Statistical Modeling of Diffusion Processes with a Fractal Structure

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Abstract. A discrete continuous-time random walk model for non-Markov diffuse processes with fractal structure is presented. On the basis of the apparatus of integro-differentiation of fractional order, finite-difference approximations of diffuse models of fractional order are obtained taking into account the effects of memory and self-organization A modification of the statistical modeling method (Monte Carlo method) was carried out and an algorithm for its implementation was constructed to study the diffusion process of fractional order in time.

Keywords: non-integer integro-differentiation apparatus, fractal structures, diffusion processes, statistical modeling method, discrete model.

1 Introduction

Today, the fractional intero-differential apparatus is well developed and is used to explain and simulate complex systems in nature. The development of the idea of using the fractional integro-differential apparatus to model complex systems is handled by many scientific schools in the world that are associated with the names: F. Mainardi [8], I. Podlubny [5], S. Samko, A. Kilbas [9], V. Uchajkin [1] and others. Such special attention and interest in using non-integer integro-differentiation is ex- plained by the fact that the mathematical apparatus of differentiation and fractional- order integration allows modeling of various processes and systems, which are char- acterized by the effects of memory, spatial nonlocality and self-organization. A particular advantage of fractional-differential models, as opposed to integer ones, is the ability to describe and explore more accurately real-world models with the above characteristics and effects. Fractal integro-differential parameters have been success- fully applied in the fields such as physics, biology, chemistry and biochemistry, hydrology, medicine, technology, finance. Fractional-order differential equations describe the evolution of physical systems with residual memory, which occupy an intermediate position between Markov systems and systems that are characterized by total memory. In particular, the fractionality index indicates the proportion of states of the system that persist throughout the entire process of its functioning.

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It is believed that the presence of a fractional derivative with time in equations is interpreted as a reflection of a special property of the process - memory (eridarity), and in the case of a stochastic process - non-Markovian behavior. Fractional spatial derivatives reflect the self-similar heterogeneity of the structure or the medium in which the process develops. Such structures are called fractal [5]. The use of fractional order differential equation apparatus is important for studying the processes of anomalous diffusion in the study of anomalous properties of complex-structured inhomogeneous structures. Such structures have significant effects on memory and spatial nonlocality.

2 Analysis of Research

Abnormal diffusion processes $< X^2(\tau) >\sim 2K_\alpha \tau^\alpha / \Gamma(1+\alpha)$ are characterized by a departure from the linear law $< X^2(\tau) >\sim K_\alpha \tau$ of mean-square displacement and the presence of the fractional index α depending on the time τ, where K_1, K_α - are the usual diffusion coefficients of the dimension $cm^2 * \sec^{-1}$ and the generalized diffusion coefficient $cm^2 * \sec^{-\alpha}$, $\Gamma()$ is Gamma-function.

The fractional index $\alpha \neq 1$ characterizes various modes of diffusion processes: $0 < \alpha < 1$ a slow diffuse process, $1 < \alpha < 2$ an accelerated diffuse process. The case $\alpha = 2$ is described by the wave equation. This approach describes the so-called non-Gaussian processes in dynamic systems.

They are characterized by the presence of correlation dependencies for arbitrarily large space-time scales. According to [10, 11], a differential apparatus based on fractional-order derivatives can be used to model anomalous diffusion processes, or direct modeling of the dynamics of particles and their collisions in the system.

Fractional-order differential equations are characterized by strong nonlocality and spatial correlation and are based on both spatial and evolutionary fractional differential operators. A characteristic feature of fractional operators of differentiation and integration is the absence of an explicit physical and geometric interpretation of such operations [1, 9, 16]. There are several approaches to solving this problem, which can conditionally be divided into three directions: probabilistic, geometric and physical [18, 19].

The presence of different approaches to the determination of fractional derivatives give rise to ambiguity regarding the correctness and physical meaningfulness of the formulation of initial and boundary conditions depending on the type of fractional derivative [5, 7, 16].

It is also important that the fractional derivatives and integrals included in the integro-differential equations and describe a certain process can be used in the sense of the Riemann-Liouville, Caputo, Wright, Weil, Grunwald-Letnikov, Marcho derivatives. At present, to solve fractional-order differential equations, both analytical [20, 21, 22] and numerical methods are used [2, 3, 6, 23, 24, 25].

In the works [4, 20, 21, 22], found are analytical solutions to heat conduction problems with boundary conditions of the first kind containing derivatives of fractional order with time and spatial variable. In particular, one-dimensional cases of problems for an infinite straight line, a semi-bounded straight line, and problems without initial conditions are considered. Relaxation processes at the phase boundary are of complex nature, which leads to nonlinear and nonlocal heat-transfer processes. However, one of the analytical methods used to solve fractional-differential equations is the Laplace transformation method [19, 22].

Analytical solutions of boundary- value problems with fractional derivatives often have considerable difficulties; therefore, numerical methods are more efficient and easier to apply. The theory of numerical methods for solving differential equations in fractional partial derivatives is fragmentary and far from being complete [26, 27]. That is why a considerable number of works is devoted to finding optimal numerical methods.

3 Formulation of Problems

The fractional-order differential equation takes the form:

$$\frac{\partial^{\alpha} u(x,\tau)}{\partial \tau^{\alpha}} = K_{\alpha} \frac{\partial^{\beta} u(x,\tau)}{\partial x^{\beta}} \tag{1}$$

where $u(x,\tau)$ - function of diffusion in the region $\Delta = \{(x,\tau): 0 \le x \le L, 0 \le \tau \le T\}$.

Note that the diffusion equation (1) with a fractional-order differential operator is associated with a random walk process with continuous time if the asymptotic behavior of the $\omega(\tau)$ - density of the waiting time is determined by the relation [1, 10]:

$$\omega(\tau) \approx \frac{\tau^{\alpha}}{\tau^{\alpha+1}}, 0 < \alpha < 1$$

According to [12, 16], the Laplace transformation for $\omega(s) = \exp(-s^{\alpha}\tau^{\alpha}) \approx 1-(s\tau)^{\alpha}$ is characterized by asymptotics, while for $0 < \alpha < 1$, the function $\omega(\tau)$ in such Laplace transformation corresponds to the conditions of distribution density. The types of some functions $\omega_{\alpha}(\tau)$ are given in [16]. In particular, $\omega(\tau)$ can be selected in the form of Mitag-Leffler functions for which the Laplace transformation has the abovegiven form.

By applying the Laplace transformation with respect to the time variable and the Fourier transformation for the spatial variable, one can obtain the fractional-order diffusion equation with the fractional Kaputo differentiation operator [5].

The differential fractional-order operators in equation (1) are defined by Riemann-Liouville formulas:

$$\frac{\partial^{\alpha} u(x,\tau)}{\partial \tau^{\alpha}} = \frac{1}{\Gamma([\alpha]+1-\alpha)} \frac{d^{[\alpha]+1}}{d\tau^{[\alpha]+1}} \int_{-\infty}^{t} (t-\tau)^{[\alpha]-\alpha} u(x,t)dt \tag{2}$$

$$\frac{\partial_+^{\beta} u(x,\tau)}{\partial x^{\beta}} = \frac{1}{\Gamma([\beta]+1-\beta)} \frac{d^{[\beta]+1}}{dx^{[\beta]+1}} \int_{-\infty}^{x} (x-t)^{[\beta]-\beta} u(\tau,t)dt \qquad (3)$$

$$\frac{\partial_-^{\beta} u(x,\tau)}{\partial x^{\beta}} = \frac{(-1)^{[\beta]+1}}{\Gamma([\beta]+1-\beta)} \frac{d^{[\beta]+1}}{dx^{[\beta]+1}} \int_{x}^{+\infty} (t-x)^{[\beta]-\beta} u(\tau,t)dt\,, \qquad (4)$$

where $\Gamma()$ - is Gamma function, $[\ ]$ - is an integer part.

It is known that analytical methods of implementing differential equations with fractional-order derivatives encounter great difficulties. Therefore, only for some cases, exact solutions of equation (1) were obtained mainly with boundary conditions of the first kind.

Finite-difference methods are used to obtain the numerical solution. They are based on the approximation of fractional derivatives using the Grunwald-Letnikov formulas. Such fractional derivatives are a direct generalization in terms of finite differences and are determined by the dependencies for function $u(x,\tau)$ on the interval $[a,b]$

$$\frac{\partial^{\alpha} u(x)}{\partial x^{\alpha}} = \lim_{h\to 0} \frac{\Delta_h^{\alpha} u(x)}{h^{\alpha}} = \lim_{h\to 0} \frac{1}{h^{\alpha}} \sum_{k=0}^{m} (-1)^k \binom{\alpha}{k} u(x-kh)\,, \qquad (5)$$

Where $m = \left[\frac{x-a}{h}\right]$, the value of $h > 0$ correspond to the left-side derivatives, and $h < 0$ to the right-side. Similarly, you can write for a function on R:

$$\lim_{h\to 0} \frac{1}{h^{\alpha}} \sum_{k=0}^{m} (-1)^k \binom{\alpha}{k} u(x-kh), \alpha > 0 \qquad (6)$$

where $(-1)^k \binom{\alpha}{k} = \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)}$.

If the function $u(x)$ is continuous, and its derivative $u'(x)$ is integrated on the interval $[a,x]$, then the Riemann-Liouville and Grunwald-Letnikov derivatives coincide, in particular, with the Caputo derivatives as well [5, 16]. For further studies, we introduce a uniform grid with respect to spatial and temporal variables in the region $\Delta = \{(x,\tau): 0 \le x \le L, 0 \le \tau \le T\}$.

$$\omega_{\Delta\tau,h} = \left\{(\tau^k, x_n): \tau^k = k\Delta\tau, k = \overline{0,K}, \Delta\tau = \frac{t}{K}, x_n = (n-1)h, n = \overline{1,N}, h = \frac{l}{N-1}\right\}$$

Then, according to (2)-(4), the fractional derivatives of equation (1) on the grid $\omega_{\Delta\tau,h}$ can be approximated by the following dependencies [9, 17]:

$$\frac{\partial^{\alpha} u(x_n, \tau_j)}{\partial \tau^{\alpha}} = \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} u(x_n, \tau_{j-k}) \tag{7}$$

$$\frac{\partial_{+}^{\beta} u(x_n, \tau_j)}{\partial x^{\beta}} = \frac{1}{h^{\beta}} \sum_{k=0}^{n+1} \frac{\Gamma(k-\beta)}{\Gamma(-\beta)\Gamma(k+1)} u(x_{n-k+1}, \tau_j) \tag{8}$$

$$\frac{\partial_{-}^{\beta} u(x_n, \tau_j)}{\partial x^{\beta}} = \frac{1}{h^{\beta}} \sum_{k=0}^{N-n-1} \frac{\Gamma(k-\beta)}{\Gamma(-\beta)\Gamma(k+1)} u(x_{n+k-1}, \tau_j) \tag{9}$$

The above approximations using shifted Grunwald-Letnikov formulas allow obtaining conditionally stable explicit and stable implicit first-order accuracy schemes for fractional differential equations.

In fractal-structured media, it was shown in [12, 28] that the fundamental solutions of fractional differential equations with respect to temporal and spatial variables are characterized by properties which are intrinsic to the distribution densities of random variables.

4 Simulation of Random Walks

Discrete models of Markov random walk for the classical Brownian motion are the basis for the application of statistical methods for studying conventional diffusion processes [10, 16]. For a one-dimensional case where displacements are possible only at two nearest points, it is possible to write

$$u(x, \tau + \Delta\tau) = p_1 u(x-h, \tau) + p_2 u(x+h, \tau)$$

Where p_1, p_2 are the probabilities of particle displacement by one step $p_1 + p_2 = 1, x = nh, \tau = k\Delta\tau, p_n^k = u(nh, k\Delta\tau)$ - is the probability that at the n^{th} step the process is at the k^{th} point. $\frac{\partial u(x,\tau)}{\partial \tau} = a^2 \frac{\partial^2 u(x,\tau)}{\partial x^2}, a = const$

The implementation of the statistical test method involves the use of appropriate difference schemes [4, 14, 16]. The diffusion equation in the region $\Delta = \{(x,\tau) : 0 \le x \le L, 0 \le \tau \le T\}$ takes the form:

$$\frac{\partial u(x,\tau)}{\partial \tau} = a^2 \frac{\partial^2 u(x,\tau)}{\partial x^2}, a = const \tag{10}$$

To use the statistical test method in order to study the model (10), we use the Crank-Nicholson difference scheme [4]. In this case, the algorithm for calculating the probability of a random variable location at a point of time τ_j takes the form:

$$u_n^{j+1} = \frac{1}{1+\frac{2\sigma a\Delta\tau}{h^2}} \cdot \left(\frac{\sigma a\Delta\tau}{h^2}\left(u_{n+1}^{j+1}+u_{n-1}^{j+1}\right)+\frac{(1-\sigma)a\Delta\tau}{h^2}\left(u_{n+1}^{j}+u_{n-1}^{j}\right)+\left(1-\frac{2(1-\sigma)a\Delta\tau}{h^2}\right)u_n^j \right) \tag{11}$$

where $x_n = (n-1)h, \tau_j = j\Delta\tau, \tau, h$ - uniform splitting steps, n, j - numbers of splitting nodes, $\sigma = 0;1$.

According to [13], the value u_n^{j+1} can be interpreted as the probability of a random variable location at the point x_n at the time τ_j. That is, over a period of time $[\tau_i, \tau_{i+1}]$ we can consider the Markov process with corresponding probabilities:

$$u_n^j = \sum_{k=-\infty}^{+\infty} p_k u_{n-k}^j \tag{12}$$

The coefficients p_k are determined from the difference relation (12) and are the probability of uniform random walks of some particle M around the nodes of the difference grid (11) of approximation of the diffusion equation (1). In particular, for a six-point pattern for two time j and $j+1$, such probabilities take the form:

$$p_0 = \frac{h^2 - 2(1-\sigma)a\Delta\tau}{h^2 + 2\sigma a\Delta\tau}, p_{\pm 1} = \frac{(1-\sigma)a\Delta\tau}{h^2 + 2\sigma a\Delta\tau}, p_{\pm 2} = \frac{\sigma a\Delta\tau}{h^2 + 2\sigma a\Delta\tau}, p_k = 0, k = \pm 3,4,... \tag{13}$$

In particular, p_{+2} in formula (13) corresponds to the value $j+1$. In addition, the transfer coefficients satisfy the condition $\sum_{k=-\infty}^{+\infty} p_k = 1$ as well as the stability condition [17] of the difference scheme (11) for $\sigma < 0.5$.

The relations (12), (13) characterize the standard random walk model for the Gaussian process. It is believed that a random particle location in the internal node of the difference scheme can move to neighboring nodes, that is, to carry out the movement of a unit length or remain in the location node, namely, to perform a zero-length step.

5 Simulation of Random Walks for Fractional-Diffusion Process

To construct a discrete model of random walk for the differential equation of diffusion of fractional order (1), we use [12, 13, 15]. Equally important in this respect is to establish the relationship of the fundamental solution of the fractional-order differential equation (1) with the time variable of the fractionally stable distributions [16]. In particular, the fundamental solution of the equation (*) with the fractional differentiation operator Caputo:

$$G(x,\tau)=\frac{1}{2a\tau^{\alpha}}\sum_{n=0}^{\infty}\frac{(-1)^{n}}{\Gamma(n+1)\Gamma(1-\alpha-\alpha n)}\frac{|x|^{n}}{a^{n}\tau^{\alpha n}}$$

is a probability density function of the fractionally stable distribution [9, 13].

For $\alpha = 0.5$ we get a Gaussian solution [16].

Then, in the equation (11) obtained in terms of the relations in discrete form, you can move from the function $u(x,\tau)$ to the probability density (or relative diffusion concentration). This, in turn, makes it possible to move on to the probability of a particle location at a nodal point of a discrete grid. In this regard, we introduce the designation.

Given the relation (7)-(9) according to [13, 17], we can write:

$$\sum_{m=0}^{\infty}\frac{\Gamma(m-\alpha)}{\Gamma(-\alpha)\Gamma(m+1)}V_{n}^{n-m}=\frac{\Delta\tau^{\alpha}K_{\alpha}}{h^{\beta}}\times \left(C_{+}\sum_{i=0}^{\infty}\frac{\Gamma(i-\beta)}{\Gamma(-\beta)\Gamma(i+1)}V_{n-i+1}^{k-1}+C_{-}\sum_{i=0}^{\infty}\frac{\Gamma(i-\beta)}{\Gamma(-\beta)\Gamma(i+1)}V_{n+i-1}^{k-1}\right) \tag{14}$$

$$V_{n}^{k}=\alpha V_{n}^{k-1}-\sum_{m=2}^{\infty}\frac{\Gamma(m-\alpha)}{\Gamma(-\alpha)\Gamma(m+1)}V_{n}^{k-m}+\frac{\Delta\tau^{\alpha}K_{\alpha}}{h^{\beta}}\times \left(C_{+}\sum_{i=0}^{\infty}\frac{\Gamma(i-\beta)}{\Gamma(-\beta)\Gamma(i+1)}V_{n-i+1}^{k-1}+C_{-}\sum_{i=0}^{\infty}\frac{\Gamma(i-\beta)}{\Gamma(-\beta)\Gamma(i+1)}V_{n+i-1}^{k-1}\right) \tag{15}$$

The relation for determining V_n^k can be considered as a modeling scheme for a random process with discrete time. The value V_n^k characterizes the probability of the particle location at the point x_n at the time τ_k during a random walk in the difference grid. The coefficients V_n^k correspond to the probability of transitions in space and time. We denote them by p_{1i}, p_{2m}. Then (15) can be written as:

$$V_{n}^{k}=\sum_{i=-\infty}^{+\infty}p_{1i}V_{n-i}^{k-1}+\sum_{m=2}^{+\infty}p_{2m}V_{n}^{k-m} \tag{16}$$

Using the relation (16) for each case of random walk, we can get a finite number of values p_{1i} and p_{2m}. In addition, these values must satisfy the conditions of non-negativity, normalizing, which are typical of probabilistic characteristics, that is $p_{1i}\ge 0,\ p_{2m}\ge 0,\ \sum_{i=-\infty}^{+\infty}p_{1i}+\sum_{m=2}^{+\infty}p_{2m}=1$. The conditions $V_n^k\ge 0,\ \sum_{i=-\infty}^{+\infty}V_i^k=\sum_{i=-\infty}^{+\infty}V_i^0$ must also be met. The second condition ensures the preservation of the total number of particles.

6 Numerical Experiment

Numerical experiments were performed for materials with density $\rho = 460 kg/m^3$, $K_2 = 0.5$. For the equation () was specified boundary conditions $u(\varepsilon, \tau) = u = b, \tau = \tau$. Initial conditions: $u(x,0) = x - a$, if $0 \le x \le (b-a)/2$, $u(x,0) = b - x$, $(b-a)/2 \le x \le b$.

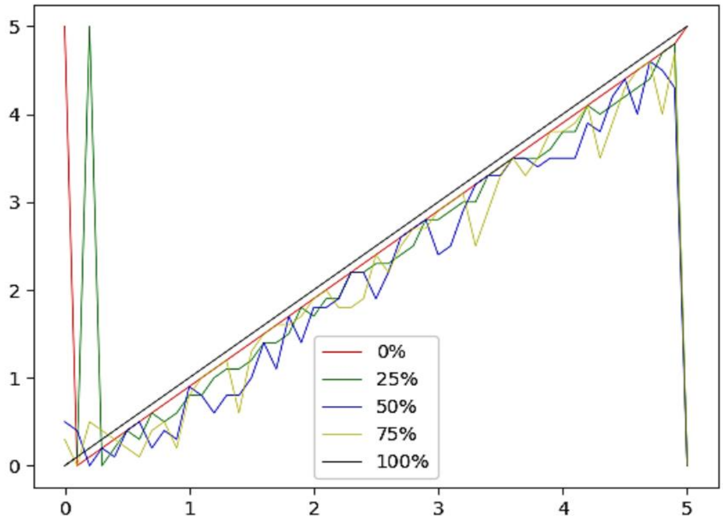

Fig. 1. Changing the function U over time for $\alpha = 0.7$ with different values x.

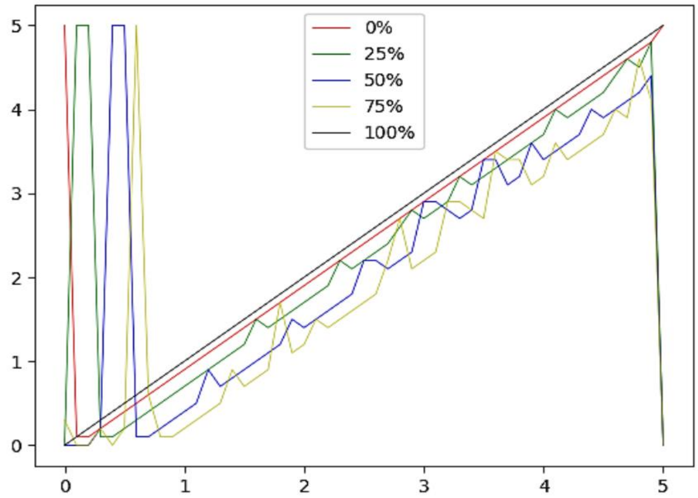

Fig. 2. Changing the function U over time for $\alpha = 0.9$ with different values x.

Quantities $h = 0.1$, $\Delta\tau = 0.1$. Figures 1 and 2 show the dependences of the function change $u(x, \tau)$, respectively, for the fractal coefficient $\alpha = 0.7$ and $\alpha = 0.9$ for different values x, which are respectively $x = 0;0.25;0.5;0.75;1$.

The analysis of graphic dependences indicates the effect of the parameter α on the function change $u(x,\tau)$. Increasing the parameter α increases the number of maximum values of the curve for different values of change of coordinates.

Conclusions

On the basis of discrete models of diffusion processes with fractional derivatives shows a modification of the method of random walk on the implementation of the mathematical model of a diffusion process subject to temporal nonlocality. For numerical implementation of such a mathematical model, finite-difference schemes are proposed, an algorithm is developed and software is created. The results of numerical experiments for the implementation of a mathematical model of diffusion processes for different values of the fractional index according to time are given by the statistical method.

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