right)}{\left(\lambda_k h\right)^2}=1-\frac{2\left(\frac{\left(\lambda_k h\right)^2}{2}-\frac{\left(\lambda_k h\right)^4}{24}+O\left(h^6\right)\right)}{\left(\lambda_k h\right)^2}=\frac{\left(\lambda_k h\right)^2}{12}+O\left(h^4\right). \tag{41}$$

From (41), we can conclude that when approximating the spatial variable using scheme (37), the numerical solution at the interior grid nodes (34) deviates from the exact solution by $O(h^2)$.

Let us now consider the approximation of the function $u(x,t)$ with respect to the spatial variable at the boundary nodes of the spatial grid (34). We construct this approximation based on the integro-interpolation method (the balance method). Without loss of generality, let us consider the approximation of $u(x,t)$ on the left boundary of the computational grid (i. e., at $x = 0$):

$$2\frac{u_1^n-u_0^n}{h^2}-2\frac{\alpha u_0^n}{h}=2\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\frac{\lambda_k\cos\lambda_k h+\alpha\sin\lambda_k h-\lambda_k}{h^2}-2\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\frac{\alpha\lambda_k}{h}=$$
$$=2\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\frac{\lambda_k\left(\cos\lambda_k h-1\right)+\alpha\left(\sin\lambda_k h-\lambda_k h\right)}{h^2}=\frac{2\lambda_k}{h^2}\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\left(1-\frac{\left(\lambda_k h\right)^2}{2}+\frac{\left(\lambda_k h\right)^4}{24}+O\left(h^6\right)-1\right)+ \tag{42}$$
$$+\frac{2\alpha}{h^2}\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\left(\lambda_k h-\frac{\left(\lambda_k h\right)^3}{6}+\frac{\left(\lambda_k h\right)^5}{120}+O\left(h^7\right)-\lambda_k h\right)=\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\left(-\lambda_k^3-\lambda_k^3\frac{\alpha h}{3}+O\left(h^2\right)\right).$$

To increase the order of approximation error for the spatial derivative of the function $u(x,t)$ at the boundary nodes of the grid (34), we consider the following approximation:

$$2\frac{u_1^n-u_0^n}{h^2}-2\alpha\frac{\gamma_1u_0^n+\gamma_2u_1^n}{h}=2\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\frac{\lambda_k\cos\lambda_k h+\alpha\sin\lambda_k h-\lambda_k}{h^2}-2\alpha\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\frac{\gamma_1\lambda_k+\gamma_2\lambda_k\cos\lambda_k h+\gamma_2\alpha\sin\lambda_k h}{h}=$$
$$=\frac{2}{h^2}\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\left(1-\gamma_2\alpha h\right)\left(\lambda_k\cos\lambda_k h+\alpha\sin\lambda_k h\right)-\frac{2}{h^2}\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\lambda_k\left(1+\gamma_1\alpha h\right)=$$
$$=\frac{2}{h^2}\left(1-\gamma_2\alpha h\right)\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\left(\lambda_k-\frac{\lambda_k^3h^2}{2}+\frac{\lambda_k^5h^4}{24}+\alpha\lambda_k h-\alpha\frac{\lambda_k^3h^3}{6}+\alpha\frac{\lambda_k^5h^5}{120}+O\left(h^6\right)\right)- \tag{43}$$
$$-\frac{2}{h^2}\left(1+\gamma_1\alpha h\right)\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\lambda_k=\frac{2\alpha}{h}\left(\gamma_2+1-\gamma_2\alpha h-\gamma_1\right)\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\lambda_k-\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\lambda_k^3+$$
$$+\frac{2}{h^2}\left(\gamma_2\alpha\frac{h^3}{2}-\alpha\frac{h^3}{6}+\gamma_2\alpha^2\frac{h^4}{6}\right)\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\lambda_k^3+\frac{h^2}{12}\sum_{k=1}^{N-1}C_k^{(u)}(t^n)\lambda_k^5+O\left(h^3\right).$$

The coefficients γ_1 and γ_2 in (43) are found as a solution to the system:

$$\begin{cases} \gamma_2 + 1 - \gamma_2 \alpha h - \gamma_1 = 0, \\ \gamma_2 - \dfrac{1}{3} + \gamma_2 \alpha \dfrac{h}{3} = 0, \end{cases}$$

from which we obtain the values of the coefficients $\gamma_1 = 2/(3 + \alpha h)$ and $\gamma_2 = 1/(3 + \alpha h)$.

Thus, we obtain the following approximation for the spatial derivative of the function $u(x,t)$ at the boundary nodes of the grid (34):

$$2\frac{u_1^n - u_0^n}{h^2} - \frac{4\alpha}{h(3+\alpha h)} u_0^n - \frac{2\alpha}{h(3+\alpha h)} u_1^n = \sum_{k=1}^{N-1} C_k^{(u)}(t^n)\left(-\lambda_k^3 + \frac{\lambda_k^5 h^2}{12} + O\left(h^3\right)\right). \quad (44)$$

Results. Assume we need to compare the computational accuracy of the spatial approximations (42) and (44) by solving test problems. We consider three test problems. The first is a steady-state problem with a constant right-hand side. The second is also a steady-state problem, but with a harmonic right-hand side corresponding to an eigenvalue λ_k. The third problem involves solving the heat conduction equation with a stepwise right-hand side.

Test Problem 1. Find the solution to the following problem:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + 2, \; 0 < x < 2, \quad (45)$$

with the initial condition:

$$u(x,t)\big|_{t=0} = 0 \quad (46)$$

and boundary conditions of the third kind

$$\left(\frac{\partial}{\partial x} u(x,t) - 2u(x,t)\right)\bigg|_{x=0} = 0, \; \left(\frac{\partial}{\partial x} u(x,t) + 2u(x,t)\right)\bigg|_{x=2} = 0. \quad (47)$$

Problem (45)–(47) is a steady-state problem.

The analytical solution to problem (45)–(47) can be written in the form: $u(x,t) = -x^2 + 2x + 1$.

Figure 1 shows the analytical solution of problem (45)–(47), as well as numerical solutions of Test Problem 1 obtained using: the first-order finite difference scheme in space (42), and the second-order finite difference scheme in space (44), for different spatial step sizes.

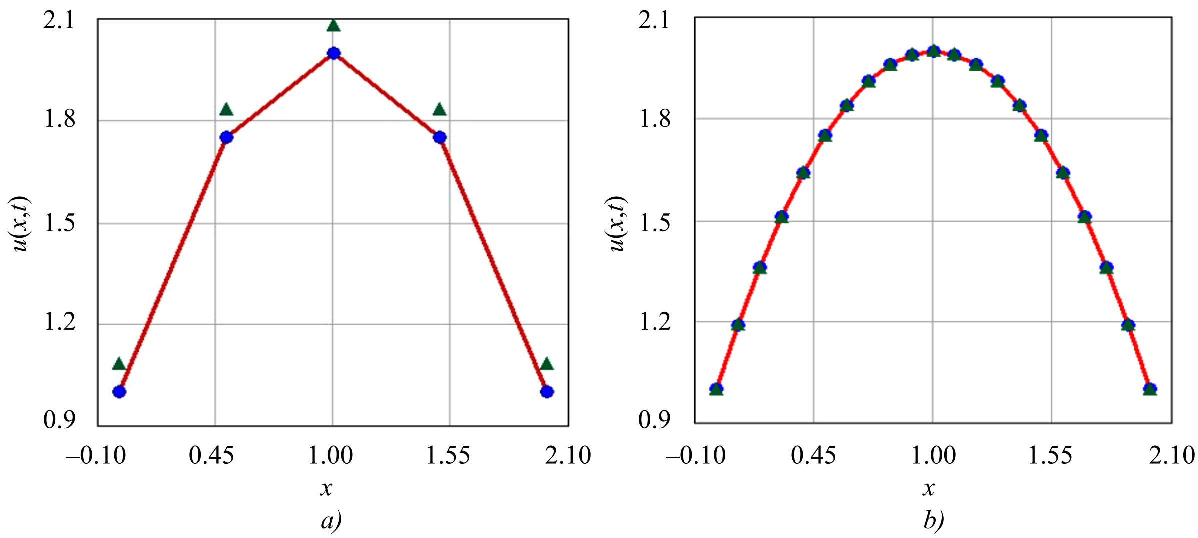

Fig. 1. Results of solving Test Problem 1:
red line — exact solution; blue dots — numerical solution using the first-order spatial approximation scheme (42);
green triangles — numerical solution using the second-order spatial approximation scheme (44);
a — spatial step size $h = 0.5$; *b* — spatial step size $h = 0.1$

In addition to the approximation error, we compute the effective order of accuracy of the scheme [28]:

$$p^{eff} = \log_r \left|\frac{R_N}{R_{rN}}\right|, \tag{48}$$

where R_N is the error of the numerical solution on the grid with step size h, R_{rN} is the error on the grid with step size h/r.

Table 1 presents the computational error of the numerical solution for Test Problem 1 based on schemes (42) and (44) for different spatial step sizes. The error was measured in the grid space norm $\Psi^n = \sum_{i=1}^{N} \left|u(x_i,t^n) - u_i^n\right| \cdot h,$ where $u(x_i,t^n)$ is the analytical solution, and u_i^n is the numerical solution.

Based on the data in Table 1, we can conclude that the proposed scheme (44), with improved boundary approximation for the heat conduction equation under third-kind boundary conditions (33), exhibits an effective order of accuracy equal to 2, which agrees with the theoretical estimate.

Table 1

Computed errors of the numerical solution for Test Problem 1 for various spatial step sizes

	The error value of the numerical solution			
	h = 1.00	h = 0.50	h = 0.25	h = 0.10
Finite difference scheme with standard boundary approximation (42)	0.000	0.000	0.000	3.286×10^{-15}
Finite difference scheme with improved boundary approximation (44)	1.000	0.208	0.047	0.007
Effective accuracy order of scheme (44)	–	2.263	2.152	2.075

Test Problem 2. Let us consider the solution of the following problem:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + X_k,\ 0 < x < 5, \tag{49}$$

with the following initial condition:

$$u(x,t)\big|_{t=0} = 0 \tag{50}$$

and third-kind boundary conditions:

$$\left(\frac{\partial}{\partial x}u(x,t) - 0{,}1u(x,t)\right)\Bigg|_{x=0} = 0,\ \left(\frac{\partial}{\partial x}u(x,t) + 0{,}1u(x,t)\right)\Bigg|_{x=5} = 0, \tag{51}$$

where X_k is an eigenfunction corresponding to an eigenvalue λ_k, which is determined by equation (11). Problem (49)–(51) is a steady-state problem.

The analytical solution to problem (49)–(51) in the steady-state formulation can be expressed in the following form:

$$u(x,t) = \frac{1}{\sqrt{\alpha^2 + \lambda_k^2}} \sin\left(\lambda_k x + \arccos\left(\frac{\alpha}{\sqrt{\alpha^2 + \lambda_k^2}}\right)\right).$$

According to the conditions of the problem (49)–(51), $\alpha = 0.1$. Let us determine λ_k.

We now consider the numerical algorithm for solving equation (11) to determine the eigenvalues λ_k. Let us assume we need to find the roots of the nonlinear equation $f(\lambda) = 0$, where $f(\lambda) = 2\ \text{ctg}\ \lambda l - \frac{\lambda}{\alpha} + \frac{\alpha}{\lambda}$.

Step 1. Introduce two auxiliary functions $f_1(\lambda) = 2\ \text{ctg}\ \lambda l$ and $f_2(\lambda) = \frac{\lambda}{\alpha} - \frac{\alpha}{\lambda}$.

Step 2. Define the number of iterations K, which also determines the number of eigenvalues to be computed.

Step 3. For each eigenvalue λ_k define the initial guess using the following expression:

$$w_k = \frac{(2k+1)\pi}{2l} - \frac{1}{l} \cdot \text{arctg}\left(\frac{1}{2} \cdot f_2\left(\frac{(2k+1)\pi}{2l}\right)\right),$$

where k is the iteration index or the index of the corresponding eigenvalue λ_k.

Step 4. At each iteration, apply Newton's method to find the solution of the nonlinear equation $f(\lambda) = 0$. For this, define the function

$$g(\lambda) = f'(\lambda) = -\frac{2l}{\sin^2(\lambda l)} - \frac{1}{\alpha} - \frac{\alpha}{\lambda^2}.$$

Step 5. Use x_0 as the initial approximation w_k.

Step 6. Compute the value $x_{i+1} = x_i - f(x_i)/g(x_i)$.

Step 7. If $|x_{i+1} - x_i| > \varepsilon$, where ε is a predefined small tolerance, return to Step 6.

Step 8. Assign the computed value λ_k define equal x_{i+1}.

Step 9. If $k < K$, proceed to Step 4. Otherwise, terminate the eigenvalue computation algorithm λ_k.

Figure 2 presents the results of the algorithm described above. The points in the figure indicate the values λ_k, that correspond to the solution of the equation $f(\lambda) = 0$.

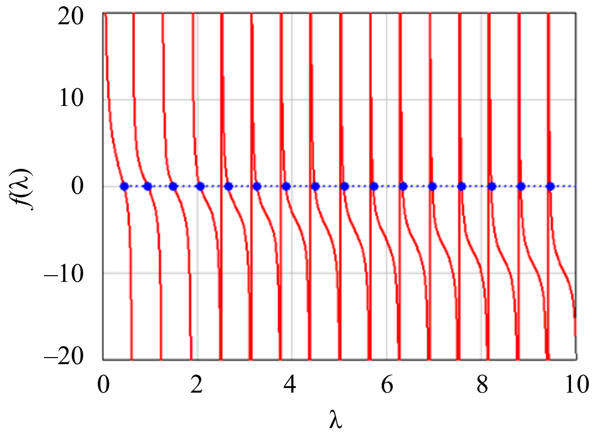

Fig. 2. Results of the eigenvalue λ_k computation algorithm: the red line represents the graph of the function $f(\lambda)$; the blue dots indicate the computed values λ_k, which correspond to the roots of the equation $f(\lambda) = 0$

Figure 3 presents the analytical solution of problem (49)–(51), as well as the numerical solutions of Test Problem 2 obtained using the first-order finite difference scheme in space (42) and the second-order finite difference scheme in space (44) for various spatial step sizes. The eigenvalue was taken for $k = 4$ and is equal to $\lambda_4 \approx 2{,}529$.

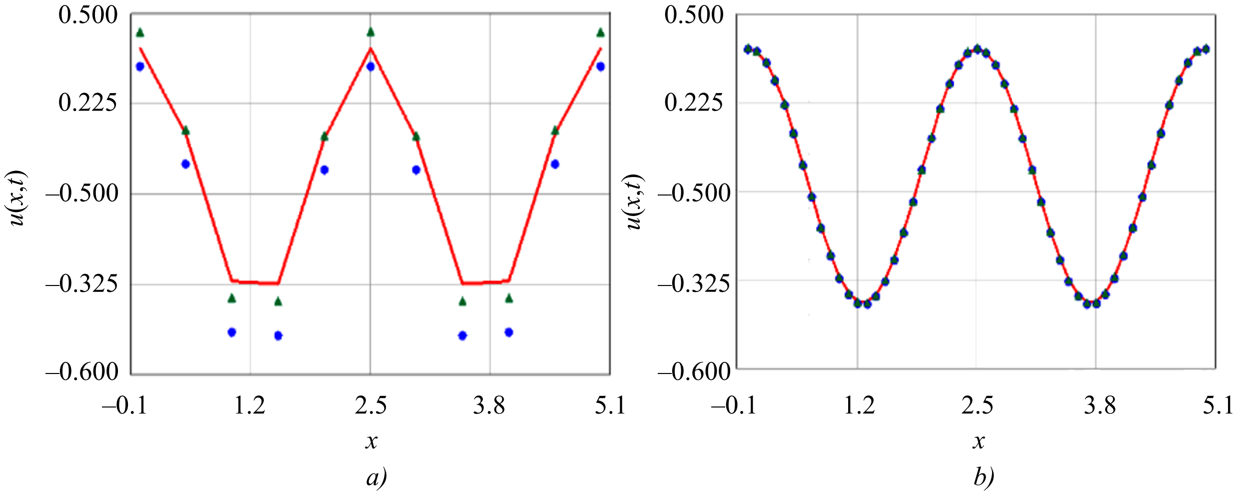

Fig. 3. Results of solving Test Problem 2 for $k = 4$: the red line represents the exact solution; blue dots represent the numerical solution based on the first-order spatial approximation scheme (42); green triangles represent the numerical solution based on the second-order spatial approximation scheme (44); *a* — spatial step size $h = 0.5$; *b* — spatial step size $h = 0.1$

Table 2 presents data on the computed error of the numerical solution of Test Problem 2 obtained using schemes (42) and (44) for various spatial step sizes.

Table 2

Computed Error Values of the Numerical Solution of Test Problem 2 for Various Spatial Step Sizes

	Values of the Numerical Solution Error			
	$h = 1.00$	$h = 0.50$	$h = 0.25$	$h = 0.10$
Finite Difference Scheme (42)	2.916	0.581	0.136	0.021
Effective Order of Accuracy of Scheme (42)	–	2.327	2.094	2.028
Finite Difference Scheme with Improved Boundary Approximation (44)	1.126	0.206	0.047	6.964×10^{-3}
Effective Order of Accuracy of Scheme (44)	–	2.455	2.133	2.080

Based on the data in Table 2, it can be observed that the proposed scheme (44), which incorporates improved boundary approximation for the heat conduction equation with third-kind boundary conditions (33), demonstrates an effective order of accuracy equal to 2, which is consistent with the theoretical estimate. The finite difference scheme (42), employing standard boundary approximation, also exhibits an effective order of accuracy close to 2, despite the lower theoretical approximation error order at the boundary nodes. It is worth noting that the proposed scheme (44) reduces the numerical solution error by approximately 2.5 to 3 times, depending on the spatial step size. As the spatial step size decreases, the difference in accuracy between schemes (42) and (44) becomes more pronounced.

Test Problem 3. Let us find the solution to the following problem:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - \theta(x-1) + \theta(x-3),\ 0 < x < 5,\ 0 < T < 10 \tag{52}$$

with the following initial condition

$$u(x,t)\big|_{t=0} = 0 \tag{53}$$

and third-order boundary conditions

$$\left(\frac{\partial}{\partial x}u(x,t) - u(x,t)\right)\Bigg|_{x=0} = 0,\ \left(\frac{\partial}{\partial x}u(x,t) + u(x,t)\right)\Bigg|_{x=5} = 0, \tag{54}$$

where $\theta(x)$ is a piecewise-defined Heaviside function.

According to (30), the analytical solution to the problem (52)–(54) can be written in the following form:

$$u(x,t) = \sum_{k=1}^{\infty} C_k^{(w)}(t)\left(\lambda_k \cos\lambda_k x + \alpha \sin\lambda_k x\right),$$

where $C_k^{(w)}(t)$ is determined based on (29), while taking into account the type of the right-hand side (52)

$$C_k^{(f)}(t) = C_k^{(f)} = -\frac{2}{5\left(\lambda_k^2+1\right)+2}\int_1^3\left(\lambda_k\cos\lambda_k x + \alpha\sin\lambda_k x\right)dx = \frac{2}{5\left(\lambda_k^2+1\right)+2}\left(\frac{1}{\lambda_k}\left(\cos 3\lambda_k - \cos\lambda_k\right) + \sin\lambda_k - \sin 3\lambda_k\right). \tag{55}$$

Taking into account (29) and (55), we obtain the following form for the exact solution of the problem (52)–(54):

$$u(x,t) = \sum_{k=1}^{\infty}\frac{\exp\left(-\lambda_k^2 t\right)-1}{\lambda_k^2}C_k^{(f)}\left(\lambda_k\cos\lambda_k x + \alpha\sin\lambda_k x\right).$$

The eigenvalues λ_k are determined using the algorithm described in Test Problem 2.

In Figure 4*a*, the numerical solution to Test Problem 3, obtained using the difference scheme with improved boundary approximation (44) for a spatial step of $h = 0.5$. is presented. In these calculations, 1000 eigenvalues λ_k were used. Visually, no significant difference was observed between the numerical solutions obtained using difference schemes (42) and (44).

In Figure 4*b*, difference between the analytical and numerical solutions, calculated using formula (56) for k from 1 to 1000, is shown.

Figure 5 presents the analytical solution of the problem (52)–(54) at a fixed time $t = 2$, as well as the numerical solutions of Test Problem 3 obtained using the first-order spatial approximation scheme (42) and the second-order spatial approximation scheme (44) for different spatial step sizes. The calculations accounted for the sum of the first 1000 eigenvalues λ_k.

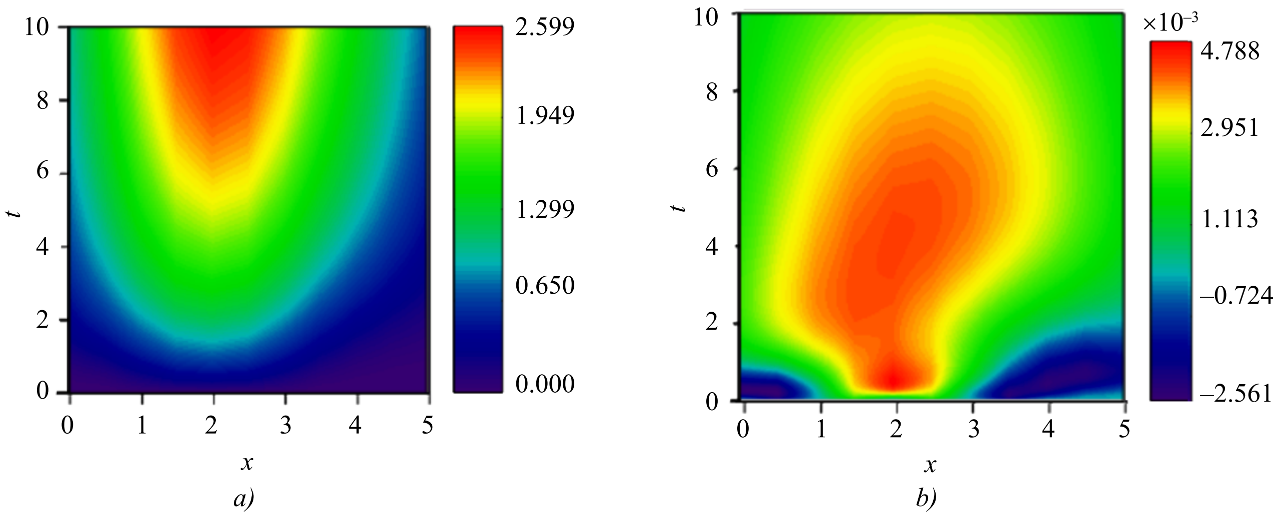

Fig. 4. Results of solving Test Problem 3 considering 1000 λ_k and time steps $\tau = 0.001$ and spatial steps $h = 0.5$:
a — numerical solution based on the second-order spatial approximation scheme (42);
b — difference between the analytical and numerical solutions based on (44)

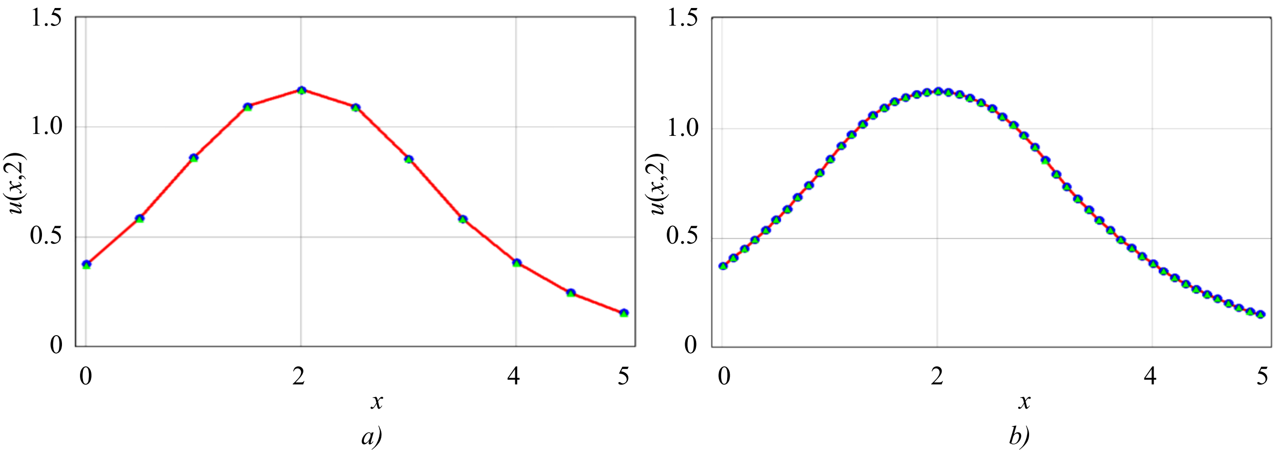

Fig. 5. Results of solving Test Problem 3 at $t = 2$:
red line — analytical solution; blue dots — numerical solution based on the first-order spatial approximation scheme (42); green triangles — numerical solution based on the second-order spatial approximation scheme (44);
a — spatial step $h = 0.5$; *b* — spatial step $h = 0.1$

Table 3 presents information on the computational error of the numerical solution of Test Problem 3 based on schemes (42) and (44) for different spatial step sizes.

Table 3

Computed values of the error for the numerical solution of Test Problem 3 at $t = 2$ for different spatial step sizes

	Error values of the numerical solution			
	$h = 1.00$	$h = 0.50$	$h = 0.25$	$h = 0.10$
Solution based on the first-order spatial approximation scheme (42)	0.0503	0.0102	0.002	2.6797×10^{-4}
Effective order of accuracy of scheme (42)	–	2.3010	2.231	2.2860
Solution based on the second-order spatial approximation scheme (44)	0.0530	0.0130	2.914×10^{-3}	2.0397×10^{-4}
Effective order of accuracy of scheme (44)	–	2.0570	2.132	2.9020

From the data in Table 3 (similarly to Test Problem 2), it can be observed that the proposed scheme (44) with improved boundary approximation for the heat conduction equation under third-kind boundary conditions (33) exhibits an effective order of accuracy equal to 2, which is consistent with the theoretical estimate. The difference scheme (42) with standard boundary approximation also demonstrates an effective order of accuracy close to 2, despite the theoretical estimate of the approximation error order at the boundary nodes. At the same time, for the proposed scheme (44), the numerical solution error decreases significantly faster than for the solution based on scheme (42).

Discussion and Conclusion. This study examined the heat conduction equation with third-kind boundary conditions, for which an exact solution was obtained. The problem was discretized, and it was shown that under standard boundary approximation, the theoretical order of approximation error for the second-order differential operator in the diffusion equation is $O(h)$. Based on this estimate, it follows that for the heat conduction equation with third-kind boundary conditions, the standard discretization yields a first-order accurate scheme. To improve the accuracy of the numerical solution, a finite difference scheme was proposed that provides an approximation error of $O(h^2)$, for the second-order differential operator, both at interior and boundary nodes of the computational domain. This scheme is applicable to third-kind boundary conditions of a specific form.

Numerical experiments demonstrate that the proposed scheme, featuring enhanced boundary approximation for the heat conduction equation with third-kind boundary conditions of a specific type, achieves an effective order of accuracy close to 2, which aligns with the theoretical estimate. It is also worth noting that the finite difference scheme with standard boundary approximation exhibits an effective order of accuracy close to 2, despite the theoretical approximation error estimate at the boundary nodes. The observed discrepancy between the theoretical approximation error and the achieved numerical accuracy calls for further investigation. Importantly, the numerical error of the proposed scheme decreases significantly faster than that of the scheme with standard boundary approximation.

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