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Algorithms for Numerical Solving of 2D Anomalous Diffusion Problems

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Abstract. Fractional analog of the reaction diffusion equation is used to model the subdiffusion process. Diffusion equation with fractional Riemann–Liouville operator is analyzed in this paper. We offer finite-difference methods that can be used to solve the initial-boundary value problems for some time-fractional order differential equations. Stability and convergence theorems are proved.

Keywords: subdiffusion process, fractional order differential equation.

AMS Subject Classification: 65N06; 65N12; 65Z05; 92C10; 92C05.

1 Introduction

Cell membrane is a complicated heterogeneous dynamic bio-structure that can be considered as fractal media. Here a lateral raft diffusion is not classic Brownian motion [7]. Such physical processes as the diffusion in the fractal media lead to various types of "anomalies" like jump (hop), fractional, sub- and superdiffusion. These processes are well described by the fractional order partial differential equations [14]. Time-space fractional diffusion equations extend the classical model, substituting fractional derivatives for their integer-order analog.

Some models of reversible reaction in subdiffusive regime are constructed using fractional reaction diffusion equation [4]

$$\partial_t u(x,t) = {}_0D_t^{1-\gamma}\big(k(x)\nabla^2 u(x,t)\big) + f(x,t), \quad 0<\gamma<1. \tag{1.1}$$

Physical interpretation was presented by [3, 4, 11, 20]. In this framework some authors investigated the front reaction in biomolecular reactions [7].

In papers [1, 15] authors suggested to use a well-known factorization method as a numerical method for solving the Dirichlet problem of anomalous diffusion equation. Estimation of fractional order shifted mixed derivatives was adapted, in order to construct a factorization numerical model using the general theory of the finite difference schemes [16].

We also mention interesting applications of fractional time derivatives to formulate the exact and approximate discrete transparent boundary conditions for solution of Schrōdinger type problems [5, 6].

In present paper we consider two approaches how to solve numerically the 2D fractional partial differential equations. These approaches are based on the construction of finite difference schemes and the application of Grunwald–Letnikov formula and L_1-approximation for time fractional derivative. Analytical solution for considered problems can be obtained only for some special cases. Moreover, the number of the published papers, that are devoted to this theme, is limited. This fact is our motivation to investigate the modifications of multilayer difference schemes for this class of problems.

2 Statement of the Problem

In the present paper, we investigate numerical methods to solve initial-boundary value problems for equation (1.1).

Let us define continuous function $u(x,t)$ in cylinder $Q_T = \overline{G} \times [0 \le t \le T]$, where $\overline{G} = G \cup \Gamma$ is two dimensional domain with boundary Γ and $x = (x_1, x_2)$ satisfies the following equation

$$\frac{\partial u}{\partial t} = {}_0D_t^{1-\gamma}\left(\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2}\right) + r(x,t), \quad x \in G,\ t > 0, \tag{2.1}$$

and special conditions

$$u(x,0) = u_0(x), \quad x \in \overline{G}, \qquad u(x,t) = \mu(x,t), \quad x \in \Gamma,\ t \ge 0. \tag{2.2}$$

Here ${}_0D_t^{1-\gamma}$ denotes the fractional Riemann–Liouville operator that is defined by

$$ {}_0D_t^{1-\gamma} v(t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t \frac{v(s)}{(t-s)^\gamma}\, ds,$$

where $0 < \gamma < 1$ and $\Gamma(\cdot)$ is the Gamma function [9]. Let the problem (2.1), (2.2) has a unique and sufficiently smooth solution. Riemann–Liouville fractional derivative is considered in the class of a function, that is continuous across the segment $[0,T]$. Also, these functions have derivatives at this segment till $|\gamma|$-order and exist almost everywhere [9, 12]. We assume that fractional γ-order derivative of the function $r(x,t)$ across the value t in initial time $t = 0$ exists. Here $r(x,t) = \frac{a(x)t^{\gamma-2}}{\Gamma(\gamma-1)}$ and $a(x)$ is given function at point x.

According to [10, 12, 13], we obtain

$$ {}_0D_t^{1-\gamma}\left[{}_0D_t^{\gamma} u(x,t) - \frac{u(x,0)t^{-\gamma}}{\Gamma(1-\gamma)}\right] = {}_0D_t^{1-\gamma} \nabla^2 u(x,t).$$

Then the equivalent form of the equation (2.1) is

$$ {}_0D_t^{\gamma} u(x,t) - \frac{u(x,0)t^{-\gamma}}{\Gamma(1-\gamma)} = Lu(x,t),$$

where $L = \sum_{m=1}^2 \partial^2/\partial x_m^2$.

3 Difference Schemes

Let us introduce the discrete-time domain $\overline{w}_\tau = \{t_j = j\tau,\ j = 0,\dots,M;\ M\tau = T\}$ and the discrete-space domain $\overline{w}_h = \{x_i = (i_1h_1, i_2h_2),\ i_\alpha = 0,1,\dots,N_\alpha,\ h_\alpha = l_\alpha/N_\alpha\}$. We use the following notation [16, 17]

$$y^{(\pm 1_\alpha)} = y\bigl(x_i^{(\pm 1_\alpha)}, t\bigr), \qquad x^{\pm 1_\alpha} = x_\alpha^{1_\alpha} \pm h_\alpha, \qquad x_\alpha^{i_\alpha} = h_\alpha i_\alpha, \quad \alpha = \overline{1,2},$$

here y is the value of the function $y(x,t)$ in the fixed node $x = (i_1h_1, i_2h_2)$. For numerical approximation of Lu we use the second difference derivative along any space direction

$$\Lambda u = \sum_{\alpha=1}^{2} \Lambda_\alpha u, \Lambda_\alpha u = u_{\overline{x}_\alpha x_\alpha} = \frac{u^{(+1_\alpha)} - 2u + u^{(-1_\alpha)}}{h_\alpha^2} + O\bigl(h_\alpha^2\bigr) \sim \frac{\partial^2 u}{\partial x_\alpha^2}(x, t_j). \tag{3.1}$$

Time-derivative is approximated by the finite difference operator that is obtained from the Grunwald–Letnikov formula and L_1-approximation [9, 10]. Therefore we have

$${}_0D_t^\gamma u(x,t_j) - \frac{u(x,0)t_j^{-\gamma}}{\Gamma(1-\gamma)} \sim u_t^{(\gamma)} + O(\tau), \tag{3.2}$$

$${}_0D_t^\gamma u(x,t_j) - \frac{u(x,0)t_j^{-\gamma}}{\Gamma(1-\gamma)} \sim \widetilde{u}_t^{(\gamma)} + O\bigl(\tau^{2-\gamma}\bigr), \tag{3.3}$$

where

$$u_t^{(\gamma)} = \tau^{-\gamma} \sum_{k=0}^{j} g_{\gamma,k}\bigl[u^{j-k} - u^0\bigr], \quad g_{\gamma,k} = (-1)^k \binom{\gamma}{k},$$

$$\widetilde{u}_t^{(\gamma)} = \frac{\tau^{-\gamma}}{\Gamma(2-\gamma)} \left[u^j - \sum_{k=1}^{j-1} (a_{\gamma,j-k-1} - a_{\gamma,j-k}) u^k - a_{\gamma,j-1} u^0 \right],$$

$$a_{\gamma,k} = (k+1)^{1-\gamma} - k^{1-\gamma}.$$

Modified difference schemes on the basis of the approximations (3.1) and (3.2) have the following form

$$y_t^\gamma = \Lambda\bigl(\sigma y^j + (1-\sigma) y^{j-1}\bigr), \tag{3.4}$$

$$y^0 = u_0(x), \quad x \in \overline{w}_h, \tag{3.5}$$

$$y^j\big|_{\gamma^*} = \mu(x,t), \quad x \in \gamma^*,\ t \ge 0 \tag{3.6}$$

and on the basis of the approximations (3.1) and (3.3)

$$\widetilde{y}_t^\gamma = \Lambda\bigl(\sigma y^j + (1-\sigma) y^{j-1}\bigr), \tag{3.7}$$

$$y^0 = u_0(x), \quad x \in \overline{w}_h, \tag{3.8}$$

$$y^j\big|_{\gamma^*} = \mu(x,t), \quad x \in \gamma^*,\ t \ge 0. \tag{3.9}$$

Here γ^* is a set of the nodes that belong to Γ, $0 \le \sigma \le 1$.

4 Consistency and Stability

The conditional stability of the explicit scheme (3.4)–(3.6) as $0 \leq \sigma < 1$ is obtained in [2] and the following theorem holds:

Theorem 1. *Suppose that the condition* $\tau^\gamma \leq \frac{\gamma}{2(1-\sigma)}[\sum_{\alpha=1}^{2} h_\alpha^{-2}]^{-1}$ *is valid, then the finite-difference scheme* (3.4)–(3.6) *is stable.*

The stability and consistency of the difference scheme are proved in [18] for (3.7)–(3.9) as $0 < \sigma < 1$. This proof is based on the maximum principle and the realization of the following condition

$$\tau^\gamma < \frac{2 - 2^{1-\gamma}}{2\Gamma(2-\gamma)(1-\gamma)} \left(\sum_{k=1}^{2} \frac{1}{h_k^2} \right)^{-1}.$$

For difference functions we define the scalar product and the norm in the following way

$$(v, w) = \sum_{x \in w_h} v(x) w(x) h_1 h_2, \qquad \|v\| = \sqrt{(v, v)}.$$

According to [16], we have

$$(\Lambda_\alpha z, z) = -(z_{\overline{x}_\alpha}, z_{\overline{x}_\alpha}]_\alpha.$$

where $z = 0$ as $x \in \gamma_h^*$ and

$$\sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2-1} v(i_1 h_1, i_2 h_2) w(i_1 h_1, i_2 h_2) h_1 h_2 := (v, w]_1,$$

$$\sum_{i_1=1}^{N_1-1} \sum_{i_2=1}^{N_2} v(i_1 h_1, i_2 h_2) w(i_1 h_1, i_2 h_2) h_1 h_2 := (v, w]_2.$$

Lemma 1. *The implicit scheme* (3.4)–(3.6) *is unconditionally stable for* $\sigma = 1$.

Proof. Let ρ^0 is a perturbation solution. Then the corresponding error of (3.4) as $\sigma = 1$ is defined by the following equation

$$\tau^{-\gamma} \Big[\rho^j + \sum_{k=1}^{j-1} g_{\gamma,k} \rho^{j-k} - \sum_{k=0}^{j-1} g_{\gamma,k} \rho^0 \Big] = \Lambda \rho^j.$$

Here $i_1 = 1, 2, \ldots, N_1 - 1$, $i_2 = 1, 2, \ldots, N_2 - 1$ and $\rho^j|_{\gamma_h^*} = 0$ for all $j \in N$. Multiplying (4.1) by $\tau^\gamma h_1 h_2 \rho^j$ and summing over $i_1 = \overline{1, N_1 - 1}$, $i_2 = \overline{1, N_2 - 1}$, we have

$$\|\rho^j\|^2 = -\Big(\sum_{k=1}^{j-1} g_{\gamma,k} \rho^{j-k}, \rho^j \Big) + \Big(\sum_{k=0}^{j-1} g_{\gamma,k} \rho^0, \rho^j \Big) + \tau^\gamma (\Lambda \rho^j, \rho^j). \qquad (4.1)$$

We remind some important properties of binomial coefficients [2, 8, 9]

$$g_{\gamma,k} = \Big(1 - \frac{1+\gamma}{k}\Big) g_{\gamma,k-1}, \quad g_{\gamma,0} = 1, \quad g_{\gamma,1} = -\gamma,$$
$$g_{\gamma,2} = \frac{\gamma(\gamma-1)}{2!}, \quad g_{\gamma,3} = -\frac{\gamma(\gamma-1)(\gamma-2)}{3!}, \quad \sum_{k=0}^{+\infty} g_{\gamma,k} = 0,$$
$$\text{as } k = 1,2,\dots, \quad g_{\gamma,k} < 0, \quad \sum_{k=0}^{j-1} g_{\gamma,k} > 0, \quad (0 < \gamma < 1).$$

They give us the following estimates according to (4.1)

$$-\Big(\sum_{k=1}^{j-1} g_{\gamma,k}\rho^{j-k}, \rho^j\Big) \le -\frac{1}{2}\sum_{k=1}^{j-1} g_{\gamma,k}\|\rho^{j-k}\|^2 - \frac{1}{2}\sum_{k=1}^{j-1} g_{\gamma,k}\|\rho^j\|^2,$$
$$\Big(\sum_{k=0}^{j-1} g_{\gamma,k}\rho^0, \rho^j\Big) \le \frac{1}{2}\sum_{k=0}^{j-1} g_{\gamma,k}\big(\|\rho^0\|^2 + \|\rho^j\|^2\big),$$
$$\tau^\gamma\big(\Lambda\rho^j, \rho^j\big) = -\tau^\gamma\sum_{\alpha=1}^{2}\|\rho^j_{\overline{x}_\alpha}\|_\alpha^2 \le -\tau^\gamma\Big(\frac{8}{l_1^2} + \frac{8}{l_2^2}\Big)\|\rho^j\|^2 \le 0. \quad (4.2)$$

Using the obtained estimates, (4.1) and (4.2), we have

$$\|\rho^j\|^2 \le \sum_{k=0}^{j-1} g_{\gamma,k}\|\rho^0\|^2 - \sum_{k=1}^{j-1} g_{\gamma,k}\|\rho^{j-k}\|^2.$$

Let $j = 1$ and $\|\rho^1\|^2 \le \|\rho^0\|^2$. Then according to mathematical induction the estimate

$$\|\rho^j\|^2 \le \sum_{k=0}^{j-1} g_{\gamma,k}\|\rho^0\|^2 - \sum_{k=1}^{j-1} g_{\gamma,k}\|\rho^{j-k}\|^2 \le \sum_{k=0}^{j-1} g_{\gamma,k}\|\rho^0\|^2 - \sum_{k=1}^{j-1} g_{\gamma,k}\|\rho^0\|^2$$

is valid. Thus we obtain $\|\rho^j\|^2 \le \|\rho^0\|^2$, $\forall j \in N$. □

Theorem 2. *The scheme* (3.4)–(3.6) *approximates the problem* (2.1) *and* (2.2), *it is stable and the following accuracy estimate is valid:*

$$\|z(x^j)\| = \|u(x,t_j) - y(x,t_j)\| \le M\big(\tau + h_1^2 + h_2^2\big), \quad M > 0.$$

Proof. We get the expression that is similar to (4.2). Moreover, this expression contains $\tau^\gamma(\psi^j, z^j)$, $|\psi^j| \le M_1(\tau + \sum_{\alpha=1}^2 h_\alpha^2)$ where $M_1 > 0$ is constant. To estimate the obtained equality we use ε-inequality in the following form

$$\tau^\gamma\big(\psi^j, z^j\big) \le \frac{1}{4\varepsilon}\tau^\gamma\|\psi^j\|^2 + \varepsilon\tau^\gamma z^j.$$

Let $\varepsilon = (-\sum_{k=j}^{\infty} g_{\gamma,k})(2\tau^\gamma)^{-1}$. Then according to the inequality [18]

$$-\sum_{k=j}^{\infty} g_{\gamma,k} > \frac{1}{j^\gamma\Gamma(1-\gamma)},$$

we can define

$$\frac{1}{4\varepsilon}\tau^{\gamma}\|\psi^j\|^2 = \frac{\tau^{2\gamma}}{-2\sum_{k=j}^{\infty} g_{\gamma,k}}\|\psi^j\|^2 \le \frac{\tau^{2\gamma} j^{\gamma}\Gamma(1-\gamma)}{2}\|\psi^j\|^2$$

$$\le \frac{T^{\gamma}\tau^{\gamma}\Gamma(1-\gamma)}{2} l_1 l_2 M_1\Big(\tau+\sum_{\alpha=1}^{2} h_\alpha\Big)^2 = \frac{M_2}{2}\tau^{\gamma}\Big(\tau+\sum_{\alpha=1}^{2} h_\alpha^2\Big)^2, \tag{4.3}$$

$$\varepsilon\tau^{\gamma}\|z^j\|^2 = \frac{-\sum_{k=j}^{\infty} g_{\gamma,k}}{2}\|z^j\|^2.$$

Thus we obtain the estimate

$$\|z^j\|^2 \le -\sum_{k=1}^{j-1} g_{\gamma,k}\|z^{j-k}\|^2 + M_2\tau^{\gamma}\Big(\tau+\sum_{\alpha=1}^{2} h_\alpha^2\Big)^2. \tag{4.4}$$

By (4.4), we get that $\sum_{k=0}^{j-1} g_{\gamma,k} = -\sum_{k=j}^{\infty} g_{\gamma,k}$, and the mathematical induction proves that

$$\|z^j\|^2 \le M_2\Big(-\sum_{k=j}^{\infty} g_{\gamma,k}\Big)^{-1}\tau^{\gamma}\Big(\tau+\sum_{\alpha=1}^{2} h_\alpha^2\Big)^2, \quad \forall j \in N.$$

Using the estimates (4.3), (4.4), we get

$$\|z^j\|^2 \le M_2 j^{\gamma}\Gamma(1-\gamma)\tau^{\gamma}\Big(\tau+\sum_{\alpha=1}^{2} h_\alpha\Big)^2 \le C_2 T^{\gamma}\Gamma(1-\gamma)\Big(\tau+\sum_{\alpha=1}^{2} h_\alpha^2\Big)^2$$

$$= M^2\Big(\tau+\sum_{\alpha=1}^{2} h_\alpha^2\Big)^2.$$

The theorem is proved. □

In analogous way we can prove the following theorem:

Theorem 3. *Difference scheme* (3.7)–(3.9) *is stable under the initial data in the norm* $\|\cdot\| = \sqrt{(\cdot,\cdot)}$ *and for the solution of this scheme the following estimate*

$$\|z^j\| \le M\Big(\tau^{2-\gamma}+\sum_{\alpha=1}^{2} h_\alpha^2\Big), \quad M > 0 \tag{4.5}$$

is satisfied for $\sigma = 1$.

Proof. We limit the proof of Theorem 3 to the part, that includes the essential addition to Theorem 2. Multiplying the perturbed solution of (3.7), (3.9) by $\tau^{\gamma}\Gamma(2-\gamma) = A$ we get the following equation

$$(\rho^j,\rho^j) = \Big(\sum_{k=1}^{j-1}(a_{\gamma,j-k-1}-a_{\gamma,j-k})\rho^k, \rho^j\Big) + a_{\gamma,j-1}(\rho^0,\rho^j) + A(\Lambda\rho^j,\rho^j).$$

Since $a_{\gamma,m} > a_{\gamma,m+1}$ $(m = 0, 1, \ldots)$, it follows that

$$\Bigl(\sum_{k=1}^{j-1}(a_{\gamma,j-k-1} - a_{\gamma,j-k})\rho^k, \rho^j\Bigr)$$
$$\le \frac{1}{2}\sum_{k=1}^{j-1}(a_{\gamma,j-k-1} - a_{\gamma,j-k})\|\rho^k\|^2 + \frac{1}{2}\sum_{k=1}^{j-1}(a_{\gamma,j-k-1} - a_{\gamma,j-k})\|\rho^j\|^2$$
$$= \frac{1}{2}\sum_{k=1}^{j-1}(a_{\gamma,j-k-1} - a_{\gamma,j-k})\|\rho^k\|^2 + \frac{1}{2}(a_{\gamma,0} - a_{\gamma,j-1})\|\rho^j\|,$$
$$a_{\gamma,j-1}(\rho^0, \rho^j) \le \frac{1}{2}a_{\gamma,j-1}(\|\rho^0\|^2 + \|\rho^j\|^2).$$

We obviously have $\|\rho^1\|^2 \le \|\rho^0\|^2$ at $j = 0$. From here we obtain

$$\|\rho^{j+1}\|^2 \le \sum_{k=1}^{j-1}(a_{\gamma,j-k-1} - a_{\gamma,j-k})\|\rho^k\|^2 + a_{\gamma,j-1}\|\rho^0\|^2. \tag{4.6}$$

Using the recurrent calculus from (4.6), we get

$$\|\rho^{j+1}\|^2 \le \sum_{k=1}^{j-1}(a_{\gamma,j-k-1} - a_{\gamma,j-k})\|\rho^k\|^2 + a_{\gamma,j-1}\|\rho^0\|^2$$
$$\le \sum_{k=1}^{j-1}(a_{\gamma,j-k-1} - a_{\gamma,j-k})\|\rho^0\|^2 + a_{\gamma,j-1}\|\rho^0\|^2$$
$$= (1 - a_{\gamma,j-1})\|\rho^0\|^2 + a_{\gamma,j-1}\|\rho^0\|^2 = \|\rho^0\|^2.$$

The theorem is proved. □

The error of the observed method is defined by the following estimate

$$\|z^j\|^2 \le a_{\gamma,j-1}^{-1}M_2\tau^\gamma(\tau^{2-\gamma} + h^2)^2, \quad \forall j \in N,$$

where M_2 is constant. Since $a_{\gamma,j-1} > \frac{1-\gamma}{(j)^\gamma}$, $\forall j \in N$, we see that

$$\|z^j\|^2 \le \frac{M_2T^\gamma}{1-\gamma}(\tau^{2-\gamma} + h^2)^2.$$

Using $M = \bigl(M_2T^\gamma/(1-\gamma)\bigr)^{\frac{1}{2}}$, we obtain the estimate (4.5).

Remark. In the case when the approximation has the second order with respect to spatial variables, coefficients $k_\alpha(x) \ne const$ and the convection term $-{}_0D_t^{1-\gamma}(\sum_{\alpha=1}^{2} v_\alpha(x)\frac{\partial u}{\partial x_\alpha})$ is presented in the model, all obtained results are still valid. Modificated schemes (3.4)–(3.6), (3.7)–(3.9) are closely related to n-layer finite–difference schemes [16] and its solution can be expressed via the solution of the system of equations, that contain the operator matrix $(c_{ij}) = c$. The size of this matrix is $m \times m$, $(m = 1)$. Therefore, using the concept of compound schemes with m period, we can construct a local additive scheme for the considered class of problems [16]. These FDS allow us to take into account the memory effect of the considered system [19].

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