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θ-FUNCTION METHOD FOR A TIME-FRACTIONAL REACTION-DIFFUSION EQUATION

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ABSTRACT. In this paper, the initial-boundary-value problems with both the Dirichlet and the Neumann boundary conditions for a nonlinear time-fractional reaction-diffusion equation are considered. The proposed solution method consists in employing a suitable generalization of the θ-function that is constructed based on the fundamental solution of the corresponding linear time-fractional diffusion equation. For the solutions of the initial-boundary-value problems for the time-fractional reaction-diffusion equation, the integral equations of the Volterra type with the generalized θ-function in the kernel are obtained. These equations are useful, e.g., for the numerical solutions of the problems under consideration.

1. Introduction

It is well known that under the usual assumptions placed on the jump probability density functions of the diffusing microscopic particles, the underlaying diffusion process can be modeled by the diffusion equation

$$\frac{\partial u}{\partial t} - \nabla \cdot (D\nabla u(\mathbf{x}, t)) = 0 \tag{1}$$

that describes the substance concentration $u = u(\mathbf{x}, t),\ t \geq 0,\ \mathbf{x} \in \Omega \subseteq \mathbf{R}^N$, where $D = D(\mathbf{x}, t, u)$ is the diffusion coefficient and ∇ is the gradient operator. This equation can be also derived by combining the continuity equation $\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{j} = 0$ and the Fick's first law $\mathbf{j} = -D\nabla u(\mathbf{x}, t)$, where $\mathbf{j}$ is the flux of the substance.

Whereas the diffusion equation (1) has been successfully applied in many areas of physics and engineering, recently some other phenomena called **anomalous diffusion** have been observed ([**1, 4, 10, 23**]). In the case of the classical diffusion equation (1), the diffusive profile is connected with the Gaussian distribution. The main feature of this process is the linear relation between the mean square displacement of the diffusing particles and time, namely $\langle x^2(t)\rangle = 2Dt$. In the

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case of the anomalous diffusion, this relation is not linear anymore and can be often written in the form $\langle x^2(t)\rangle = D_\gamma\, t^\gamma$ with $\gamma \neq 1$.

One of the most powerful models of the anomalous diffusion is the continuous time random walk model that under some realistic assumptions on the jump probability density functions leads to the time-, space-, or time-space-fractional diffusion and diffusion-wave equations on the large time- and space-scales (see e.g. [**2, 18, 19, 27**]). In the literature, a lot of attention was given to the initial-value problems for the linear fractional diffusion and diffusion-wave equations (see e.g. [**8, 13, 14, 16, 25, 26**]). A fundamental solution of the linear one-dimensional time-fractional diffusion equation was derived in [**25**] in terms of the special functions of the Wright type. In [**21**], a maximum principle for the generalized multi-dimensional time-fractional diffusion equation was proved. For some regularity results of the solutions of the time-fractional diffusion equations we refer the reader to [**29**]. As to the initial-boundary-value problems for these equations, they were analyzed in [**17, 20, 21**] by applying the Fourier method of variables separation. In general, this method leads to a generalized solution in form of a Fourier series that in some cases can be shown to be a solution in the classical sense ([**17**]).

In contrast to the linear case, only few analytical results are known for the nonlinear fractional diffusion and diffusion-wave equations. One research direction in this field is the qualitative theory of the fractional partial differential equations (see e.g. [**5, 6**] and references therein). In this paper, we introduce another method for analytical treatment of the initial-boundary-value problems for a factional reaction-diffusion equation that is based on the fractional θ-function that is constructed using the known fundamental solution of the initial-value problem for the linear time-fractional diffusion equation. In the case of the conventional diffusion equation, this technique is described e.g. in [**3**]. For the solutions of the initial-boundary-value problems for the fractional reaction-diffusion equations, the integral equations of the Volterra type with the fractional θ-function in the kernel are derived. These equations can be used e.g. for the numerical treatment of the problems under consideration.

Let us note that initial-boundary-value problems for linear and nonlinear fractional partial differential equations can be numerically solved by the finite differences method (see e.g. [**7, 15**]) or by the finite elements method (see e.g. [**11, 12**]), too. In the final section of our paper, we compare the results derived by employing our method and the method of the finite differences.

The rest of this paper is organized as follows. In the 2nd section, a fractional generalization of the θ-function is constructed and studied. In particular, its properties that are employed for solving the initial-boundary-value problems we are dealing with in this paper are derived. The 3rd section is devoted to construction of the Volterra type integral equations for the solutions of the initial-boundary-value problems for the time-fractional reaction-diffusion equations with both Dirichlet and Neumann boundary conditions. Finally, in the last section, some numerical examples are presented.

2. Fractional θ_α-function and its properties

We start with an initial-boundary-value problem for a linear one-dimensional fractional diffusion equation in the form

$$\begin{cases} \partial_t^\alpha u - u_{xx} = 0, \quad 0<\alpha<1,\ x\in\mathbb{R},\ t\in\mathbb{R}_+ \\ u(x,0) = f(x), \quad x\in\mathbb{R}, \\ u(\pm\infty,t) = 0, \quad t\in\mathbb{R}_+, \end{cases} \tag{2}$$

$\partial_t^\alpha u,\ 0<\alpha<1$ being the Caputo fractional derivative defined by

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

Let us mention that for $\alpha = 1$ the fractional Caputo derivative is defined as the first order derivative and thus the problem (2) is just an initial-value problem for the conventional diffusion equation:

$$\begin{cases} \partial_t u - u_{xx} = 0, \quad x\in\mathbb{R},\ t\in\mathbb{R}_+ \\ u(x,0) = f(x), \quad x\in\mathbb{R}, \\ u(\pm\infty,t) = 0, \quad t\in\mathbb{R}_+. \end{cases} \tag{3}$$

The fundamental solution (the Green function) of the problem (2) is called a solution to this problem with the initial condition $f(x) = \delta(x)$, where δ is the Dirac δ-function. Let us denote the fundamental solution of the problem (2) by $K_\alpha(x,t)$. Then it is known that

$$u(x,t) = \int_{-\infty}^{\infty} K_\alpha(\xi,t) f(x-\xi) d\xi \tag{4}$$

is a solution to the general problem (2).

Following [**25, 26**], the fundamental solution can be represented in the form

$$K_\alpha(x,t) = \frac{1}{2}t^{-\alpha/2}M_{\alpha/2}(|x|/t^{\alpha/2}), \qquad x\in\mathbb{R},\ t\in\mathbb{R}_+ \tag{5}$$

in terms of an auxiliary function of the Wright type that is often referred to as the Mainardi function. The M-function is represented by

$$M_\mu(z) := W_{-\mu,1-\mu}(-z),\ 0<\mu<1 \tag{6}$$

in terms of the Wright function that is defined as a convergent series (see e.g. [**9**]):

$$W_{\alpha,\beta}(z) = \sum_{k=0}^{\infty}\frac{z^k}{k!\Gamma(\alpha k+\beta)},\ \alpha>-1,\ \beta\in\mathbb{C},\ z\in\mathbb{C}. \tag{7}$$

For $\mu = 1/2$ ($\alpha = 1$ in the equation (2)), the M-function becomes the familiar Gaussian function:

$$M_{1/2}(z) = \frac{1}{\sqrt{\pi}}\exp(-z^2/4). \tag{8}$$

For the conventional diffusion equation (3), a method of representation of the solutions to the boundary-value-problems for the linear and nonlinear diffusion equations in terms of the fundamental solutions to the initial-value problems for the linear equations is known (see e.g. [**3**]). This representation is constructed in terms of the so called θ-function.

For the reader's convenience, some basic results regarding the conventional diffusion equation are now presented. The θ-function is defined as

$$\theta(x,t) = \sum_{m=-\infty}^{\infty} K(x+2m,t), \tag{9}$$

where K is the fundamental solution to the initial-value problem for the linear diffusion equation (3) given by

$$K(x,t) = \frac{1}{\sqrt{4\pi t}} \exp(-\frac{x^2}{4t}). \tag{10}$$

The main result we are going to generalize in this paper for the case of the fractional diffusion equation is given in the following lemma.

Lemma 2.1. *Let f be a continuous function and u_0, g_1, g_2 be piecewise continuous functions on the suitable intervals. Then the function*

(11)

$$u(x,t) = \int_0^1 \{\theta(x-\xi,t) - \theta(x+\xi,t)\} u_0(\xi) d\xi - 2\int_0^t \frac{\partial\theta}{\partial x}(x,t-\tau) g_1(\tau) d\tau +$$
$$2\int_0^t \frac{\partial\theta}{\partial x}(x-1,t-\tau) g_2(\tau) d\tau + \int_0^t \int_0^1 \{\theta(x-\xi,t-\tau) - \theta(x+\xi,t-\tau)\} f(u(\xi,\tau)) d\xi d\tau$$

is a solution of the following initial-boundary value problem for the reaction-diffusion equation

$$\begin{cases} u_t - u_{xx} = f(u), & 0 < x < 1,\ t > 0 \\ u(x,0) = u_0(x), & 0 < x < 1, \\ u(0,t) = g_1(t), & u(1,t) = g_2(t), \quad t > 0. \end{cases} \tag{12}$$

Remark. *A similar result is valid for the problem of type (12) with the Neumann boundary conditions instead of the Dirichlet boundary conditions. In this case, the terms $\frac{\partial\theta}{\partial x}(x,t-\tau)$ have to be replaced by $\theta(x,t-\tau)$ in the representation (11).*

Now the main object of our paper - a fractional generalization θ_α of the θ-function - is defined as follows:

$$\theta_\alpha(x,t) = \sum_{m=-\infty}^{+\infty} K_\alpha(x+2m,t), \qquad x \in \mathbb{R},\ t > 0 \tag{13}$$

with the function K_α as in (5).

Because of the formula (8), our θ_α coincides with the conventional θ-function for $\alpha = 1$.

Before we start with investigation of the relevant properties of θ_α, some results needed for further discussions are formulated. In the next section, we need some properties of the Riemann-Liouville fractional derivative D^α_{a+} that for $0 < \alpha < 1$ is defined by

$$D^\alpha_{a+}u(t) = \frac{1}{\Gamma(1-\alpha)}\frac{d}{dt}\int_a^t \frac{u(s)}{(t-s)^\alpha}ds.$$

Lemma 2.2. *(Lemma 2.2 in [**13**]) Let $u(t) \in AC([a,b])$. Then the Riemann-Liouville fractional derivative $D^\alpha_{a+}u$ exists almost everywhere on $[a,b]$.*

Lemma 2.3. *Let f, $g \in AC([0,b])$ with $f(0) = g(0) = 0$ and $0 < \alpha < 1$. Then the integration by parts formula*

$$\int_0^t D^\alpha_{0+}f(t-\tau)g(\tau)d\tau = \int_0^t f(t-\tau)D^\alpha_{0+}g(\tau)d\tau \tag{14}$$

holds true for $t \in [0,b]$.

Proof. The proof is by direct computation. Using Lemma 2.2, the left hand side of (14) can be transformed to the form

$$\begin{aligned}
\int_0^t D^\alpha_{0+}f(t-\tau)g(\tau)d\tau &= \int_0^t \frac{1}{\Gamma(1-\alpha)}\left(\int_0^{t-\tau}\frac{f'(s)}{\big((t-\tau)-s\big)^\alpha}ds + \frac{f(0)}{(t-\tau)^\alpha}\right)g(\tau)d\tau\\
&= \frac{1}{\Gamma(1-\alpha)}\int_0^t\int_0^{t-\tau}\frac{f'(s)g(\tau)}{\big((t-\tau)-s\big)^\alpha}dsd\tau + \frac{f(0)}{\Gamma(1-\alpha)}\int_0^t\frac{g(\tau)}{(t-\tau)^\alpha}d\tau\\
&=: J_1
\end{aligned}$$

since $f(0) = 0$.

By the change of variables $\mu = t - \tau$ and then $\rho = t - \mu$ and $t - s = \tau$ we get the following chain of equalities:

$$\begin{aligned}
J_1 &= \frac{1}{\Gamma(1-\alpha)}\int_0^t\int_0^\mu \frac{f'(s)g(t-\mu)}{\big(\mu-s\big)^\alpha}dsd\mu = \frac{1}{\Gamma(1-\alpha)}\int_0^t\int_s^t\frac{g(t-\mu)}{(\mu-s)^\alpha}d\mu f'(s)ds\\
&= \frac{f(s)}{\Gamma(1-\alpha)}\int_s^t\frac{g(t-\mu)}{(\mu-s)^\alpha}d\mu\Big|_{s=0}^{s=t} - \frac{1}{\Gamma(1-\alpha)}\int_0^t\frac{\partial}{\partial s}\Big(\int_s^t\frac{g(t-\mu)}{(\mu-s)^\alpha}d\mu\Big)f(s)ds\\
&= -\frac{f(0)}{\Gamma(1-\alpha)}\int_0^t\frac{g(t-\mu)}{\mu^\alpha}d\mu + \frac{1}{\Gamma(1-\alpha)}\int_0^t\frac{\partial}{\partial s}\Big(\int_0^{t-s}\frac{g(\rho)}{(t-s-\rho)^\alpha}d\rho\Big)f(s)ds\\
&= \frac{1}{\Gamma(1-\alpha)}\int_0^t\frac{\partial}{\partial\tau}\Big(\int_0^\tau\frac{g(\rho)}{(\tau-\rho)^\alpha}d\rho\Big)f(t-\tau)d\tau\\
&= \int_0^t f(t-\tau)D^\alpha_{0+}g(\tau)d\tau.
\end{aligned}$$

This completes the proof. □

Now we start with investigation of the properties of the θ_α-function that are needed in the next section for our treatment of the initial-boundary-value problems for a fractional reaction-diffusion equation.

Lemma 2.4. *The function $\theta_\alpha(x,t)$ is a C^∞ function in both $x \in \mathbb{R}$ and $t > 0$. It is an even function with respect to the spatial variable x. Moreover, for $0 < \alpha < 1$ the relations*

$$\lim_{x\to 0+} \mathcal{L}\Big\{\frac{\partial\theta_\alpha}{\partial x}(x,t);s\Big\} = -\frac{1}{2}s^{\alpha-1}, \tag{15}$$

$$\lim_{x\to 0+} \mathcal{L}\Big\{\frac{\partial}{\partial x}D_{0+}^{1-\alpha}\theta_\alpha(x,t);s\Big\} = -\frac{1}{2}, \tag{16}$$

$$\lim_{t\to 0}\theta_\alpha(x,t) = 0, \tag{17}$$

$$\lim_{x\to 1}\frac{\partial\theta_\alpha}{\partial x}(x,t) = 0, \forall t > 0 \tag{18}$$

hold true, where $\mathcal{L}$ denotes the Laplace transform and $D_{0+}^{1-\alpha}$ is the Riemann-Liouville fractional derivative.

Proof. Using the notation $r_m = |x+2m|/t^{\alpha/2}$, $m \in \mathbb{Z}$, the formula (13) can be represented in the form

$$\theta_\alpha(x,t) = \sum_{m=-\infty}^{\infty}\frac{1}{2}t^{-\alpha/2}M_{\alpha/2}(r_m), \tag{19}$$

where M_μ is defined as in (6). The asymptotic behavior of $M_\mu(r)$ as $r \to \infty$ is known (see e.g. [**26**]):

$$M_\mu(r) \sim Ar^a\exp(-br^c), \quad r\to\infty \tag{20}$$

with

$$A = \Big(2\pi(1-\mu)\mu^{\frac{1-2\mu}{1-\mu}}\Big)^{-1/2},\ a = \frac{2\mu-1}{2-2\mu},\ b = (1-\mu)\mu^{\frac{\mu}{1-\mu}},\ c = \frac{1}{1-\mu}.$$

Now we apply the asymptotical formula (20) with $\mu = \alpha/2$ and $r = r_m$ to the representation (19) of the θ_α-function. For $0 < \alpha < 1$, the value of μ is between 0 and $\frac{1}{2}$ and thus for the constants in (20) the inequalities $b > 0$ and $1 < c < 2$ hold true. We then obtain

(21)

$$|\theta_\alpha(x,t)| < \sum_{m=-\infty}^{\infty}\frac{1}{2}t^{-\alpha/2}Ar_m^a\exp(-br_m^c) < C\sum_{m=-\infty}^{\infty}\frac{1}{2}t^{-\alpha/2}Ar_m^a\exp(-br_m),$$

where C is a constant. If the inequality $e^{-br_m^c} < e^{-br_m}$ holds for all $t > 0$, then we can simply take $C = 1$. For a fixed t, we can find an integer M, such that $r_m > 1$ for all $m > M$ and then we get $e^{-br_m^c} < e^{-br_m}$. Now we split the last series in (21) into a finite part with the indices $|m| \le M$ and the remaining terms with $|m| > M$. Since all terms of the series are positive, the finite part can be bounded by a constant times the sum that contains e^{-br_m} while the remaining terms allow the bound $C = 1$.

Let us denote the function $t^{-\alpha/2}Ar_m^a\exp(-br_m)$ by $u_m(x,t)$. Then for any $t_0 > 0$, $t \ge t_0 > 0$, there is an integer M such that the equality $|r_{m+1}|-|r_m| = \frac{2}{t^{\alpha/2}}$

holds if $m > M$. Restricting m to this range we obtain

$$\lim_{m\to\infty}\frac{u_{m+1}}{u_m}=\lim_{m\to\infty}\left(\frac{|x+2(m+1)|}{|x+2m|}\right)^a\exp\left(-\frac{2b}{t^{\alpha/2}}\right)=\exp\left(-\frac{2b}{t^{\alpha/2}}\right)<1$$

since $b > 0$ and $t \geq t_0 > 0$. Thus the series $\sum_{m=0}^{\infty} u_m(x,t)$ is uniformly convergent for $x \in \mathbb{R}$ and $t \geq t_0 > 0$. Similarly, there exists an integer N such that for all $m < N$, we have $|r_{m-1}| - |r_m| = \frac{2}{t^{\alpha/2}}$ and

$$\lim_{m\to-\infty}\frac{u_{m-1}}{u_m}=\lim_{m\to-\infty}\left(\frac{|x+2(m-1)|}{|x+2m|}\right)^a\exp\left(-\frac{2b}{t^{\alpha/2}}\right)=\exp\left(-\frac{2b}{t^{\alpha/2}}\right)<1,$$

so that the series $\sum_{m=-\infty}^{0} u_m(x,t)$ also uniformly converges for $x \in \mathbb{R}$ and $t > 0$. Thus the series for $\theta_\alpha(x,t)$ is uniformly convergent one for $x \in \mathbb{R}$ and $t \geq t_0 > 0$, too. Using the same technique, we can show that the series for all partial derivatives of θ_α are also uniformly convergent for $x \in \mathbb{R}$ and $t > 0$ that shows that θ_α is in $C^\infty(0,\infty)$ with respect to the time variable t and in $C^\infty(\mathbb{R})$ with respect to the spatial variable x.

Now we move to the proof of the relation (15). By direct calculation, for $m = 1, 2, \ldots$ we get the relations

$$\frac{\partial}{\partial x}(K_\alpha(x+2m,t)) = -\frac{1}{2}t^{-\alpha}\sum_{k=0}^{\infty}\frac{(-\frac{|x+2m|}{t^{\alpha/2}})^k}{k!\Gamma(-\frac{\alpha}{2}k+(1-\alpha))},$$
$$\frac{\partial}{\partial x}(K_\alpha(x-2m,t)) = \frac{1}{2}t^{-\alpha}\sum_{k=0}^{\infty}\frac{(-\frac{|x-2m|}{t^{\alpha/2}})^k}{k!\Gamma(-\frac{\alpha}{2}k+(1-\alpha))}.$$

Thus

$$\lim_{x\to 0+}\left(\frac{\partial}{\partial x}(K_\alpha(x+2m,t))+\frac{\partial}{\partial x}(K_\alpha(x-2m,t))\right)=0. \tag{22}$$

We use now the uniform convergence of the series for θ_α and the equality (22) to obtain

$$\lim_{x\to 0+}\frac{\partial\theta_\alpha(x,t)}{\partial x}=\lim_{x\to 0+}\frac{\partial}{\partial x}\left(\sum_{m=-\infty}^{\infty}K_\alpha(x+2m,t)\right)=\lim_{x\to 0+}\sum_{m=-\infty}^{\infty}\frac{\partial}{\partial x}(K_\alpha(x+2m,t))$$
$$=\lim_{x\to 0+}\sum_{m=1}^{\infty}\left(\frac{\partial}{\partial x}(K_\alpha(x+2m,t))+\frac{\partial}{\partial x}(K_\alpha(x-2m,t))\right)+\lim_{x\to 0+}\frac{\partial}{\partial x}(K_\alpha(x,t))$$
$$=\lim_{x\to 0+}\frac{\partial}{\partial x}(K_\alpha(x,t)).$$

The last formula along with the series representation of K_α leads to the relation

$$\lim_{x\to 0+}\frac{\partial\theta_\alpha(x,t)}{\partial x}=\lim_{x\to 0+}-\frac{1}{2}t^{-\alpha}\sum_{k=0}^{\infty}\frac{(-\frac{x}{t^{\alpha/2}})^k}{k!\Gamma(-\frac{\alpha}{2}k+(1-\alpha))}$$
$$=\lim_{x\to 0+}-\frac{1}{2}t^{-\alpha}W_{-\frac{\alpha}{2},1-\alpha}(x,t).$$

Using the Laplace transform formula (see [**9**])

$$\mathcal{L}\{t^{-\alpha}W_{-\frac{\alpha}{2},1-\alpha};s\} = s^{-(1-\alpha)}\exp(-|x|s^{\alpha/2}),$$

we obtain

$$\lim_{x\to 0+}\mathcal{L}\Big\{\frac{\partial\theta_\alpha(x,t)}{\partial x};s\Big\} = \lim_{x\to 0+} -\frac{1}{2}s^{-(1-\alpha)}\exp(-|x|s^{\alpha/2}) = -\frac{1}{2}s^{\alpha-1},$$

which proves formula (15).

In order to prove (16), we show that the formula

$$\lim_{x\to 0+}\int_0^t \frac{\partial}{\partial x}D_{0+}^{1-\alpha}\theta_\alpha(x,t-\tau)\varphi(\tau)d\tau = -\frac{1}{2}\varphi(t) \tag{23}$$

holds true for all $\varphi(t)\in C_0^\infty(0,\infty)$. By Lemma 2.2, $D_{0+}^{1-\alpha}\theta_\alpha(x,t)$ exists and is continuous for $x\in\mathbb{R}$ and $t>0$, so that the Laplace transform formula $\mathcal{L}\{D_{0+}^{\alpha}\varphi(t);s\} = s^\alpha\mathcal{L}\{\varphi(t);s\}$ is valid because $(D_{0+}^{\alpha-1}\varphi(t))|_{t=0}=0$. Applying the Laplace transform to the left hand side of (23) and using Lemma 2.3, we obtain the following chain of equalities

$$\begin{aligned}
&\lim_{x\to 0+}\mathcal{L}\Big\{\int_0^t \frac{\partial}{\partial x}D_{0+}^{1-\alpha}\theta_\alpha(x,t-\tau)\varphi(\tau)d\tau;s\Big\}\\
&= \lim_{x\to 0+}\mathcal{L}\Big\{\int_0^t \frac{\partial}{\partial x}\theta_\alpha(x,t-\tau)D_{0+}^{1-\alpha}\varphi(\tau)d\tau;s\Big\}\\
&= \lim_{x\to 0+}\mathcal{L}\Big\{\frac{\partial}{\partial x}\theta_\alpha(x,t);s\Big\}\times\mathcal{L}\Big\{D_{0+}^{1-\alpha}\varphi(t);s\Big\}\\
&= -\frac{1}{2}s^{\alpha-1}\times s^{1-\alpha}\mathcal{L}\Big\{\varphi(t);s\Big\}\\
&= \mathcal{L}\Big\{-\frac{1}{2}\varphi(t);s\Big\}
\end{aligned}$$

that immediately leads to (23).

In order to prove (17), we employ the Proposition 1 from [**8**] with $n=1$ and $m=0$ (note that our notations are different from those used in [**8**], where in particular the notation Z_0 stays in place of our θ_α). This gives the estimate $|\theta_\alpha|\le Ct^{-\alpha/2}\exp(-\sigma t^{-\frac{\alpha}{2-\alpha}}|x|^{\frac{2}{2-\alpha}})$ that for $t\to 0$ leads to (17).

To show (18), we first calculate the value of $\frac{\partial\theta_\alpha}{\partial x}(x,t)$ at the point $x=1$ for $t>0$:

$$\begin{aligned}
\frac{\partial\theta_\alpha}{\partial x}(x,t)\Big|_{x=1} &= -\frac{1}{2}t^{-\alpha}\sum_{m=1}^{\infty}\sum_{k=0}^{\infty}\frac{(-\frac{|1+2m|}{t^{\alpha/2}})^k}{k!\Gamma(-\frac{\alpha}{2}k+(1-\alpha))}\\
+\frac{1}{2}t^{-\alpha}\sum_{m=1}^{\infty}\sum_{k=0}^{\infty}&\frac{(-\frac{|1-2m|}{t^{\alpha/2}})^k}{k!\Gamma(-\frac{\alpha}{2}k+(1-\alpha))} - \frac{1}{2}t^{-\alpha}\sum_{k=0}^{\infty}\frac{(-\frac{1}{t^{\alpha/2}})^k}{k!\Gamma(-\frac{\alpha}{2}k+(1-\alpha))} = 0.
\end{aligned}$$

Thus by the continuity of $\frac{\partial\theta_\alpha}{\partial x}(x,t)$ with respect to x, we obtain

$$\lim_{x\to 1}\frac{\partial\theta_\alpha}{\partial x}(x,t) = \frac{\partial\theta_\alpha}{\partial x}(x,t)\Big|_{x=1} = 0$$

that is the relation (18). □

3. Initial-boundary-value problems with the Dirichlet and Neumann boundary conditions

The θ_α-function introduced and studied in the previous section is now used to derive the Volterra type integral equations for the solutions of the initial-boundary-value problems with the Dirichlet and with the Neumann boundary conditions for a fractional reaction-diffusion equation. First we consider the case of the Dirichlet boundary conditions. In this case, the following result is valid:

Theorem 3.1. *Let u_0, g_1, and g_2 be piecewise continuous functions on the suitable intervals. Then a solution u of the initial-boundary-value problem for the fractional reaction-diffusion equation given by*

$$\begin{cases} \partial_t^\alpha u - u_{xx} = f(u) + \gamma(x,t), \qquad 0 < x < 1,\ 0 < t < T \\ u(x,0) = u_0(x), \quad 0 < x < 1, \\ u(0,t) = g_1(t), \qquad u(1,t) = g_2(t), \quad 0 \le t \le T \end{cases} \tag{24}$$

can be represented in the form

$$u(x,t) = w(x,t) + v_1(x,t) + v_2(x,t) + v_3(x,t) \tag{25}$$

with the functions w, v_1, v_2, v_3 given by

$$w(x,t) = \int_0^1 \Big[\theta_\alpha(x-\xi,t) - \theta_\alpha(x+\xi,t)\Big] u_0(\xi) d\xi,$$

$$v_1 = -2\int_0^t \frac{\partial(D_{0+}^{1-\alpha}\theta_\alpha)}{\partial x}(x,t-\tau) g_1(\tau) d\tau,$$

$$v_2 = -2\int_0^t \frac{\partial(D_{0+}^{1-\alpha}\theta_\alpha)}{\partial x}(x-1,t-\tau) g_2(\tau) d\tau,$$

$$v_3 = \int_0^t\int_0^1 \big[(D_{0+}^{1-\alpha}\theta_\alpha)(x-\xi,t-\tau) + (D_{0+}^{1-\alpha}\theta_\alpha)(x+\xi,t-\tau))\big][f(u(\xi,\tau) + \gamma(\xi,\tau)] d\xi d\tau.$$

Proof. The problem of existence and uniqueness of a solution to (24) has been considered in [**24**] and we refer the interested reader to this paper for more information. In this paper, the focus is on the solution formula (25).

By definition of the θ_α-function, we have

$$\begin{aligned} \partial_t^\alpha w &= \int_0^1 \Big[\partial_t^\alpha \theta_\alpha(x+\xi,t) + \partial_t^\alpha \theta_\alpha(x-\xi,t)\Big] u_0(\xi) d\xi \\ &= \int_0^1 \Big[\theta_\alpha(x+\xi,t) + \theta_\alpha(x-\xi,t)\Big]_{xx} u_0(\xi) d\xi = w_{xx}. \end{aligned}$$

Then by direct calculations, we get the following chain of equalities:

$$\begin{aligned}
\partial_t^\alpha v_1 &= -2\partial_t^\alpha \left(\int_0^t D_{0+}^{1-\alpha} (\frac{\partial \theta_\alpha}{\partial x})(x, t-\tau) g_1(\tau) d\tau \right) \\
&= -2\partial_t^\alpha \left(\int_0^t \frac{\partial \theta_\alpha}{\partial x}(x, t-\tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau \right) \\
&= -2 \left(\int_0^t \frac{\partial}{\partial x}(\partial_t^\alpha \theta_\alpha)(x, t-\tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau \right) \\
&= -2 \left(\int_0^t \frac{\partial}{\partial x}((\theta_\alpha)_{xx})(x, t-\tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau \right) \\
&= -2 \left(\int_0^t D_{0+}^{1-\alpha} (\frac{\partial \theta_\alpha}{\partial x})_{xx}(x, t-\tau) g_1(\tau) d\tau \right) \\
&= -2 \left(\int_0^t (\frac{\partial D_{0+}^{1-\alpha} \theta_\alpha}{\partial x})_{xx}(x, t-\tau) g_1(\tau) d\tau \right) \\
&= \left(-2 \int_0^t \frac{\partial (D_{0+}^{1-\alpha} \theta_\alpha)}{\partial x}(x, t-\tau) g_1(\tau) d\tau \right)_{xx} = (v_1)_{xx},
\end{aligned}$$

where we change of the order of the derivatives $D_{0+}^{1-\alpha}$ and $\frac{\partial}{\partial x}$ is guaranteed by the uniformly convergence of the series for θ_α and its fractional derivatives.

Using the same technique, the equality

$$\partial_t^\alpha v_2 = (v_2)_{xx}$$

can be derived, too.

Finally, it follows from the Duhamel principle for the fractional order differential equations that was formulated in [**30**] that v_3 is a solution to the problem

$$\begin{cases} \partial_t^\alpha v - v_{xx} = f(v) + \gamma(x,t), & 0 < x < 1,\ 0 < t < T, \\ v(x,0) = 0, \quad 0 < x < 1, \\ v(0,t) = 0, \qquad -v(1,t) = 0, \quad 0 \le t \le T. \end{cases} \tag{26}$$

By combining the above four equations, we arrive at the conclusion that the function (25) satisfies the fractional reaction-diffusion equation formulated in (24).

To verify the initial condition, the value $t = 0$ is substituted into the formula (25). Simple calculations show that (25) satisfies the initial condition formulated in (24).

To prove that the function given by (25) satisfies the boundary conditions from (24), the formulas (16)-(18) from Lemma 2.4 are employed. We restrict ourselves to the function v_1; all other cases can be treated along the same lines.

On the left boundary, $x = 0$, the formula (16) presented in Lemma 2.4 leads to the equality

$$\lim_{x\to 0+} v_1(x,t) = -2 \lim_{x\to 0+} \int_0^t \frac{\partial}{\partial x}(D_{0+}^{1-\alpha}\theta_\alpha)(x, t-\tau) g_1(\tau) d\tau$$
$$= g_1(x,t).$$

On the right boundary, $x = 1$, we apply the formula (18) of Lemma 2.4 to get the desired boundary condition

$$\lim_{x\to 1-} v_1(x,t) = -2 \int_0^t D_{0+}^{1-\alpha}(\lim_{x\to 1+} \frac{\partial}{\partial x}(\theta_\alpha(x, t-\tau)) g_1(\tau) d\tau$$
$$= 0.$$

□

Now we consider the initial-boundary-value problems for the fractional reaction-diffusion equation with the Neumann boundary conditions. In this case, the main result is given in the following statement.

Theorem 3.2. *Let u_0, g_1, and g_2 be piecewise continuous functions on the suitable intervals. Then a solution u of the initial-boundary-value problem for the fractional reaction-diffusion equation*

$$\begin{cases} \partial_t^\alpha u - u_{xx} = f(u) + \gamma(x,t), & 0 < x < 1,\ 0 < t < T \\ u(x,0) = u_0(x), \quad 0 < x < 1, & \\ u_x(0,t) = g_1(t), \qquad -u_x(1,t) = g_2(t), & 0 \le t \le T \end{cases} \tag{27}$$

can be represented in the form

$$u(x,t) = w(x,t) + v_1(x,t) + v_2(x,t) + v_3(x,t), \tag{28}$$

where

$$w(x,t) = \int_0^1 \Big[\theta_\alpha(x-\xi, t) - \theta_\alpha(x+\xi, t)\Big] u_0(\xi) d\xi,$$
$$v_1 = -2\int_0^t (D_{0+}^{1-\alpha}\theta_\alpha)(x, t-\tau) g_1(\tau) d\tau,$$
$$v_2 = 2\int_0^t (D_{0+}^{1-\alpha}\theta_\alpha)(x-1, t-\tau) g_2(\tau) d\tau,$$
$$v_3 = \int_0^t\!\!\int_0^1 \big[(D_{0+}^{1-\alpha}\theta_\alpha)(x-\xi, t-\tau) + (D_{0+}^{1-\alpha}\theta_\alpha)(x+\xi, t-\tau))\big][f(u(\xi,\tau) + \gamma(\xi,\tau)] d\xi d\tau.$$

The proof of Theorem 3.2 closely follows the lines of the proof of Theorem 3.1 and is omitted here.

Remark. *In the formulas (25) and (28), the fractional θ_α-function was used to deduce the integral equations of the Volterra type for solutions of the initial-boundary-value problems with the Dirichlet and the Neumann boundary conditions for a time-fractional reaction-diffusion equation. One advantage of this integral* *representation is that it can be used to solve some inverse problems for the time-fractional reaction-diffusion equation by using a regularization via the Volterra integral equations of the second kind as it has been done for the case of the conventional reaction-diffusion equation in* [**28**] *(see also Chapter 13 of* [**3**]*).*

4. Numerical results and plots

First we shortly describe a direct solver for numerical solution of the problem (24). It is based on an implicit time step method for the fractional differential equations with the Caputo fractional derivative that is similar to one presented in [**15**], but takes into account the nonlinear source terms.

Let x_i and t_k be uniformly spaced grid points and Δx and Δt the space and the time step sizes, respectively. Let us denote $u(x_i, t_k)$ by u_i^k. For the time-fractional Caputo derivative, we use the standard approximation

$$\partial_t^\alpha u^{k+1}(x) \approx \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{k} b_j \frac{u(x, t_{k+1-j}) - u(x, t_{k-j})}{\Delta t^\alpha},$$

where $b_j = (j+1)^{1-\alpha} - j^{1-\alpha}, j = 0, 1, \ldots, k$. For the space derivative, we use the usual central difference scheme. This leads to the following system of the nonlinear equations

$$\frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{k} b_j \frac{u_i^{k+1-j} - u_i^{k-j}}{\Delta t^\alpha} - \frac{u_{i-1}^{k+1} - 2u_i^{k+1} + u_{i+1}^{k+1}}{\Delta x^2} = f(u_i^k) + \gamma(x_i, t_k)$$

for the numerical approximations u_i^k of the solution u to the problem (24) at the grid points.

Another approach for numerical solution of the problem (24) is based on numerical solution of the nonlinear integral equation (25) for the solution to this problem. This approach requires numerical evaluation of the function θ_α and its fractional derivatives. For numerical evaluation of θ_α, the Wright function has to be first evaluated that can be done e.g. using the algorithms suggested in [**22**]. For numerical evaluation of θ_α, we need to evaluate an infinite series with the terms in form of the Wright function with different arguments and this task is not trivial. Even in the classical case ($\alpha = 1$), numerical evaluation of the θ-function is a difficult problem, too. Summarizing, the second approach for numerical solution of the problem (24) is a more computationally expensive option compared with the one that employs the finite difference scheme. In Example 4.2, we apply these two approaches for a particular case of the problem (24) and show that they lead to the same numerical results.

In the rest of this section, two examples are presented to verify the numerical approaches proposed above.

Example 4.1. *In this example, the problem*

$$\begin{cases} \partial_t^\alpha u - u_{xx} = f(u) + \gamma(x,t), & 0 < x < 1,\ 0 < t < 1 \\ u(x,0) = x^2, & 0 < x < 1, \\ u_x(0,t) = 0, \quad u_x(1,t) = 2, & 0 \le t \le 1 \end{cases} \tag{29}$$

is numerically solved for the functions $\gamma(x,t) = 1/\Gamma(3-\alpha)t^{2-\alpha} - (x^2+t^2)^2 - 2$, $f(u) = u^2$ *and the derivative order* $\alpha = 0.5$ *by employing the finite difference scheme described above. The problem (29) possesses a closed-form solution* $u(x,t) = x^2 + t^2$. *The absolute errors of the numerical results obtained with our finite difference scheme are shown in Figure 1. For the grid of the size* $Nx \times Nt = 100 \times 100$, *the maximum error is equal to 0.0103. In Table 1, the deviation of the numerical values from the exact value of the solution u at the point* $(0.5, 0.5)$ *that is equal to* $1/8$ *is presented for different grid sizes.*

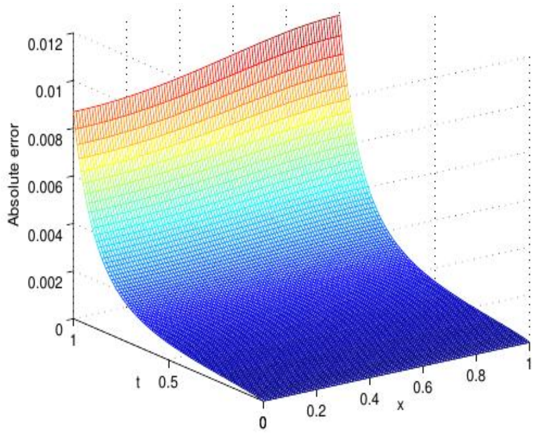

Figure 1. Absolute errors of the numerical results in Example 4.1 .

Nx× Nt	*Error*
20×20	*0.8062e-3*
40×40	*0.2939e-3*
60×60	*0.1064e-3*
80×80	*0.0383e-3*

Table 1. Deviations of the numerical results from the exact solution in Example 4.1.

Example 4.2. *In this example, we compare the numerical results obtained by the finite differences method with the results of the direct numerical integration* *using the representation (25) for the problem*

$$\begin{cases} \partial_t^\alpha u - u_{xx} = 0, \quad 0 < x < 1,\ 0 < t < 1 \\ u(x,0) = x(x-1), \quad 0 < x < 1, \\ u(0,t) = 0, \quad u(1,t) = 0, \quad 0 \le t \le 1. \end{cases} \tag{30}$$

For simplicity, the problem (30) contains the homogeneous boundary conditions and the representation (25) of the solution is as follows:

$$u(x,t) = \int_0^1 \Big[\theta_\alpha(x-\xi,t) - \theta_\alpha(x+\xi,t)\Big]\xi(\xi-1)d\xi, \tag{31}$$

where θ_α is defined as in the formula (13). The differences in numerical results obtained by the finite differences method the by the direct integration method for the solution u at the point $(0.5, 0.5)$ *are shown in Table 2 for different grid sizes. As we see in Table 2, the direct integration method that is based on our new representation (25) of the solution delivers about the same results as the finite difference method.*

N	*Variations*
100	*0.5340e-3*
200	*0.3318e-3*
400	*0.2307e-3*
800	*0.1801e-3*
1600	*0.1549e-3*

Table 2. Variations in numerical results obtained by the finite differences method the by the direct integration method in Example 4.2.

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