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IMPLICITE FINITE DIFFERENCE METHOD FOR TIME FRACTIONAL HEAT EQUATION WITH MIXED BOUNDARY CONDITIONS

Summary. This paper describes an application of the implicit finite difference method for solving the time fractional heat equation with mixed boundary conditions. In particular, the differential scheme will be presented for the non-homogeneous Neumann and Robin boundary conditions. To illustrate the accuracy of described method some computational examples will be presented as well.

SCHEMAT NIEJAWNY METODY RÓŻNIC SKOŃCZONYCH DLA RÓWNANIA PRZEWODNICTWA CIEPŁA Z POCHODNĄ RZĘDU UŁAMKOWEGO WZGLĘDEM CZASU Z MIESZANYMI WARUNKAMI BRZEGOWYMI

Streszczenie. W artykule przedstawiono zastosowanie schematu niejawnego metody różnic skończonych do przybliżonego rozwiązania równania przewodnictwa ciepła z pochodną rzędu ułamkowego względem czasu oraz mieszanymi warunkami brzegowymi. W szczególności rozpatrywane są niejednorodne warunki brzegowe Neumanna oraz Robina. Przedstawione zostały również przykłady obliczeniowe ilustrujące dokładność metody.

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1. Introduction

Recently various types of phenomena in physics, biology, control theory, electrical engineering and mechanics are modeled by using the derivatives of fractional order [1,4,10,13,17]. Not all of these models can be solved in analytical way, therefore it is so important to develop various types of approximate methods for solving differential equations of fractional order.

Murio in his paper [11] shows the implicit finite difference approximation for the time fractional diffusion equations with homogeneous Dirichlet boundary conditions. In paper [18] the numerical scheme for the fractional heat equation with Dirichlet and Neumann boundary conditions is described. By using the finite difference scheme for spatial variable the authors transform the considered equation into a system of ordinary fractional differential equations. Next, this system is expressed in integral form. Further, the integral equation is transformed into a difference equation by the modified trapezoidal rule. In paper [15] the finite difference scheme for fractional sub-diffusion equation with homogeneous Neumann boundary conditions is presented.

In paper [3] the finite difference scheme for the fractional sub-diffusion equations with non-homogeneous source term and Dirichlet boundary conditions is presented. First the authors transform the original sub-diffusion problem with the Riemann-Liouville fractional derivative on the right hand side of the equation to the form with the Caputo fractional derivative on the left hand side of the equation. Then they use the $L1$ approximation to deal with the temporal Caputo fractional derivative and the compact scheme for spatial directional derivative. The resulting difference scheme is unconditionally stable and convergent in maximum norm with the convergence order of $O((\Delta t)^{2-\alpha} + (\Delta x)^4)$. Zhao and Xu [20] consider the numerical solutions of the time fractional sub-diffusion equation with the variable coefficient subject to both Dirichlet boundary conditions and Neumann boundary conditions. A compact difference scheme is proposed for solving the equation with Dirichlet boundary conditions. The unconditional stability and the global convergence of the scheme in the maximum norm are proved rigorously with the help of the newly introduced norms regarding to the variable coefficient. The convergence order is $O((\Delta t)^{2-\alpha} + (\Delta x)^4)$. A box-type scheme is derived by introducing new intermediate variable for the problem with Neumann boundary conditions. Stability and the global convergence of the box-type scheme in maximum norm are also investigated.

In paper [2] the authors present the numerical method for the time fractional diffusion equations with Dirichlet boundary condition. In the discretization formulation, the finite difference scheme and the Kansa method are respectively used to discretize the time fractional derivative and the spatial derivative terms. Meerschaert with co-authors [6–8, 19] deals also with the numerical approximation for different types of the fractional partial differential equations. In papers concerning the fractional diffusion equation the authors presuppose the Dirichlet boundary conditions.

Paper [5] describes the finite volume method for solving the space fractional diffusion equation with the variable diffusion coefficient and the zero Dirichlet boundary conditions. Zheng et al. [21] present the finite element method for solving the space-fractional advection diffusion equation with the non-homogeneous Dirichlet boundary condition. Computational aspects of the finite element method approximation of the fractional advective dispersion equation are described in paper [16].

In paper [12] two numerical methods, namely, the $L2$ approximation and the shifted Grünwald scheme for the Riesz fractional diffusion equation with the zero Dirichlet boundary conditions are compared. Numerical solution of the fractional diffusion-wave equation is presented in paper [9].

The current paper describes the implicit finite difference method for solving the time fractional heat equation with mixed boundary conditions. In particular, we intend to present the differential scheme for the non-homogeneous Neumann and Robin boundary conditions and the Dirichlet boundary conditions. To illustrate the accuracy of described method some computational examples will be presented as well.

2. Formulation of the problem

We consider the fractional order differential equation

$$c\varrho\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}=\lambda\frac{\partial^2 u(x,t)}{\partial x^2}+g(x,t), \tag{1}$$

defined in domain $D=\{(x,t): x\in[0,L], t\in[0,T]\}$, where c denotes the specific heat, ϱ is the density and λ describes the thermal conductivity coefficient.

The above equation is a differential equation with the fractional derivative with respect to the time variable. It is called the time fractional diffusion equation. Equations of this type are used to describe the transport processes with a long memory. Derivative with respect to the time variable is the fractional derivative of order $\alpha \in (0,1)$. Derivatives of this type are used to describe the problems associated with the fluid mechanics and subdiffusion process. Fractional derivative with respect to time, occuring in equation (1), will be the Caputo fractional derivative which is determined as follows

$$\frac{{}_a\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(n-\alpha)} \int_a^t \frac{\partial^n u(x,s)}{\partial s^n}(t-s)^{n-\alpha-1} ds, \tag{2}$$

where $n = \lceil \alpha \rceil$ and $\Gamma(\cdot)$ is the Gamma function [14]. In our case $\alpha \in (0,1)$, therefore $n = 1$. In addition, we assume that $a = 0$. Then we get

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x,s)}{\partial s}(t-s)^{-\alpha} ds, \quad \alpha \in (0,1). \tag{3}$$

To ensure the uniqueness of solution we pose the initial-boundary conditions

$$u(x,0) = f(x), \qquad x \in [0,L], \tag{4}$$

$$-\lambda \frac{\partial u}{\partial x}(0,t) = q(t), \qquad t \in [0,T], \tag{5}$$

$$-\lambda \frac{\partial u}{\partial x}(L,t) = h(t)(u(L,t) - u^\infty), \qquad t \in [0,T], \tag{6}$$

where h is the heat transfer coefficient and u^∞ denotes the ambient temperature. At the left and right end of the space interval we pose the Neumann and Robin boundary conditions, respectively. In this paper we also consider the Dirichlet boundary condition

$$u(0,t) = \phi(t), \qquad t \in [0,T], \tag{7}$$

$$u(L,t) = \psi(t), \qquad t \in [0,T]. \tag{8}$$

3. Numerical solution

We will now describe the approximate solution of equation (1) obtained by using the finite difference method. Let $N, M \in \mathbb{N}$ will be the grid sizes in the space and time intervals, respectively. We define the following steps of the grid $\Delta x = L/N,\ \Delta t = T/M$. Points of the grid in interval $[0,L]$ are then the following numbers $x_i = i\ \Delta x,\ i = 0,1,2,\ldots,N$, and in interval $[0,T]$ we have numbers $t_k = k\ \Delta t,\ k = 0,1,2,\ldots,M$. Values of functions $f, q, h, g, u, \phi, \psi$ in the grid points will be denoted as follows: $f_i = f(x_i),\ q_k = q(t_k), h_k = h(t_k), g_i^k = g(x_i,t_k), \phi_k =$

$\phi(t_k), \psi_k = \psi(t_k)$ and $u_i^k = u(x_i, t_k)$. Values of the approximate function in points (x_i, t_k) will be denoted by U_i^k.

Equation (1) may be written as

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = a\frac{\partial^2 u(x,t)}{\partial x^2} + \overline{g}(x,t), \tag{9}$$

where $a = \frac{\lambda}{c\varrho}$ is the thermal diffusivity coefficient and $\overline{g}(x,t) = \frac{g(x,t)}{c\varrho}$.

Now we derive the formula for approximating the fractional derivative (3) [11]:

$$\frac{\partial^\alpha u(x_i,t_k)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)}\int_0^{t_k} \frac{\partial u(x_i,s)}{\partial t}(t_k - s)^{-\alpha} ds =$$

$$= \frac{1}{\Gamma(1-\alpha)}\sum_{j=1}^{k}\int_{(j-1)\Delta t}^{j\Delta t}\left[\frac{u_i^j - u_i^{j-1}}{\Delta t} + O(\Delta t)\right](k\Delta t - s)^{-\alpha} ds =$$

$$= \frac{1}{\Gamma(1-\alpha)}\frac{1}{1-\alpha}\times$$

$$\times\sum_{j=1}^{k}\left\{\left[\frac{u_i^j - u_i^{j-1}}{\Delta t} + O(\Delta t)\right]\left[(k-j+1)^{1-\alpha} - (k-j)^{1-\alpha}\right]\right\}\Delta t^{1-\alpha} =$$

$$= \frac{1}{\Gamma(1-\alpha)}\frac{1}{1-\alpha}\frac{1}{\Delta t^\alpha}\sum_{j=1}^{k}(u_i^j - u_i^{j-1})\left[(k-j+1)^{1-\alpha} - (k-j)^{1-\alpha}\right] +$$

$$+ \frac{1}{\Gamma(1-\alpha)}\frac{1}{1-\alpha}\sum_{j=1}^{k}\left[(k-j+1)^{1-\alpha} - (k-j)^{1-\alpha}\right]O(\Delta t^{2-\alpha}).$$

Thus, the approximation of fractional derivative (3) is given by

$$D_t^{(\alpha)}U_i^k = \sigma(\alpha,k)\sum_{j=1}^{k}\omega(\alpha,j)(U_i^{k-j+1} - U_i^{k-j}), \tag{10}$$

where

$$\sigma(\alpha,\Delta t) = \frac{1}{\Gamma(1-\alpha)(1-\alpha)\Delta t^\alpha},$$
$$\omega(\alpha,j) = j^{1-\alpha} - (j-1)^{1-\alpha}.$$

Using approximations of the Neumann and Robin boundary conditions we obtain

$$-\lambda\frac{U_1^k - U_{-1}^k}{2\Delta x} = q_k \implies U_{-1}^k = U_1^k + \frac{2\Delta x q_k}{\lambda}, \tag{11}$$

$$-\lambda\frac{U_{N+1}^k - U_{N-1}^k}{2\Delta x} = h_k(U_N^k - u^\infty) \implies U_{N+1}^k = U_{N-1}^k - \frac{2\Delta x h_k}{\lambda}(U_N^k - u^\infty). \quad (12)$$

Applying these relations and the difference quotient for derivative of the second order with respect to space, we get the following difference equations:

$k \geqslant 1,\ i = 0$:

$$\Big(\sigma(\alpha,\Delta t) + \frac{2a}{(\Delta x)^2}\Big)U_0^k - \frac{2a}{(\Delta x)^2}U_1^k =$$
$$= \sigma(\alpha,\Delta t)U_0^{k-1} - \sigma(\alpha,\Delta t)\sum_{j=2}^{k}\omega(\alpha,j)(U_0^{k-j+1} - U_0^{k-j}) + \overline{g}_i^k + \frac{2}{\Delta x c\varrho}q_k, \quad (13)$$

$k \geqslant 1,\ i = 1,2,\ldots,N-1$:

$$-\frac{a}{(\Delta x)^2}U_{i-1}^k + \Big(\sigma(\alpha,\Delta t) + \frac{2a}{(\Delta x)^2}\Big)U_i^k - \frac{a}{(\Delta x)^2}U_{i+1}^k =$$
$$= \sigma(\alpha,\Delta t)U_i^{k-1} - \sigma(\alpha,\Delta t)\sum_{j=2}^{k}\omega(\alpha,j)(U_i^{k-j+1} - U_i^{k-j}) + \overline{g}_i^k, \quad (14)$$

$k \geqslant 1,\ i = N$:

$$-\frac{2a}{(\Delta x)^2}U_{N-1}^k + \Big(\sigma(\alpha,\Delta t) + \frac{2a}{(\Delta x)^2} + \frac{2}{\Delta x c\varrho}h_k\Big)U_N^k = \sigma(\alpha,\Delta t)U_N^{k-1} -$$
$$-\sigma(\alpha,\Delta t)\sum_{j=2}^{k}\omega(\alpha,j)(U_N^{k-j+1} - U_N^{k-j}) + \overline{g}_i^k + \frac{2}{\Delta x c\varrho}h_k u^\infty. \quad (15)$$

In case of boundary conditions of the first kind, functions ϕ and ψ on the boundary are known, hence we get the following relations

$$U_0^k = \phi_k, \quad U_N^k = \psi_k, \qquad k \geqslant 1. \quad (16)$$

Thus for $k \geqslant 1,\ i = 1,2,\ldots,N-1$, we obtain the following difference equations

$$-\frac{a}{(\Delta x)^2}U_{i-1}^k + \Big(\sigma(\alpha,\Delta t) + \frac{2a}{(\Delta x)^2}\Big)U_i^k - \frac{a}{(\Delta x)^2}U_{i+1}^k =$$
$$= \sigma(\alpha,\Delta t)U_i^{k-1} - \sigma(\alpha,\Delta t)\sum_{j=2}^{k}\omega(\alpha,j)(U_i^{k-j+1} - U_i^{k-j}) + \overline{g}_i^k. \quad (17)$$

The resulting difference scheme is unconditionally stable and has the convergence order of $O(\Delta t + (\Delta x)^2)$.

4. Examples

Example 1. Let us consider equation (1) with the initial condition

$$u(x,0) = 0,$$

and homogeneous boundary conditions of the second kind

$$-\lambda \frac{\partial u}{\partial x}(0,t) = 0,$$

$$-\lambda \frac{\partial u}{\partial x}(1,t) = 0.$$

We assume that $\alpha = 0.5,\ \lambda = 1,\ c = 1,\ \varrho = 1$ and $h(t) \equiv 0$, whereas function $g(x,t)$ is expressed by the following formula

$$g(x,t) = \frac{1}{2} e^x t^2 \left[-2t^\alpha (2 + x(x^3 + 6x^2 + x - 8)) + x^2 (x-1)^2 \Gamma(3+\alpha) \right].$$

Exact solution of this problem is given by function

$$u(x,t) = e^x x^2 (1-x)^2 t^{(2+\alpha)}.$$

Plot of the exact solution $u(x,t)$ is shown in Figure 1.

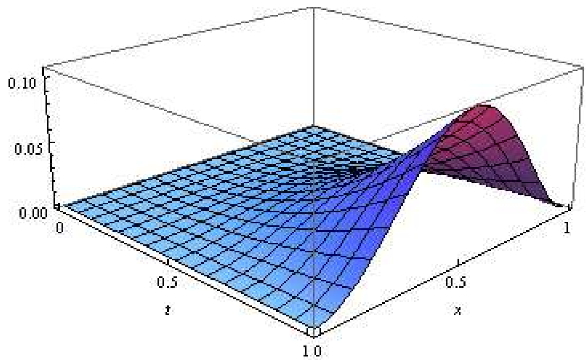

Fig. 1. Exact solution $u(x,t)$
Rys. 1. Rozwiązanie dokładne $u(x,t)$

The calculations were made on the grid of discretization intervals equal to $\Delta x = \Delta t = \frac{1}{100}$ $(N = M = 100)$. Plot of the obtained approximate solution is presented in Figure 2. Maximal error of this approximate solution in this case is the following

$$E(\Delta x, \Delta t) = \max_{\substack{0 \leqslant i \leqslant N \\ 1 \leqslant k \leqslant M}} |u_i^k - U_i^k| = 0.000372632.$$

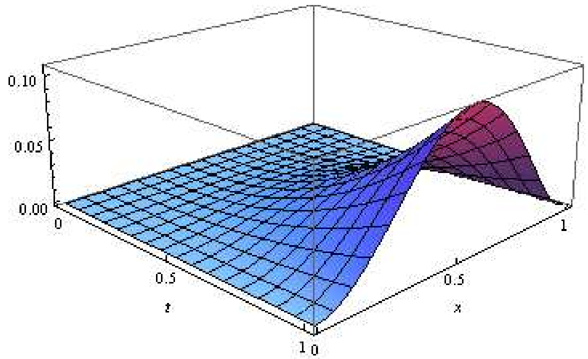

Fig. 2. Approximate solution for Example 1 ($N = M = 100$)
Rys. 2. Przybliżone rozwiązanie dla przykładu 1 ($N = M = 100$)

Distribution of errors in points of the grid is presented in Figure 3. In Figures 4 and 5 there are presented the exact and approximate solution for the moment of time $t = 0.75,\ 1.0$ together with errors of this approximation.

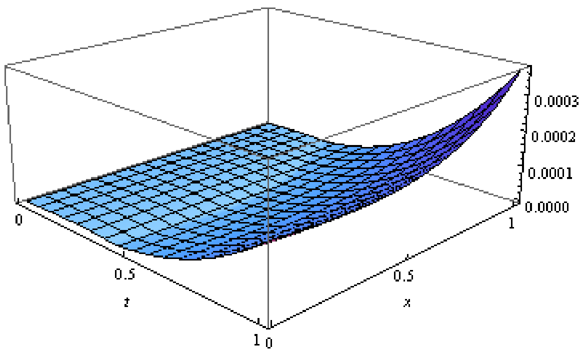

Fig. 3. Distribution of errors for Example 1 ($N = M = 100$)
Rys. 3. Rozkład błędów dla przykładu 1 ($N = M = 100$)

Increasing four times the number of the grid points ($N = M = 200$) we obtain the following maximal error $E(\Delta x, \Delta t) = 0.000088636$. In Figure 6 the distribution of errors is presented in case of the grid size $N = M = 200$.

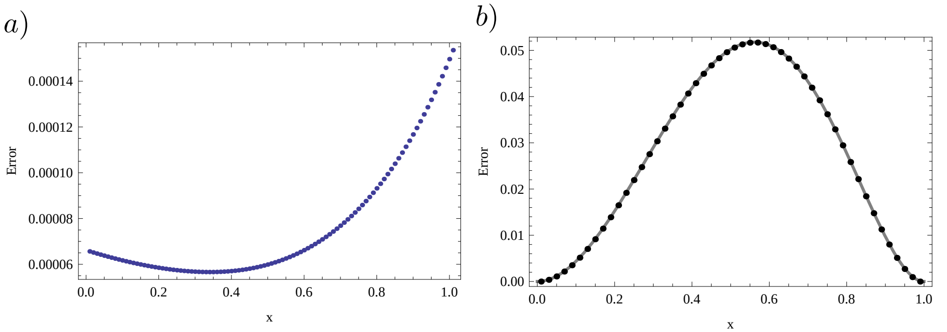

Fig. 4. Distribution of errors (a) and the comparison of approximate (points) and exact (solid line) solution (b) in moment of time $t = 0.75$ for Example 1 ($N = M = 100$)

Rys. 4. Rozkład błędów (a) oraz porównanie przybliżonego (punkty) i dokładnego (linia ciągła) rozwiązania (b) w chwili $t = 0{,}75$ dla przykładu 1 ($N = M = 100$)

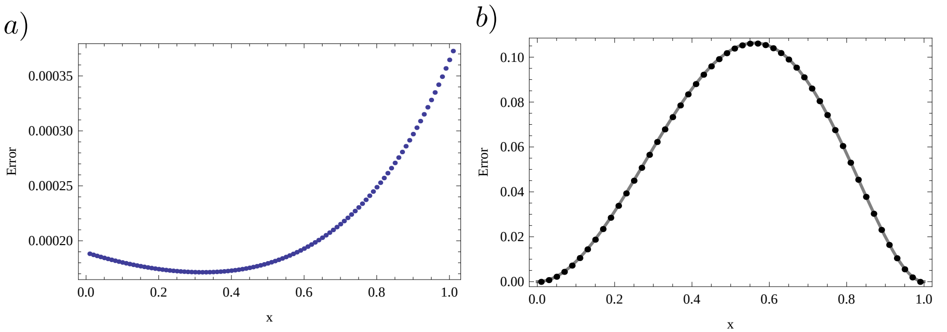

Fig. 5. Distribution of errors (a) and the comparison of approximate (points) and exact (solid line) solution (b) in moment of time $t = 1$ for Example 1 ($N = M = 100$)

Rys. 5. Rozkład błędów (a) oraz porównanie przybliżonego (punkty) i dokładnego (linia ciągła) rozwiązania (b) w chwili $t = 1$ dla przykładu 1 ($N = M = 100$)

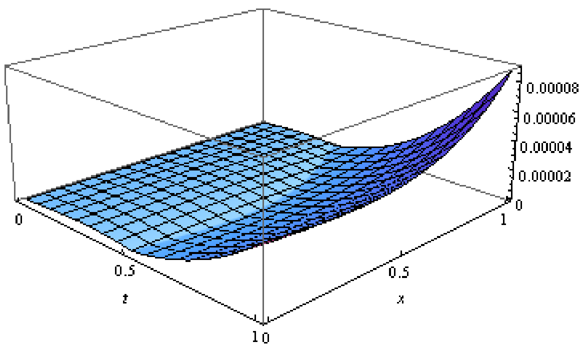

Fig. 6. Distribution of errors for Example 1 ($N = M = 200$)

Rys. 6. Rozkład błędów dla przykładu 1 ($N = M = 200$)

Example 2. Let us consider again the equation from Example 1. This time, instead of boundary conditions of the second and third kind, we assume boundary conditions of the first kind

$$u(0,t) = u(1,t) = 0, \qquad t \in [0,T].$$

Exact solution of this problem is given again by function

$$u(x,t) = e^x x^2 (1-x)^2 t^{(2+\alpha)}.$$

The calculations are made on the grid of discretization intervals equal to $N = M = 100$. Maximal error of obtained approximate solution is the following

$$E(\Delta x, \Delta t) = \max_{\substack{0 \leqslant i \leqslant N \\ 1 \leqslant k \leqslant M}} |u_i^k - U_i^k| = 0.0041865.$$

In Figure 7 distribution of the errors of approximate solution is displayed.

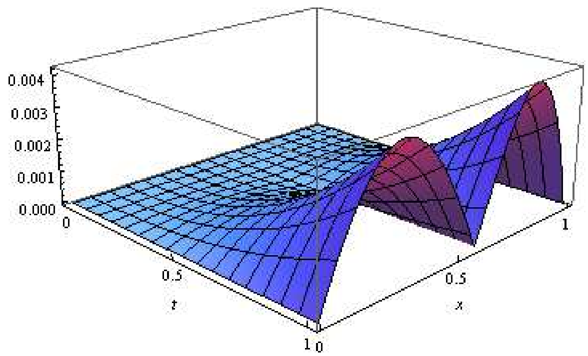

Fig. 7. Distribution of errors for Example 2 ($N = M = 100$)
Rys. 7. Rozkład błędów dla przykładu 2 ($N = M = 100$)

For the grid size $N = M = 200$ the maximal error is equal to $E(\Delta x, \Delta t) = 0.00229827$. In Figures 9 and 10 there are displayed the distribution of errors and the exact and approximate solutions in moment of time $t = 1$ for the grid of size $N = M = 200$.

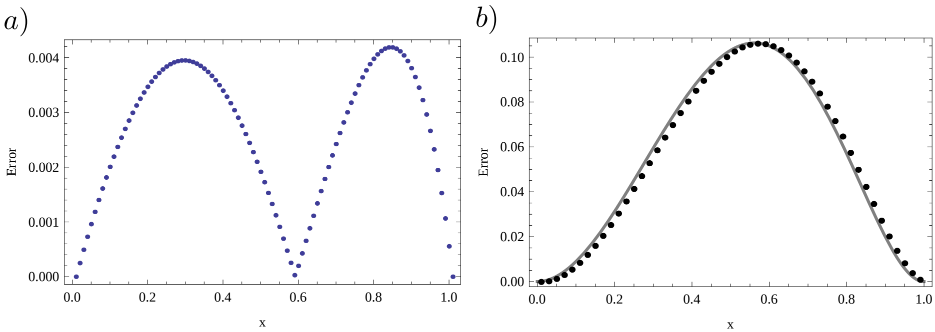

Fig. 8. Distribution of errors (a) and the comparison of approximate (points) and exact (solid line) solution (b) in moment of time $t = 1$ for Example 2 ($N = M = 100$)

Rys. 8. Rozkład błędów (a) oraz porównanie przybliżonego (punkty) i dokładnego (linia ciągła) rozwiązania (b) w chwili $t = 1$ dla przykładu 2 ($N = M = 100$)

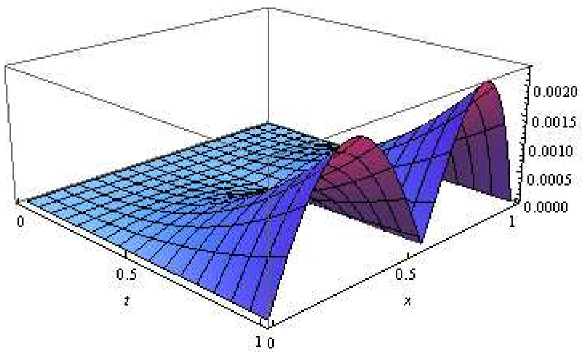

Fig. 9. Distribution of errors for Example 2 ($N = M = 200$)

Rys. 9. Rozkład błędów dla przykładu 2 ($N = M = 200$)

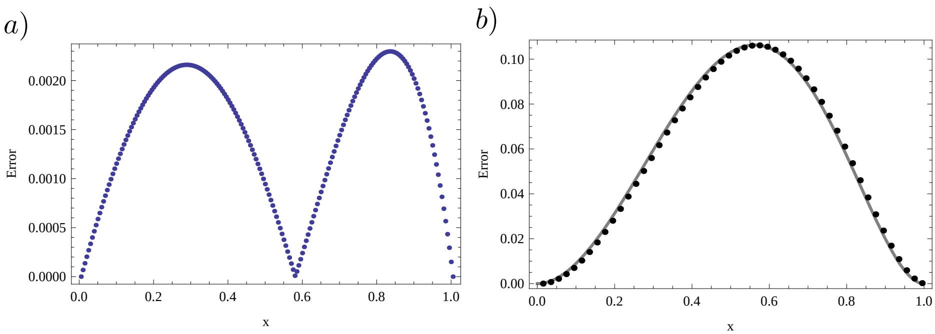

Fig. 10. Distribution of errors (a) and the comparison of approximate (points) and exact (solid line) solution (b) in moment of time $t = 1$ for Example 2 ($N = M = 200$)

Rys. 10. Rozkład błędów (a) oraz porównanie przybliżonego (punkty) i dokładnego (linia ciągła) rozwiązania (b) w chwili $t = 1$ dla przykładu 2 ($N = M = 200$)

Example 3. We consider equation (1) in domain $D = \{(x,t) : x,t \in [0,1]\}$. We also include the initial condition

$$u(x,0) = 0,$$

and boundary conditions of the second and third kind

$$-\lambda \frac{\partial u}{\partial x}(0,t) = q(t),$$

$$-\lambda \frac{\partial u}{\partial x}(1,t) = h(t)(u(L,t) - u^{\infty}),$$

where $q(t) = -t^{1+\alpha}$ and $h(t) \equiv -1,\ u^{\infty} = 0$. We assume that $\alpha = 0.5,\ \lambda = 1,\ c = 1,\ \varrho = 1$. Function $g(x,t)$ is in the form

$$g(x,t) = e^x t^{\alpha}\Big(-t + \frac{\sqrt{t}\,\Gamma[2+\alpha]}{\Gamma[\frac{3}{2}+\alpha]}\Big).$$

Exact solution of this problem is represented by function

$$u(x,t) = e^x t^{1+\alpha}.$$

For the grid size $N = M = 100$ the maximal error is equal to $E(\Delta x, \Delta t) = 0.0108085$. Distribution of errors of the approximate solution in domain D is presented in Figure 11.

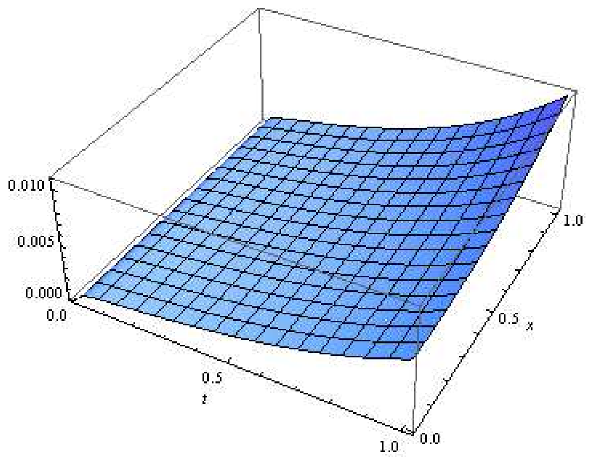

Fig. 11. Distribution of errors for Example 3 ($N = M = 100$)
Rys. 11. Rozkład błędów dla przykładu 3 ($N = M = 100$)

By increasing density of the grid in the time domain we can observe the decrease of the maximal error. In Table 1 there are collected the maximal errors for different sizes of the grid.

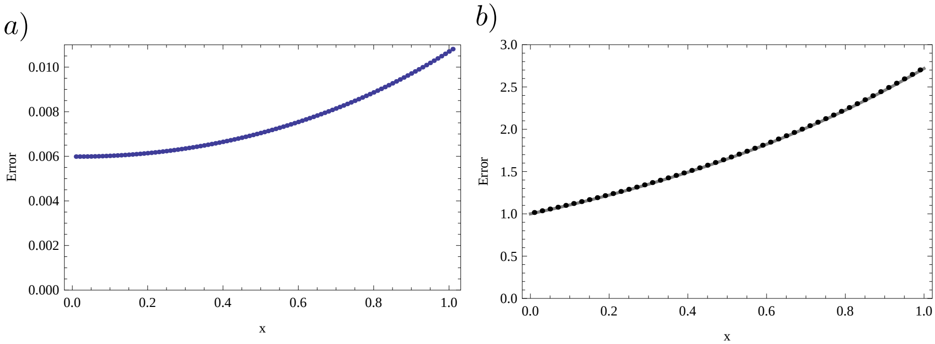

Fig. 12. Distribution of errors (a) and the comparison of approximate (points) and exact (solid line) solution (b) in moment of time $t = 1$ for Example 3 ($N = M = 100$)
Rys. 12. Rozkład błędów (a) oraz porównanie przybliżonego (punkty) i dokładnego (linia ciągła) rozwiązania (b) w chwili $t = 0{,}75$ dla przykładu 3 ($N = M = 100$)

Table 1
Maximal errors $E(\Delta x, \Delta t)$ for different sizes of the grid

Grid ($\Delta x \times \Delta t$)	$E(\Delta x, \Delta t)$
$1/100 \times 1/100$	0.01080850
$1/100 \times 1/200$	0.00384188
$1/100 \times 1/300$	0.00205081

5. Conclusions

In the paper the implicit finite difference method used for solving the time fractional diffusion equation with mixed boundary conditions has been presented. The resulting difference scheme is unconditionally stable and has the convergence order of $O(\Delta t + (\Delta x)^2)$. To illustrate the accuracy of described method some computational examples have been presented. Results received in calculations confirm usefulness of the proposed approach.

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