UDC 519.63 MSC2020 65N06

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Numerical methods for systems of diffusion and superdiffusion equations with Neumann boundary conditions and with delay

A feature of many mathematical models is the presence of two equations of the diffusion type with Neumann boundary conditions and the delay effect, for example, in the model of interaction between a tumor and the immune system. In this paper we construct and study the orders of convergence of analogues of the implicit method and the Crank-Nicolson method. Also, for a system of space fractional superdiffusion-type equations with delay and Neumann boundary conditions, an analogue of the Crank-Nicolson method is constructed. To approximate the two-sided fractional Riesz derivatives, the shifted Grunwald-Letnikov formulas are used; to take into account the delay effect, interpolation and extrapolation of the discrete history of the model are used.

Key words: Systems of diffusion equations, Neumann conditions, delay, superdiffusion, Crank-Nicolson method.

DOI: https://doi.org/10.47910/FEMJ202229

Introduction

Systems of partial differential equations, as well as systems of ordinary differential equations, are widely used in mathematical modeling. In many equations of the diffusion type, boundary conditions of the second type (Neumann conditions) are considered, which creates difficulties in the construction and study of numerical algorithms. Models can also contain the effect of time-delay. An example is the model of interaction between a tumor and the immune system [1]. Besides, in recent years systems of fractional differential equations [2] have become more and more popular.

In this work, numerical calculations are essentially used, but the justification of the convergence of numerical methods for such problems has not been previously carried out.

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For boundary conditions of the first kind (Dirichlet conditions), numerical algorithms for solving diffusion-type equations with functional delay were previously developed in [3]. Convergence was proved using the technique of embedding difference schemes with heredity in the general scheme and determining stability using the general theory of difference schemes. For the Neumann problems of equations of diffusion type, this technique turned out to be inapplicable. However, the simplest difference schemes can be studied based on the properties of the resulting system of linear algebraic equations.

But the Neumann problem for systems of equations of superdiffusion type, the technique of embedding in the general scheme is applicable in the same way as for the Dirichlet problem [4].

1 Diffusion-type equations

1.1 Problem definition

Let us consider a system of equations of the diffusion type with a functional delay of the form

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} = a_1 \frac{\partial^2 u}{\partial x^2} + f_1(x,t,u(x,t),u_t(x,\cdot),v(x,t),v_t(x,\cdot)), \\ \frac{\partial v(x,t)}{\partial t} = a_2 \frac{\partial^2 v}{\partial x^2} + f_2(x,t,u(x,t),u_t(x,\cdot),v(x,t),v_t(x,\cdot)), \end{cases}$$
(1)

where $0 \leqslant t \leqslant T$, $0 \leqslant x \leqslant X$ are independent variables, u(x,t), v(x,t) are desired functions, $u_t(x,\cdot) = \{u(x,t+s), \tau \leqslant s < 0\}$ and $v_t(x,\cdot) = \{v(x,t+s), \tau \leqslant s < 0\}$ are stories of desired functions by the time $t, \tau > 0$ is the value of delay, $a_1 > 0$, $a_2 > 0$.

Initial conditions are given

$$u(x,t) = \varphi(x,t), \quad 0 \leqslant x \leqslant X, \ -\tau \leqslant t \leqslant 0,$$

$$v(x,t) = \psi(x,t), \quad 0 \leqslant x \leqslant X, \ -\tau \leqslant t \leqslant 0.$$
(2)

Homogeneous boundary conditions of the second type (Neumann conditions) are also set

$$\frac{\partial u(x,t)}{\partial x}\Big|_{x=0} = 0, \quad \frac{\partial u(x,t)}{\partial x}\Big|_{x=X} = 0, \quad 0 < t \leqslant T,$$

$$\frac{\partial v(x,t)}{\partial x}\Big|_{x=0} = 0, \quad \frac{\partial v(x,t)}{\partial x}\Big|_{x=X} = 0, \quad 0 < t \leqslant T.$$
(3)

We introduce vector notation

$$U = \begin{pmatrix} u \\ v \end{pmatrix}, F = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, A = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix},$$

then the system (1) can be written as

$$\frac{\partial U(x,t)}{\partial t} = A \diamond \frac{\partial^2 U}{\partial x^2} + F(x,t,U(x,t),U_t(x,\cdot)),$$

where $A \diamond U$ denotes the vector with coordinates $\begin{pmatrix} a_1 u \\ a_2 v \end{pmatrix}$, if $A = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$.

1.2 Implicit method

Introduce the time step $\Delta = \frac{\tau}{M_0}$, where M_0 is a natural number and let $M = [\frac{T}{\Delta}]$. Introduce points $t_j = j\Delta$, $j = -M_0, \ldots, M$. Let us divide the segment [0, X] into parts with a step h = X/N, N is an integer, $N \geq 2$, by introducing the points $x_i = ih$, $i = 0, \ldots, N$. The approximation of the vector function $U(x_i, t_j)$ at the grid nodes will be denoted by the vector V_i^j with coordinates $\left(u_i^j, v_i^j\right)$.

Using the fictitious knot method, we construct an implicit numerical method

$$\left(1 + 2\frac{\Delta}{h^{2}}A\diamond\right)V_{0}^{m+1} - 2\frac{\Delta}{h^{2}}A\diamond V_{1}^{m+1} = V_{0}^{m} + \Delta F\left(x_{0}, t_{m+1}, V^{m}(t_{m+1})_{0}, V_{t_{m+1}}^{m}(\cdot)_{0}\right), (4)$$

$$-\frac{\Delta}{h^{2}}A\diamond V_{i-1}^{m+1} + \left(1 + 2\frac{\Delta}{h^{2}}A\diamond\right)V_{i}^{m+1} - \frac{\Delta}{h^{2}}A\diamond V_{i+1}^{m+1} =$$

$$= V_{i}^{m} + \Delta F\left(x_{i}, t_{m+1}, V^{m}(t_{m+1})_{i}, V_{t_{m+1}}^{m}(\cdot)_{i}\right), \qquad i = 1, \dots, N-1,$$

$$-2\frac{\Delta}{h^{2}}A\diamond V_{N-1}^{m+1} + \left(1 + 2\frac{\Delta}{h^{2}}A\diamond\right)V_{N}^{m+1} =$$

$$= V_{N}^{m} + \Delta F\left(x_{N}, t_{m+1}, V^{m}(t_{m+1})_{N}, V_{t_{m+1}}^{m}(\cdot)_{N}\right), \tag{6}$$

where $V_{t_{m+1}}^m(\cdot)_i$ is the result of piecewise constant interpolation with extrapolation by continuation at the point $t_m + \Delta$ [3].

The system (4)–(6) is two systems corresponding to the coordinates of the vector V, each of which has a tridiagonal structure with diagonal dominance equal to one. This implies the effective solvability of the system by the sweep method and the stability of the algorithm.

Theorem 1. If the exact solution of the problem (1)–(3) u(x,t), v(x,t) is four times continuously differentiable with respect to x and continuously differentiable with respect to t, then the error of the method (4)–(6) has order $h^2 + \Delta$.

The theorem is proved using the properties of a system with a tridiagonal matrix.

1.3 Crank-Nicholson method

We construct an analog of the Crank-Nicolson method

$$\left(1 + \frac{\Delta}{h^2} A \diamond\right) V_0^{m+1} - \frac{\Delta}{h^2} A \diamond V_1^{m+1} = \left(1 - \frac{\Delta}{h^2} A \diamond\right) V_0^m + \frac{\Delta}{h^2} A \diamond V_1^m + \\
+ \Delta F \left(x_0, t_{m+1/2}, V^m (t_{m+1/2})_0, V_{t_{m+1/2}}^m (\cdot)_0\right), \\
- \frac{\Delta}{2h^2} A \diamond V_{i-1}^{m+1} + \left(1 + \frac{\Delta}{h^2} A \diamond\right) V_i^{m+1} - \frac{\Delta}{2h^2} A \diamond V_{i+1}^{m+1} = \\
= \frac{\Delta}{2h^2} A \diamond V_{i-1}^m + \frac{\Delta}{2h^2} A \diamond V_{i+1}^m + \left(1 - \frac{\Delta}{h^2} A \diamond\right) V_i^m + \\
+ \Delta F \left(x_i, t_{m+1/2}, V^m (t_{m+1/2})_i, V_{t_{m+1/2}}^m (\cdot)_i\right), \ i = 1, \dots, N-1, \tag{8}$$

$$-\frac{\Delta}{h^2} A \diamond V_{N-1}^{m+1} + \left(1 + \frac{\Delta}{h^2} A \diamond\right) V_N^{m+1} = +\frac{\Delta}{h^2} A \diamond V_{N-1}^m + \left(1 - \frac{\Delta}{h^2} A \diamond\right) V_N^m + + \Delta F\left(x_N, t_{m+1/2}, V^m(t_{m+1/2})_N, V_{t_{m+1/2}}^m(\cdot)_N\right).$$
(9)

where $V_{t_{m+1/2}}^m(\cdot)_i$ is the result of piecewise linear interpolation with extrapolation by continuation at the point $t_m + \Delta/2$ [3].

Theorem 2. If the exact solution of the problem (1)–(3) u(x,t), v(x,t) is four times continuously differentiable with respect to x, twice continuously differentiable with respect to t and conditions $a_1 \frac{\Delta}{h^2} \leq 1$, $a_2 \frac{\Delta}{h^2} \leq 1$ are met, then the error of the method (7)–(9) has order $h^2 + \Delta^2$.

The theorem is proved using the properties of a system with a tridiagonal matrix.

The results of numerical experiments carried out on test examples and on model examples [1] confirm the theoretical results.

2 Superdiffusion-type equations

2.1 Problem definition

Let us consider a system of equations of the superdiffusion type with fractional Riesz derivatives with respect to space and with a functional delay of the form

$$\begin{cases}
\frac{\partial u(x,t)}{\partial t} = a_1 \frac{\partial^{\alpha} u}{\partial |x|^{\alpha}} + f_1(x,t,u(x,t),u_t(x,\cdot),v(x,t),v_t(x,\cdot)), \\
\frac{\partial v(x,t)}{\partial t} = a_2 \frac{\partial^{\alpha} v}{\partial |x|^{\alpha}} + f_2(x,t,u(x,t),u_t(x,\cdot),v(x,t),v_t(x,\cdot)),
\end{cases} (10)$$

where Riesz derivatives of order α (1 < α < 2) are defined by the relations

$$\frac{\partial^{\alpha} u}{\partial |x|^{\alpha}} = K \Big(\frac{\partial^{\alpha} u(x,t)}{\partial_{+} x^{\alpha}} + \frac{\partial^{\alpha} u(x,t)}{\partial_{-} x^{\alpha}} \Big), \quad K = -\frac{1}{2 \cos \alpha \frac{\pi}{2}},$$

where the left and right Riemann-Liouville partial derivatives of order α are defined respectively as

$$\frac{\partial^{\alpha} u(x,t)}{\partial_{+} x^{\alpha}} = \frac{1}{\Gamma(2-\alpha)} \frac{d^{2}}{dx^{2}} \int_{0}^{x} \frac{u(\xi,t)}{(x-\xi)^{\alpha-1}} d\xi, \quad \frac{\partial^{\alpha} u(x,t)}{\partial_{-} x^{\alpha}} = \frac{1}{\Gamma(2-\alpha)} \frac{d^{2}}{dx^{2}} \int_{x}^{X} \frac{u(\xi,t)}{(x-\xi)^{\alpha-1}} d\xi.$$

Derivatives $\frac{\partial^{\alpha} v}{\partial |x|^{\alpha}}$, $\frac{\partial^{\alpha} v(x,t)}{\partial_{+}x^{\alpha}}$ and $\frac{\partial^{\alpha} v(x,t)}{\partial_{-}x^{\alpha}}$ are defined similarly.

Initial conditions (2) and boundary conditions (3) are given.

The system (10) can be written as

$$\frac{\partial U(x,t)}{\partial t} = A \diamond \frac{\partial^{\alpha} U}{\partial |x|^{\alpha}} + F(x,t,U(x,t),U_t(x,\cdot)), \tag{11}$$

2.2 Crank-Nicholson method

Let us discretize and interpolate in the same way as for diffusion equations.

To approximate the left and right fractional Riemann-Liouville derivatives, we will use the shifted Grunwald formulas [5]

$$\frac{\partial^{\alpha} U(x_i, t_j)}{\partial_{+} x^{\alpha}} = \frac{1}{h^{\alpha}} \sum_{k=0}^{i+1} g_{\alpha, k} U(x_{i-k+1}, t_j) + R_i^j, \tag{12}$$

$$\frac{\partial^{\alpha} U(x_i, t_j)}{\partial_{-} x^{\alpha}} = \frac{1}{h^{\alpha}} \sum_{k=0}^{N-i+1} g_{\alpha, k} U(x_{i+k-1}, t_j) + Q_i^j, \tag{13}$$

where the normalized weights are defined as

$$g_{\alpha,0} = 1$$
, $g_{\alpha,k} = (-1)^k \frac{(\alpha)(\alpha - 1)\dots(\alpha - k + 1)}{k!}$, $k = 1, 2, 3, \dots$

If the exact solution U(x,t) is four times continuously differentiable with respect to x, then

$$||R_i^j|| \leqslant Ch^{\alpha}, ||Q_i^j|| \leqslant Ch^{\alpha}.$$

From (12)–(13) for the Riesz derivative we get the representation

$$\frac{\partial^{\alpha} U(x_i, t_j)}{\partial_{|x|}^{\alpha}} = \frac{K}{h^{\alpha}} \left(\sum_{k=0}^{i+1} g_{\alpha, k} U(x_{i-k+1}, t_j) + \sum_{k=0}^{N-i+1} g_{\alpha, k} U(x_{i+k-1}, t_j) \right) + P_i^j. \tag{14}$$

If the exact solution U(x,t) is four times continuously differentiable with respect to x, then

$$||P_i^j|| \leqslant Ch^{\alpha}.$$

Let us discretize (11) at the nodes $(x_i, t_{m+1/2})$, applying a two-site approximation to the middle for the time derivative, using the shifted formulas (14) for the Riesz derivative with respect to space on the m-th and m+1-th time layers and using piecewise linear interpolation (with extrapolation by half a step) of the prehistory of the discrete model, we obtain an analog of the Crank-Nicolson scheme

$$\frac{V_i^{m+1} - V_i^m}{\Delta} = A \diamond \frac{K}{2h^{\alpha}} \left(\sum_{s=0}^{i+1} g_{\alpha,s} V_{i-s+1}^m + \sum_{s=0}^{i+1} g_{\alpha,s} V_{i-s+1}^{m+1} + \sum_{s=0}^{N-i+1} g_{\alpha,s} V_{i+s-1}^m + \sum_{s=0}^{N-i+1} g_{\alpha,s} V_{i+s-1}^m \right) + F_i^{m+1/2},$$
(15)

$$F_i^{m+1/2} = F\left(x_i, t_m + \Delta/2, V^m(t_{m+1/2})_i, V^m_{t_{m+1/2}}(\cdot)_i\right), i = 1, \dots, N-1, m = 0, \dots, M-1,$$

where $V^m(t_{m+1/2})_i$ is the result of piecewise linear interpolation with extrapolation by continuation at the point $t_m + \Delta/2$, $V^m_{t_{m+1/2}}(\cdot)_i$ is the history of interpolation with extrapolation at this point.

Using the formulas for numerical differentiation by the boundary and the Neumann boundary conditions (3), we supplement the scheme (15) with the equalities

$$V_0^{m+1} = V_1^{m+1}, \quad V_N^{m+1} = V_{N-1}^{m+1}, \quad V_0^m = V_1^m, \quad V_N^m = V_{N-1}^m,$$

then the scheme (15) will take the form

$$\frac{V_i^{m+1} - V_i^m}{\Delta} = A \diamond \frac{K}{2h^{\alpha}} \left(\sum_{s=0}^i g_{\alpha,s} V_{i-s+1}^m + g_{\alpha,i+1} V_1^m + \sum_{s=0}^i g_{\alpha,s} V_{i-s+1}^{m+1} + g_{\alpha,i+1} V_1^{m+1} + \sum_{s=0}^{N-i} g_{\alpha,s} V_{i+s-1}^m + g_{\alpha,N-i+1} V_{N-1}^m + \sum_{s=0}^{N-i} g_{\alpha,s} V_{i+s-1}^{m+1} + g_{\alpha,N-i+1} V_{N-1}^{m+1} \right) + F_i^{m+1/2}, \quad i = 1, \dots, N-1, m = 0, \dots, M-1.$$
(16)

Scheme (16) is completed with initial conditions from (2)

$$V_i^j = \begin{pmatrix} u_i^j = \varphi(x_i, t_j) \\ v_i^j = \psi(x_i, t_j) \end{pmatrix}, \quad i = 0, \dots, N, j = -M_0, \dots, 0.$$
 (17)

The scheme (16) represents, for each fixed m, two systems of linear algebraic equations of order N-1.

Theorem 3. If the exact solution of the problem (10), (2), (3) u(x,t), v(x,t) is four times continuously differentiable with respect to x and twice continuously differentiable with respect to t, then the error of the method (16), (17) has order $h + \Delta^2$.

The theorem is proved by embedding the method in the general scheme similarly [4]. In this case, stability is proved using the Greschgorin theorem [5].

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Received by the editors June 1, 2022 The work is supported by the Russian Science Foundation, project 22-21-00075.

Пименов В. Г., Ложников А. Б., Ибрагим М. Численные методы для систем диффузионных и супердиффузионных уравнений с краевыми условиями Неймана и с запаздыванием. Дальневосточный математический журнал. 2022. Т. 22. № 2. С. 218–224.

RИЦАТОННА

Особенностями многих математических моделей (например, в модели взаимодействия опухоли и иммунной системы) является наличие двух уравнений диффузионного типа с краевыми условиями Неймана и эффекта запаздывания. В статье сконструированы и исследованы порядки сходимости аналогов неявного метода и метода Кранка – Никольсон. Также для системы дробных по пространству уравнений супердиффузионного типа с запаздыванием и краевыми условиями Неймана построен аналог метода Кранка – Никольсон. Для аппроксимации двухсторонних дробных производных Рисса применены сдвинутые формулы Грюнвальда – Летникова, для учета эффекта запаздывания применены интерполяция и экстраполяция дискретной предыстории модели.

Ключевые слова: *системы диффузионных уравнений, условия Неймана,* запаздывание, супердиффузия, метод Кранка – Никольсон.