COMENIUS UNIVERSITY IN BRATISLAVA

FACULTY OF MATHEMATICS, PHYSICS AND INFORMATICS

FRACTIONAL DIFFUSION EQUATION

MASTER THESIS

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COMENIUS UNIVERSITY IN BRATISLAVA
FACULTY OF MATHEMATICS, PHYSICS AND INFORMATICS

FRACTIONAL DIFFUSION EQUATION

MASTER THESIS

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Department:	Department of Applied Mathematics and Statistics
Supervisor:	prof. RNDr. Marek Fila, DrSc.

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Cieľ: Cieľom práce je študovať fundamentálne riešenia rovnice vedenia tepla, v ktorej je prvá časová aj druhá priestorová derivácia nahradená deriváciami neceločíselného rádu.

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Petra Strišovská

Bratislava, 2017

Declaration on Word of Honour

I declare that all parts of this thesis have been written by myself using only the references explicitly referred to in the text and consultations with my supervisor.

Petra Strišovská

Bratislava, 2017

Abstrakt

STRIŠOVSKÁ, Petra: Difúzna rovnica s neceločíselnými deriváciami [Diplomová práca], Univerzita Komenského v Bratislave, Fakulta matematiky, fyziky a informatiky, Katedra aplikovanej matematiky a štatistiky; školiteľ: prof. RNDr. Marek Fila, DrSc., Bratislava, 2017, 57 s.

V tejto práci sa zaoberáme fundamentálnymi riešeniami časovej a priestorovo-časovej difúznej rovnice. Po stručnom uvedení to teórie neceločíselného integrálneho a diferenciálneho počtu je našim prvým cieľom nájdenie riešenia rovnice vedenia tepla, v ktorej bola časová derivácia nahradená Caputovou neceločíselnou deriváciou, na intervale pre dané okrajové a počiatočné podmienky. Ďalšími cieľmi je študovanie fundamentálnych riešení časovej a priestorovo-časovej neceločíselnej difúznej rovnice na nekonečnej jedno-dimenzionálnej tyči. V časovej neceločíselnej rovnici je prvá derivácia podľa časovej premennej zamenená za Caputovu neceločíselnú deriváciu a v priestorovo-časovej neceločíselnej rovnici je navyše druhá derivácia podľa priestorovej premennej nahradená Rieszovou neceločíselnou deriváciou.

Kľúčové slová: difúzna rovnica, rovnica vedenia tepla, Caputova neceločíselná derivácia, Rieszova neceločíselná derivácia, integrálne transformácie

Abstract

STRIŠOVSKÁ, Petra: Fractional diffusion equation [Master Thesis], Comenius University in Bratislava, Faculty of Mathematics, Physics and Informatics, Department of Applied Mathematics and Statistics; Supervisor: prof. RNDr. Marek Fila, DrSc., Bratislava, 2017, 57 p.

The purpose of this thesis is to study the fundamental solutions of the time and space-time fractional diffusion equations. After a brief introduction to the fractional calculus, the first goal is to find the solution of the diffusion equation, in which the derivative with respect to time is replaced by Caputo fractional derivative, on an interval for given boundary and initial conditions. Further goals are to study the fundamental solutions of the time fractional and space-time fractional diffusion equation on an infinite one-dimensional rod. In the time fractional equation, the first order time derivative is substituted with the Caputo fractional derivative and in addition to that, in the space-time fractional equation, the second order space derivative is replaced by Riesz fractional derivative.

Keywords: diffusion equation, heat equation, Caputo fractional derivative, Riesz fractional derivative, integral transforms

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Introduction

In 1695, L'Hôpital asked in a letter to Leibniz, what would happen, if the order of the derivative $d^n y/dx^n$ was $1/2$ instead of n. In his response, Leibniz states, that this would lead to a paradox, but he also predicts, that from this paradox "useful consequences will be drawn". This discussion is considered as the origin of the fractional calculus, field of mathematics, which is nowadays studied by increasing numbers of mathematicians and physicists and applied on many problems in physics, engineering or probability theory. In this master thesis we would like to study the application of the fractional calculus on one of the most famous partial differential equations, the diffusion equation

$$u_t(x,t) = u_{xx}(x,t).$$

The aim of this thesis is to study the solutions of the fractional diffusion equation, an equation which is gained from the standard diffusion equation above by replacing the time derivative with a Caputo fractional derivative and the space derivative with a Riesz fractional derivative. Our first goal will be to study the solutions of the time fractional diffusion equation, first on an interval, where we will search for a particular solution, which should satisfy given boundary and initial conditions, and then also on the one-dimensional infinite rod, where we will seek a fundamental solution. Furthermore we aim to study the fundamental solutions of the space-time fractional equation on the one-dimensional infinite rod.

In the first chapter, we will provide the theoretical background required for completing our goals. We will introduce some special functions of the fractional calculus, as well as some of their useful properties. We will also give the definitions of Laplace and Fourier integral transforms with some examples. In the end of this chapter we will give a brief introduction into the theory of fractional calculus with the definitions of several fractional derivatives and their comparisons. We will also try to explain, why there are different definitions used for fractional derivatives with respect to time and with respect to space.

The second chapter will be dedicated to the time fractional diffusion equation. In the first section we will search for a particular solution of the equation on an interval

$x \in [0, L]$ for given boundary and initial conditions. We will try to do so, by using similar tools as are used to solve the standard diffusion equation on an interval, namely the separation of variables and integral transforms. The integral transforms will be used also in the second section, where the solution of the equation on the entire one-dimensional rod $x \in R$ will be studied.

In the third chapter, the space-time fractional diffusion equation will be studied and we will try to obtain its fundamental solution by using the Fourier and Laplace integral transforms. In both chapters we will compare our results with other works, which treated this problems, as we are aware that the fractional diffusion equation has been studied by many authors already. In spite of that, we will be trying to obtain the solutions in the cases named above by means, which are approachable and understandable also for students.

1 Preliminaries

The history of fractional calculus is nearly as old as the history of the notation $d^n y/dx^n$ used for the derivative of $n-$th order which was developed by Leibniz. Shortly after the publishing of his works containing this notation, in 1695 Leibniz received a letter from L'Hôpital, asking him about the meaning of the notation for n equal 1/2. This was the birth of the fractional calculus. In the following decades the meaning of the derivatives of non-integer order intrigued some of the most famous mathematicians and physicists like Bernoulli, Lacroix or Abel, but the biggest progress was brought by Liouville and Riemann in the 19th century. The topic was then explored only by a few scientists and the true renaissance of fractional calculus began in 1974 at the first international conference on fractional calculus in New Haven, Connecticut. Since then the interest in the topic have risen significantly and there have been a lot of works and articles published, dedicated to the topic of fractional calculus an its applications.

Before we begin with the main topic of this master thesis, which is the finding of fundamental solutions to the diffusion equation containing fractional derivatives we would like to introduce some of the special functions which are often used in the fractional calculus as well as give an introduction to the fractional calculus itself containing some of the mostly used definitions of the fractional derivative and their properties.

1.1 Special Functions of the Fractional Calculus

1.1.1 Gamma Function

The first special function to be introduced is the gamma function $\Gamma(z)$, which is very helpful when considering a generalization of the factorial function $n!$ for non-integer or even complex values.

Definition 1.1
The function $\Gamma : \mathbb{R}^+ \to \mathbb{R}^+$ defined by the integral

$$\Gamma(x) = \int_0^\infty \mathrm{e}^{-t}\, t^{x-1} dt, \tag{1}$$

is called the gamma function.

The gamma function is helpful mostly because of its properties, from which we state the following:

- $\Gamma(z+1) = z\Gamma(z)$,
- $\Gamma(1) = 1$
- for $n \in \mathbb{N}:\ \Gamma(n+1) = n!$, (2)
- $\Gamma(z)\Gamma(1-z) = \dfrac{\pi}{\sin(\pi z)}$. (3)

1.1.2 Mittag-Leffler Function

The one-parameter Mittag-Leffler function defined by the series expansion

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)} \tag{4}$$

is the generalization of the exponential function e^z and it was introduced by Mittag-Leffler in 1903 in [Mittag-Leffler (1903)]. The generalization of this function, the two-parameter Mittag-Leffler function, was firstly defined by Wiman in [Wiman (1905)], but the main progress in the study of its properties was brought by Agarwal and Humbert 50 years later in their works [Agarwal (1953)], [Humbert (1953)] and [Agarwal, Humbert (1953)].

Definition 1.2
The two-parameter Mittag-Leffler function is defined by the series expansion

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \qquad \alpha > 0, \beta > 0. \tag{5}$$

Both of this functions were studied by many other authors since than, mostly due to the fact, that they play a very important role in the fractional calculus.

It can be seen directly from the definition, that for $\beta = 1$ we obtain the one-parameter Mittag-Leffler function:

$$E_{\alpha,1}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)} = E_\alpha(z)$$

Example 1.3

This example gives some special cases of the Mittag-Leffler function for some given values of the parameters α and β:

$$E_{1,1}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k+1)} = \sum_{k=0}^{\infty} \frac{z^k}{k!} = \mathrm{e}^z, \tag{6}$$

$$E_{1,2}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k+2)} = \sum_{k=0}^{\infty} \frac{z^k}{(k+1)!} = \frac{1}{z} \sum_{k=0}^{\infty} \frac{z^{k+1}}{(k+1)!} = \frac{\mathrm{e}^z - 1}{z}. \tag{7}$$

In general, the following holds:

$$E_{1,k}(z) = \frac{1}{z^{k-1}} \left[\mathrm{e}^z - \sum_{j=0}^{k-2} \frac{z^j}{j!} \right].$$

Other well-known particular cases of the Mittag-Leffler function are the hyperbolic sine and cosine:

$$E_{2,1}(z^2) = \sum_{k=0}^{\infty} \frac{z^{2k}}{\Gamma(2k+1)} = \sum_{k=0}^{\infty} \frac{z^{2k}}{(2k)!} = \cosh(z),$$

$$E_{2,2}(z^2) = \sum_{k=0}^{\infty} \frac{z^{2k}}{\Gamma(2k+2)} = \frac{1}{z} \sum_{k=0}^{\infty} \frac{z^{2k+1}}{(2k+1)!} = \frac{\sinh(z)}{z}.$$

The most common example of a two-parameter Mittag-Leffler function with non-integer parameter is

$$E_{1/2,1}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k/2+1)} = \mathrm{e}^{z^2}\, erfc(-z),$$

where

$$erfc(z) = \frac{2}{\sqrt{\pi}} \int_z^{\infty} \mathrm{e}^{-t^2}\, dt$$

is the error function complement.

1.1.3 M-Wright Function

In this subsection, we would like to introduce some functions of the Wright type. The definitions and theorems are given according to [Mainardi, Mura, Pagnini (2010)].

Let us first define the general Wright function:

Definition 1.4

The Wright function is defined by the series representation

$$W_{\lambda,\mu}(z) = \sum_{n=0}^{\infty} \frac{z^n}{n!\Gamma(\lambda n + \mu)}, \qquad \lambda > -1, \qquad \mu \in \mathbb{C}\,. \tag{8}$$

This function is convergent in the whole complex z-plane. More interesting for us will be an auxiliary function of the Wright type, known as the M-Wright function, which can be defined as a special case of the Wright function:

$$M_\nu(z) = W_{-\nu,1-\nu}(-z), \qquad 0 < \nu < 1.$$

Using the reflection formula (3) of the Gamma function, the following series representation of the M-Wright function can be given:

$$M_\nu(z) = \sum_{n=0}^{\infty} \frac{(-z)^n}{n!\Gamma(-\nu n + 1 - \nu)} = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{(-z)^{n-1}}{(n-1)!} \Gamma(\nu n) \sin(\pi \nu n). \tag{9}$$

One of the properties of the M-Wright functions, which will be later useful is the rule for absolute moments.

Theorem 1.5

Let $M_\nu(x)$ denote the M-Wright function of a real variable x. Than the following identity holds for $0 \leq \nu < 1$ and $x \in \mathbb{R}^+$

$$\int_0^\infty x^\delta M_\nu(x) dx = \frac{\Gamma(\delta+1)}{\Gamma(\nu\delta+1)}, \quad \delta \in \mathbb{R}, \ \ \delta > -1. \tag{10}$$

The proof of this identity requires the use of the integral representation of the M-Wright function, as well as complex analysis methods, and can be found in [Mainardi, Mura, Pagnini (2010), p. 11ff].

1.2 Integral Transforms

This section will be used to define the Integral Transforms as well as to state and prove some of their properties, which will be used in the subsequent chapters.

1.2.1 Laplace Transform

In the following we would like to define the Laplace transform and give some of its properties according to [Pinkus, Zafrany (1997)].

Definition 1.6

Let the function $f : [0, \infty) \to \mathbb{C}$ be piecewise continuous. Then the Laplace transform of the function f is given by the formula

$$\mathcal{L}[f](s) = \int_0^\infty \mathrm{e}^{-st} f(t)dt, \quad s \in D \subset \mathbb{R} \tag{11}$$

if the integral exists.

One of the main properties of the Laplace transform, which will be used, is the Laplace transform of a convolution of two functions $f : [0, \infty) \to \mathbb{C}$ and $g : [0, \infty) \to \mathbb{C}$. The convolution is defined as

$$(f * g)(t) = \int_0^t f(t-y)g(y)dy, \tag{12}$$

if $t \geq 0$.

Theorem 1.7

If there exists $a \in \mathbb{R}$, $K > 0$ such that $|f(t)| \leq K e^{at}$, $|g(t)| \leq K\,\mathrm{e}^{at}$, $t \geq 0$, then $|(f * g)(t)| \leq K^2 t\,\mathrm{e}^{at}$, $t \geq 0$ and

$$\mathcal{L}[f * g](s) = \mathcal{L}[f](s) \cdot \mathcal{L}[g](s), \quad s > a. \tag{13}$$

Other well known property of the Laplace transform is the rule for computing the Laplace transform of a derivative.

Theorem 1.8

Let f, f',... $f^{(n)}$ be continuous, $|f(t)| \leq K\,\mathrm{e}^{at}$ for $K > 0$, $a \in \mathbb{R}$, and all $t \geq 0$, then $\mathcal{L}[f^{(n)}(t)](s)$ is defined for all $s > a$ and

$$\begin{aligned}\mathcal{L}[f^{(n)}(t)](s) &= s^n\,\mathcal{L}[f(t)](s) - s^{n-1}f(0) - s^{n-2}f'(0) - \dots - f^{(n-1)}(0) \\ &= s^n\,\mathcal{L}[f(t)](s) - \sum_{k=1}^{n} s^{n-k} f^{(k-1)}(0).\end{aligned} \tag{14}$$

Using this property we can compute for example the Laplace transform of the function $f(t) = t^n$, $n \in \mathbb{N}$:

$$\begin{aligned}f^n(t) &= \frac{d^n}{dt^n}t^n = n! \\ \mathcal{L}[f^{(n)}(t)](s) &= \mathcal{L}[n!](s) = \frac{n!}{s} \\ \mathcal{L}[f(t)](s) &= \mathcal{L}[t^n](s) = \mathcal{L}[f^{(n)}(t)](s)\cdot\frac{1}{s^n} = \frac{n!}{s}\cdot\frac{1}{s^n} = \frac{n!}{s^{n+1}}.\end{aligned}$$

This can be generalized for $a \in \mathbb{R}$, $a > -1$ using the Gamma function:

$$\mathcal{L}[t^a](s) = \frac{\Gamma(a+1)}{s^{a+1}}. \tag{15}$$

Using the property (13) and the Heaviside function

$$h_c(t) = \begin{cases} 0, & \text{if } 0 \leq t < c \\ 1, & \text{if } t \geq c, \end{cases}$$

as well as its Laplace transform

$$\mathcal{L}[h_c(t)] = \frac{\mathrm{e}^{-cs}}{s}, \qquad c \geq 0,$$

we can show, that the following property holds

$$\mathcal{L}\left[\int_0^t f(\tau)d\tau\right](s) = \mathcal{L}[h_0 * f](s) = \mathcal{L}[h_0](s)\cdot\mathcal{L}[f](s) = \frac{1}{s}\,\mathcal{L}[f](s). \tag{16}$$

1.2.2 Fourier Transform

In this subsection we would like to introduce the Fourier transform and some of its properties. We will use the notations based on [Mainardi, Luchko, Pagnini (2001)]. In the further discussions, let us use the notation $L^c(\mathcal{I})$ for a class of complex-valued functions of a real variable ($f : \mathbb{R} \to \mathbb{C}$) for which the improper Riemann integral on a given open interval $\mathcal{I} = (a, b)$ absolutely converges.

Definition 1.9 (**Fourier Transform and Inverse Fourier Transform**)
Let us define the Fourier transform of a function $f(x) \in L^c(\mathbb{R})$ as follows:

$$F(\kappa) = \mathcal{F}[f(x)](\kappa) = \int_{-\infty}^{\infty} f(x)\, \mathrm{e}^{+i\kappa x}\, dx, \qquad \kappa \in \mathbb{R}\,. \tag{17}$$

Then, the inverse Fourier transform can be defined as

$$f(x) = \mathcal{F}^{-1}[F(\kappa)](x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\kappa)\, \mathrm{e}^{-i\kappa x}\, d\kappa, \qquad x \in \mathbb{R}\,. \tag{18}$$

The second formula holds true for any piecewise differentiable function $f(x)$ at all points, where $f(x)$ is continuous. The integral in the formula has to be understood in the sense of the Cauchy principal value.

The first property of the Fourier transform, which we would like to state and prove, is the following scaling property:

Theorem 1.10
Let $f(x) \in L^c(\mathbb{R})$, a, $b \in \mathbb{R}$, $a \neq 0$. Then $g(x) = f(ax + b)$ belongs to $L^c(\mathbb{R})$ and

$$\mathcal{F}[g(x)](\kappa) = \frac{1}{|a|}\, \mathrm{e}^{\frac{-i\kappa b}{a}}\, \mathcal{F}\left[f(x)\right] \left(\frac{\kappa}{a}\right). \tag{19}$$

Proof. Let us prove the property for the case, when $a > 0$:

$$\begin{aligned}
\mathcal{F}[g(x)](\kappa) &= \int_{-\infty}^{\infty} f(ax+b)\, \mathrm{e}^{i\kappa x}\, dx \\
&= \left[\begin{smallmatrix} y=ax+b, \\ dy=a\ dx \end{smallmatrix}\right] = \int_{-\infty}^{\infty} f(y)\, \mathrm{e}^{i\kappa \frac{y-b}{a}}\, \frac{dy}{a} \\
&= \frac{1}{a}\, \mathrm{e}^{-i\kappa \frac{b}{a}} \int_{-\infty}^{\infty} f(y)\, \mathrm{e}^{iy\frac{\kappa}{a}}\, dy.
\end{aligned}$$

For $a < 0$ the proof would unfold equivalently. $\square$

One of the properties of the Fourier transform, which will be used later, helps to compute the Fourier transform of the derivative:

Theorem 1.11

Let the function $f(x)$ be continuous and $f(x),\ f'(x) \in L^c(\mathbb{R})$. Then

$$\mathcal{F}[f'(x)](\kappa) = -i\kappa \cdot F(\kappa). \tag{20}$$

Proof. To prove this property, we will use the inverse Fourier transform:

$$\begin{aligned} f'(x) &= \frac{d}{dx}\,\mathcal{F}^{-1}[F(\kappa)](x) \\ &= \frac{d}{dx}\frac{1}{2\pi}\int_{-\infty}^{\infty} F(\kappa)\,\mathrm{e}^{-i\kappa x}\,d\kappa \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\kappa)\frac{d}{dx}\,\mathrm{e}^{-i\kappa x}\,d\kappa \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} -i\kappa \cdot F(\kappa)\,\mathrm{e}^{-i\kappa x}\,d\kappa. \end{aligned}$$

$\square$

From this we can see, that the Fourier transform of a derivative of the function $f(x)$ can be computed using the Fourier transform of the function $f(x)$ itself. This property can be used also to compute the Fourier transform for higher order derivatives of the function $f(x)$.

Corollary 1.12

If $f(x),\ f'(x),\ \ldots\ ,\ f^{(n-1)}(x)$ are continuous, $f(x),\ f'(x),\ \ldots\ ,\ f^{(n)}(x) \in L^c(\mathbb{R})$, then

$$\mathcal{F}[f^{(n)}(x)](\kappa) = (-i\kappa)^n \cdot F(\kappa). \tag{21}$$

Another very useful property of the Fourier transform gives us similarly to the Laplace transform a relationship for the Fourier transform of a convolution.

Theorem 1.13

The Fourier transform of a convolution of two functions $f(x)$, $g(x) \in L^c(\mathcal{R})$:

$$(f * g)(x) = \int_{-\infty}^{\infty} f(x-y)g(y)dy = \int_{-\infty}^{\infty} f(y)g(x-y)dy$$

can be computed as the product of the Fourier transforms of the two functions

$$\mathcal{F}[(f * g)(x)](\kappa) = \mathcal{F}[f(x)](\kappa) \cdot \mathcal{F}[(g(x)](\kappa). \tag{22}$$

Proof.

$$\begin{aligned}
\mathcal{F}[(f * g)(x)](\kappa) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(y)g(x-y)dy \, \mathrm{e}^{i\kappa x} \, dx \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(y) \, \mathrm{e}^{i\kappa y} \, g(x-y) \, \mathrm{e}^{i\kappa(x-y)} \, dx \;\; dy \\
&= \int_{-\infty}^{\infty} f(y) \, \mathrm{e}^{i\kappa y} \, dy \int_{-\infty}^{\infty} g(x-y) \, \mathrm{e}^{i\kappa(x-y)} \, dx.
\end{aligned}$$

□

One of the Fourier transforms, which will be useful in the following, is the Fourier transform of the M-Wright function:

$$\mathcal{F}[M_\nu(|x|)](\kappa) = 2E_{2\mu}(-\kappa^2), \tag{23}$$

which was proven in [Mainardi, Mura, Pagnini (2010), p. 13ff] in a similar way, as we will use now:

$$\begin{aligned}
\mathcal{F}[M_\nu(|x|)](\kappa) &= \int_{-\infty}^{\infty} M_\nu(|x|) \, \mathrm{e}^{i\kappa x} \, dx \\
&= \int_{-\infty}^{\infty} M_\nu(|x|)(\cos(\kappa x) + i \sin(\kappa x))dx \\
&= 2 \int_0^{\infty} M_\nu(x) \cos(\kappa x) dx \\
&= 2 \int_0^{\infty} M_\nu(x) \sum_{j=0}^{\infty} \frac{(-1)^j (\kappa x)^{2j}}{(2j)!} dx
\end{aligned}$$

$$= 2\sum_{j=0}^{\infty} \frac{(-1)^j \kappa^{2j}}{(2j)!} \int_0^{\infty} x^{2j} M_\nu(x) dx.$$

Using the identity (10) for the absolute moments of the M-Wright function, the following equation can be satisfied:

$$\begin{aligned}
\mathcal{F}[M_\nu(|x|)](\kappa) &= 2\sum_{j=0}^{\infty} \frac{(-1)^j \kappa^{2j}}{(2j)!} \frac{\Gamma(2j+1)}{\Gamma(\nu 2j+1)} \\
&= 2\sum_{j=0}^{\infty} \frac{(-\kappa^2)^j}{\Gamma(2\nu j+1)} = 2E_{2\nu}(-\kappa^2).
\end{aligned}$$

1.3 Introduction to the Fractional Calculus

In this section, we would like to define some of the operators of the fractional calculus, as well as give their properties.

1.3.1 Riemann-Liouville Fractional Calculus

Starting from the definition of the n-fold repeated integral of f based at a

$$ {}_aD_t^{-n} f(t) = {}_aI_t^n f(t) = \int_a^t \int_a^{\tau_1} \int_a^{\tau_2} ... \int_a^{\tau_{n-2}} \int_a^{\tau_{n-1}} f(\tau) d\tau d\tau_{n-1} ... d\tau_3 \, d\tau_2 \, d\tau_1, \tag{24}$$

we would like to show a way to prove the Cauchy formula for the integral of order n:

$$ {}_aI_t^n f(t) = \int_a^t \frac{(t-\tau)^{n-1}}{(n-1)!} f(\tau) d\tau. \tag{25}$$

This formula was proven in [Miller, Ross (1993), p.23ff] using the method of iterated integral. This method also helps to see the connection between the classic integral operator and the Riemann-Liouville fractional integral. In the fractional calculus the connection between the integrals and the derivatives is much stronger than in the classical calculus, so that we will use the operator D^α for both integration, when $\alpha < 0$, and differentiation, when $\alpha > 0$. Let us begin with the assumption, that (24) can be written as a simple integral of the following form:

$$ \int_a^t K_n(t, \tau) f(\tau) d\tau. \tag{26}$$

The kernel $K_n(t, \tau)$ depends on n, t and τ. We look for such function $K_n(t, \tau)$, which could be than generalized also for $n \notin \mathbb{N}, n > 0$. To find this function we need to use a property of a double integral, which follows from the Fubini theorem: Suppose the function $g(\tau_1, \tau)$ is continuous for all $(\tau_1, \tau) \in [a, b] \times [a, b]$. Then the following holds:

$$ \int_a^t \int_a^{\tau_1} g(\tau_1, \tau) d\tau \, d\tau_1 = \int_a^t \int_\tau^t g(\tau_1, \tau) d\tau_1 \, d\tau. \tag{27}$$

As we can see in the figure below the integration area:

$$\begin{aligned}\Delta &= \{(\tau_1, \tau) \in \mathbb{R}^2 \mid a \le \tau \le \tau_1 \le t\} \\ &= \{(\tau_1, \tau) \in \mathbb{R}^2 \mid a \le \tau_1 \le t, a \le \tau \le \tau_1\} \\ &= \{(\tau_1, \tau) \in \mathbb{R}^2 \mid a \le \tau \le t, \tau \le \tau_1 \le t\},\end{aligned}$$

stays unchanged.

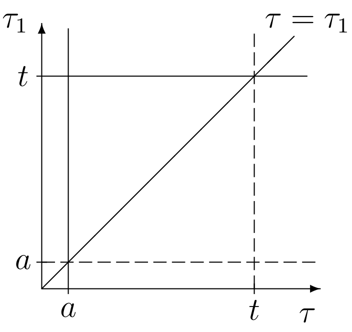

Figure 1: Integration area.

Because in this case the function

$$g(\tau_1, \tau) \equiv f(\tau)$$

does not depend on τ_1, we receive from (27):

$$\int_a^t \int_a^{\tau_1} f(\tau) d\tau \, d\tau_1 = \int_a^t \int_\tau^t f(\tau) d\tau_1 \, d\tau = \int_a^t f(\tau) \int_\tau^t d\tau_1 \, d\tau = \int_a^t f(\tau)(t - \tau) d\tau. \quad (28)$$

The double integral was reduced to a single integral. We use this result twice to compute the triple integral:

$$\begin{aligned}{}_aD_t^{-3} f(t) = {}_aI_t^3 f(t) &= \int_a^t \int_a^{\tau_1} \int_a^{\tau_2} f(\tau) d\tau \, d\tau_2 \, d\tau_1 \\ &= \int_a^t \left[\int_a^{\tau_1} \int_a^{\tau_2} f(\tau) d\tau \, d\tau_2 \right] d\tau_1 \\ &= \int_a^t \left[\int_a^t f(\tau)(\tau_1 - \tau) d\tau \right] d\tau_1\end{aligned}$$

$$= \int_a^t f(\tau) \int_\tau^t (\tau_1 - \tau) d\tau_1 \, d\tau$$
$$= \int_a^t f(\tau) \frac{(t-\tau)^2}{2} d\tau.$$

Using this approach also for the higher orders of integration would lead to the formula for the n-fold integral (24):

$$ {}_aD_t^{-n} f(t) = {}_aI_t^n f(t) = \int_a^t \frac{(t-\tau)^{n-1}}{(n-1)!} f(\tau) d\tau. \tag{29}$$

So the function satisfying the assumption (26) is:

$$K_n(t,\tau) = \frac{(t-\tau)^{n-1}}{(n-1)!}.$$

Using the fact that the Gamma function (1) is a generalization of the factorial for non-integer numbers, we can easily see that the formula above can be also generalized for non-integer order of integration. From there we receive the following operator, defined as in [Baleanu, Muslih (2007)]:

$$ {}_aD_t^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-\tau)^{\alpha-1} f(\tau) d\tau, \tag{30}$$

which is known as the Riemann-Liouville fractional integral of order $\alpha \in \mathbb{R}^+$. This integral is an important component of some of the mostly used definitions of fractional derivatives. It is also called the left Riemann-Liouville fractional integral, as it is defined for $t > a$ and the integral in the definition (30) is computed over the left-hand side of the function $f(t)$. Similarly, the right Riemann-Liouville fractional integral can be defined for $t < b$ in a following way:

$$ {}_tD_b^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_t^b (\tau - t)^{\alpha-1} f(\tau) d\tau. \tag{31}$$

In the special case, when a and b are equal 0, the operators ${}_0D_t^{-\alpha} f(t)$ and ${}_tD_0^{-\alpha} f(t)$ are referred to as Riemann fractional integrals. For $a = -\infty$ and $b = \infty$, the name Liouville fractional integral is used. The classical definition of the fractional derivative is the Riemann-Liouville fractional derivative, but one has to understand that unlike the derivative of integer order, the non-integer derivative has many definitions and the particular derivatives have only a few properties in common.

Definition 1.14 (**Left and Right Riemann-Liouville fractional derivative**) *The left Riemann-Liouville fractional derivative of order α is defined as follows:*

$$_aD_t^\alpha f(t) = \frac{d^n}{dt^n}\left({}_aD_t^{-(n-\alpha)} f(t)\right) = \frac{1}{\Gamma(n-\alpha)}\left(\frac{d}{dt}\right)^n \int_a^t (t-\tau)^{n-\alpha-1} f(\tau)d\tau, \tag{32}$$

and the right Riemann-Liouville fractional derivative of order α can be defined in the following way:

$$_tD_b^\alpha f(t) = (-1)^n \frac{d^n}{dt^n}\left({}_tD_b^{-(n-\alpha)} f(t)\right) = \frac{1}{\Gamma(n-\alpha)}\left(-\frac{d}{dt}\right)^n \int_t^b (\tau-t)^{n-\alpha-1} f(\tau)d\tau, \tag{33}$$

where $n-1 \leq \alpha < n$.

If we interpret variable t as time, the function f as a physical process in time and $f(t)$ as the state of the process at the present time t, then it can be easily understood, that the left Riemann-Liouville fractional derivative operates on the past and the right Riemann-Liouville fractional derivative on the future states of the process f. This is shown also by the following figure from [Podlubny (1999), p.89]:

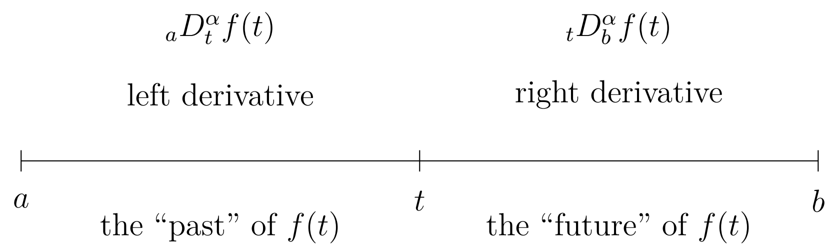

Figure 2: Interpretation of fractional derivatives as operators on a physical process f in time.

Similarly to Riemann-Liouville fractional integrals, the special cases of the above fractional derivatives $_aD_t^\alpha f(t)$ and $_tD_b^\alpha f(t)$, when a, $b = 0$ or $a = -\infty$ and $b = \infty$ are referred to as the Riemann fractional derivatives and Liouville fractional derivatives respectively.

1.3.2 Caputo fractional derivative

The next definition of a fractional derivative, which we will later use instead of the derivative with respect to time in the heat equation, is the Caputo fractional derivative.

Definition 1.15 (**Left Caputo fractional derivative**)
The left Caputo fractional derivative of order $n-1 \leq \alpha < n$ is defined as follows:

$$\begin{aligned} {}_a^C D_t^\alpha f(t) = {}_a D_t^{-(n-\alpha)} \left(\frac{d^n}{dt^n} f(t) \right) &= \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-\tau)^{n-\alpha-1} \left(\frac{d}{d\tau} \right)^n f(\tau) d\tau \\ &= \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-\tau)^{n-\alpha-1} f^{(n)}(\tau) d\tau. \end{aligned} \tag{34}$$

Although the difference between the Riemann-Liouville and the Caputo definition of the fractional derivative might seem insignificant, it can be shown even on the simple example of a constant function that the fractional and integer derivative do not commute:

Example 1.16
In this example, we differentiate the function $f(t) \equiv c$, $c \in \mathbb{R}$ to the order $\alpha = 1/2$, using first the left Riemann-Liouville and than the left Caputo definition of the fractional derivative:

$$\begin{aligned} {}_a D_t^\alpha c &= \frac{1}{\Gamma(1/2)} \frac{d}{dt} \int_a^t (t-\tau)^{-1/2}\, c\, d\tau = \frac{c}{\Gamma(1/2)} \frac{d}{dt} \left[-2\sqrt{t-\tau} \right]_a^t = \frac{1}{\Gamma(1/2)} \frac{c}{\sqrt{t-a}}, \\ {}_a^C D_t^\alpha c &= \frac{1}{\Gamma(1/2)} \int_a^t (t-\tau)^{-1/2} \frac{dc}{d\tau} d\tau = \frac{1}{\Gamma(1/2)} \int_a^t \frac{0}{\sqrt{t-\tau}} d\tau = 0. \end{aligned}$$

As we will later state, the Laplace transform is very helpful for solving fractional differential equations, especially those, which contain Caputo fractional derivatives. Because of that, we compute the Laplace transform of the left Caputo fractional derivative. It is obvious from the definition (34) that the Caputo derivative for $a = 0$ has the form of a convolution and we can use the property (13) to compute its Laplace transform:

$$\begin{aligned}\mathcal{L}[{}_0^C D_t^\alpha f(t)](s) &= \mathcal{L}\left[\frac{1}{\Gamma(n-\alpha)}\int_0^t (t-\tau)^{n-\alpha-1} f^{(n)}(\tau)d\tau\right](s)\\ &= \frac{1}{\Gamma(n-\alpha)}\,\mathcal{L}[t^{n-\alpha-1}](s)\,\mathcal{L}[f^{(n)}(t)](s).\end{aligned}$$

To compute $\mathcal{L}[t^{n-\alpha-1}](s)$ we can use the Laplace transform (15), because it follows directly from the definition of the Caputo fractional derivative, that $n-\alpha-1$ is greater than -1. This leads to the following

$$\mathcal{L}[{}_0^C D_t^\alpha f(t)](s) = \frac{1}{\Gamma(n-\alpha)}\frac{\Gamma(n-\alpha-1+1)}{s^{n-\alpha-1+1}}\,\mathcal{L}[f^{(n)}(t)](s) = \frac{1}{s^{n-\alpha}}\,\mathcal{L}[f^{(n)}(t)](s).$$

Using the property (14) of Laplace transform we receive:

$$\begin{aligned}\mathcal{L}[{}_0^C D_t^\alpha f(t)](s) &= \frac{1}{s^{n-\alpha}}\left[s^n\,\mathcal{L}[f(t)](s) - \sum_{k=1}^{n} s^{n-k} f^{(k-1)}(0)\right]\\ &= s^\alpha\,\mathcal{L}[f(t)](s) - \frac{1}{s^{n-\alpha}}\sum_{k=1}^{n} s^{n-k} f^{(k-1)}(0)\\ &= s^\alpha\,\mathcal{L}[f(t)](s) - \sum_{k=1}^{n} s^{\alpha-k} f^{(k-1)}(0). \qquad (35)\end{aligned}$$

As we mentioned before, the left Caputo fractional derivative will be used to replace the derivative with respect to time. If we use an operator on a function of time, it is understandable, that this operator should only take into account the left-hand side of the function, as this can be understood as the past values of the function. Similarly, as the functions of time are usually defined only for $t > 0$, it is clear that the fractional integral used in the definition of the Caputo time-fractional derivative is the left Riemann fractional integral. For an operator on a function of space, such approach would not be meaningful. That is why, we have to introduce another definition of fractional derivative, which could be used to substitute the derivative with respect to space in the diffusion equation.

1.3.3 Riesz fractional derivative

In this subsection, we will introduce the Riesz fractional derivative, which can be defined as a linear combination of left and right Liouville fractional derivatives. The definition and properties of the Riesz fractional derivative, as well as their proofs, will be given according to [Herrmann (2014)]. Based on [Herrmann (2014)], the Riesz fractional derivative of a function $g : \mathbb{R} \to \mathbb{R}$ is defined as

$$D^{\alpha}_{RZ} f(x) = -\frac{{}_{-\infty}D^{\alpha}_{x} f(x) + {}_{x}D^{\alpha}_{\infty} f(x)}{2\cos(\pi\alpha/2)}. \tag{36}$$

This definition can be for $0 < \alpha < 2$ explicitly written also in the following form:

$$D^{\alpha}_{RZ} f(x) = \frac{\Gamma(1+\alpha)}{\pi} \sin(\alpha\pi/2) \int_{0}^{\infty} \frac{f(x+\xi) - 2f(x) + f(x-\xi)}{\xi^{1+\alpha}} d\xi \tag{37}$$

To prove, that the definitions (36) and (37) are equivalent, we will first show, that the left and right Liouville derivatives can be written in the following alternative form:

$$\begin{aligned} {}_{-\infty}D^{\alpha}_{x} f(x) &= \frac{\alpha}{\Gamma(1-\alpha)} \int_{0}^{\infty} \frac{f(x) - f(x-\xi)}{\xi^{\alpha-1}} d\xi, \\ {}_{x}D^{\alpha}_{\infty} f(x) &= \frac{\alpha}{\Gamma(1-\alpha)} \int_{0}^{\infty} \frac{f(x) - f(x+\xi)}{\xi^{\alpha-1}} d\xi. \end{aligned}$$

This identity can be proven using the integration by parts, first for the left Liouville fractional derivative:

$$\begin{aligned} {}_{-\infty}D^{\alpha}_{x} f(x) &= \frac{1}{\Gamma(1-\alpha)} \frac{\partial}{\partial x} \int_{-\infty}^{x} (x-\xi)^{-\alpha} f(\xi) d\xi \\ &= \begin{bmatrix} x-\xi=\mu \\ -d\xi=d\mu \end{bmatrix} = \frac{1}{\Gamma(1-\alpha)} \frac{\partial}{\partial x} \int_{0}^{\infty} \mu^{-\alpha} f(x-\mu) d\mu \\ &= \frac{1}{\Gamma(1-\alpha)} \int_{0}^{\infty} \mu^{-\alpha} \frac{\partial}{\partial x} f(x-\mu) d\mu \\ &= \frac{1}{\Gamma(1-\alpha)} \int_{0}^{\infty} \mu^{-\alpha} \left(-\frac{\partial}{\partial \mu} f(x-\mu) \right) d\mu \\ &= \frac{\alpha}{\Gamma(1-\alpha)} \left(\int_{0}^{\infty} \frac{f(x)}{\mu^{\alpha+1}} d\mu - \int_{0}^{\infty} \frac{f(x-\mu)}{\mu^{\alpha+1}} d\mu \right), \end{aligned}$$

and now also for the right Liouville fractional derivative:

$$
\begin{aligned}
{}_xD^{\alpha}_{\infty}f(x) &= \frac{1}{\Gamma(1-\alpha)}\left(-\frac{\partial}{\partial x}\right)\int_x^{\infty}(\xi-x)^{-\alpha}f(\xi)d\xi \\
&= \begin{bmatrix} \scriptstyle \xi-x=\mu \\ \scriptstyle d\xi=d\mu \end{bmatrix} = -\frac{1}{\Gamma(1-\alpha)}\frac{\partial}{\partial x}\int_0^{\infty}\mu^{-\alpha}f(\mu+x)d\mu \\
&= -\frac{1}{\Gamma(1-\alpha)}\int_0^{\infty}\mu^{-\alpha}\frac{\partial}{\partial x}f(\mu+x)d\mu \\
&= -\frac{1}{\Gamma(1-\alpha)}\int_0^{\infty}\mu^{-\alpha}\left(\frac{\partial}{\partial\mu}f(\mu+x)\right)d\mu \\
&= \frac{\alpha}{\Gamma(1-\alpha)}\left(\int_0^{\infty}\frac{f(x)}{\mu^{\alpha+1}}d\mu - \int_0^{\infty}\frac{f(\mu+x)}{\mu^{\alpha+1}}d\mu\right).
\end{aligned}
$$

Using the property (3) of the gamma function as well as the basic properties of trigonometric functions, it is easy to show the following:

$$
\frac{\alpha}{\Gamma(1-\alpha)} = \Gamma(1+\alpha)\frac{\sin(\pi\alpha)}{\pi} = \frac{\Gamma(1+\alpha)}{\pi}2\sin(\pi\alpha/2)\cos(\pi\alpha/2),
$$

thus the equivalence of the two definitions of the Riesz fractional derivative of order $0<\alpha<2$ is proven.

The Riesz fractional derivative will be used instead of the second order partial derivative with respect to space. Thus we would like to show, that for $\alpha=2$, the Riesz fractional derivative is equivalent with the standard second order derivative. We start with the definition of the left Riemann-Liouville fractional derivative (32). To get the Liouville derivative, we set $a=-\infty$. As this fractional operator is defined for $n-1\leq\alpha<n$, our n for $\alpha=2$ will be 3:

$$
\begin{aligned}
{}_{-\infty}D^{2}_{x}f(x) &= \frac{1}{\Gamma(3-2)}\left(\frac{d}{dx}\right)^3\int_{-\infty}^{x}(x-\xi)^{3-2-1}f(\xi)d\xi \\
&= \left(\frac{d}{dx}\right)^3\int_{-\infty}^{x}f(\xi)d\xi = \frac{d^2}{dx^2}f(x).
\end{aligned}
$$

Similarly for the right Liouville fractional derivative, we use the definition of the right

Riemann-Liouville fractional derivative (33), for $b = \infty$, $\alpha = 2$ and $n = 3$:

$$
\begin{aligned}
{}_xD^2_\infty f(x) &= \frac{1}{\Gamma(3-2)} \left(-\frac{d}{dx}\right)^3 \int_x^\infty (\xi - x)^{3-2-1} f(\xi) d\xi \\
&= -\left(\frac{d}{dx}\right)^3 \int_x^\infty f(\xi) d\xi = -\frac{d^2}{dx^2}(-f(x)) = \frac{d^2}{dx^2} f(x).
\end{aligned}
$$

We can now use these results to compute the Riesz fractional derivative for $\alpha = 2$ according to the definition (36):

$$
D^2_{RZ} f(x) = -\frac{{}_{-\infty}D^2_x f(x) + {}_xD^2_\infty f(x)}{2\cos(\pi \cdot 2/2)} = -\frac{2f''(x)}{-2} = f''(x).
$$

Another property of the Riesz fractional derivative, which will be used later, is the rule for computing of the Fourier transform of the derivative.

Theorem 1.17

Let the Riesz fractional derivative $D^\alpha_{RZ} f(x)$ of order $\alpha > 0$ be from the class of functions $L^c(\mathbb{R})$. Then the following holds for the Fourier transform of the Riesz fractional derivative:

$$
\mathcal{F}[D^\alpha_{RZ} f(x)](\kappa) = -|\kappa|^\alpha \, \mathcal{F}[f(x)](\kappa). \tag{38}
$$

Proof. To prove this property we will use the Fourier transform of the left and right Liouville fractional integral, which was already computed in [Podlubny (1999), p. 110ff] for $0 < \beta < 1$:

$$
\begin{aligned}
\mathcal{F}[{}_{-\infty}D^{-\beta}_x f(x)](\kappa) &= (i\kappa)^{-\beta} \, \mathcal{F}[f(x)](\kappa), \\
\mathcal{F}[{}_xD^{-\beta}_\infty f(x)](\kappa) &= (-i\kappa)^{-\beta} \, \mathcal{F}[f(x)](\kappa).
\end{aligned}
$$

Using these properties, as well as (21), we can easily compute the Fourier transform of the Liouville fractional derivatives for $n-1 \le \alpha < n$:

$$\begin{aligned}\mathcal{F}[{}_{-\infty}D_x^{\alpha} f(x)](\kappa) &= \mathcal{F}\left[\left(\frac{d}{dx}\right)^n {}_{-\infty}D_x^{\alpha-n} f(x)\right](\kappa) \\ &= (-i\kappa)^n \cdot \mathcal{F}[{}_{-\infty}D_x^{\alpha-n} f(x)](\kappa) = (-i\kappa)^n (i\kappa)^{\alpha-n}\, \mathcal{F}[f(x)](\kappa) \\ &= (-1)^n (i\kappa)^{\alpha}\, \mathcal{F}[f(x)](\kappa),\end{aligned}$$

$$\begin{aligned}\mathcal{F}[{}_xD_{\infty}^{\alpha} f(x)](\kappa) &= \mathcal{F}\left[\left(-\frac{d}{dx}\right)^n {}_xD_{\infty}^{\alpha-n} f(x)\right](\kappa) \\ &= (-1)^n (-i\kappa)^n\, \mathcal{F}[{}_xD_{\infty}^{\alpha-n} f(x)](\kappa) = (-1)^n (-i\kappa)^n (-i\kappa)^{\alpha-n}\, \mathcal{F}[f(x)](\kappa) \\ &= (-1)^n (-i\kappa)^{\alpha}\, \mathcal{F}[f(x)](\kappa).\end{aligned}$$

This leads to the following formula for computing the Fourier transform of the Riesz fractional derivative for $0 < \alpha < 2$, $\alpha \neq 1$:

$$\begin{aligned}\mathcal{F}[D_{RZ}^{\alpha} f(x)](\kappa) &= \mathcal{F}\left[-\frac{{}_{-\infty}D_x^{\alpha} f(x) + {}_xD_{\infty}^{\alpha} f(x)}{2\cos(\pi\alpha/2)}\right](\kappa) \\ &= -\frac{(-1)^2 (i\kappa)^{\alpha}\, \mathcal{F}[f(x)](\kappa) + (-1)^2 (-i\kappa)^{\alpha}\, \mathcal{F}[f(x)](\kappa)}{2\cos(\pi\alpha/2)} \\ &= -\frac{(i\kappa)^{\alpha} + (-i\kappa)^{\alpha}}{2\cos(\pi\alpha/2)}\, \mathcal{F}[f(x)](\kappa) = -|\kappa|^{\alpha}\, \mathcal{F}[f(x)](\kappa).\end{aligned}$$

□

2 Time-Fractional Diffusion Equation

In this chapter, we would like to compute the solution of the diffusion equation we receive, when we replace the first derivative with respect to time with a Caputo derivative of fractional order $\alpha \in (0,2] \subset \mathbb{R}$:

$$ {}_0^C D_t^\alpha u(x,t) = D_x^2 u(x,t). \tag{39}$$

2.1 Time-Fractional Diffusion Equation on an Interval

At first, we consider this equation on a one-dimensional rod of length L with the boundary conditions

$$u(0,t) = u(L,t) = 0, \qquad t \geq 0 \tag{40}$$

and a parabolic initial condition given by

$$u(x,0) = u_0(x) = -\frac{a}{L}x^2 + ax, \qquad a \in \mathbb{R}, \tag{41}$$

if $\alpha \in (0,1]$. For $\alpha \in (1,2]$ we impose an additional initial condition

$$u_t(x,0) = u_1(x) = -\frac{b}{L}x^2 + bx, \qquad b \in \mathbb{R}\,. \tag{42}$$

In the following, we will use the notation D_t^α instead of ${}_0^C D_t^\alpha$ to make the computation clearer.

A solution of this equation is also given in [Kelow, Hayden (2013)], but as the method to solve this equation is not stated clearly, we would like to find the solution using the separation of variables and the Laplace transform. We assume, that the solution is a separable function of the form $u(x,t) = T(t)X(x)$. Inserting this function into the equation (39) leads to the following equation:

$$\begin{aligned} D_t^\alpha T(t) \cdot X(x) &= T(t) \cdot X''(x), \\ \frac{D_t^\alpha T(t)}{T(t)} &= \frac{X''(x)}{X(x)} = -\lambda^2, \qquad \lambda \in \mathbb{R}\,. \end{aligned}$$

$$\begin{cases} X''(x) = -\lambda^2 X(x) \\ D_t^\alpha T(t) = -\lambda^2 T(t) \end{cases} \tag{43}$$

The solution of the first differential equation is of the type $X(x) = C_1 \cos(\lambda x) + C_2 \sin(\lambda x)$. We search for a non-trivial solution (for example one that is not zero for all $t \geq 0$) to satisfy the boundary condition $u(0,t) = T(t)X(0) = 0$ for all $t \geq 0$, we assume that $X(0) = 0$, which requires $C_1 = 0$. To satisfy the other boundary condition $u(L,t) = T(t)X(L) = 0$ we search for λ which satisfies $X(L) = C_2 \sin(\lambda L) = 0$. Thus we receive

$$\lambda_n = \frac{n\pi}{L}, \quad n \in \mathbb{N}\,. \tag{44}$$

Therefore the boundary value problem (39), (40) has infinitely many solutions and we search for a solution satisfying (41) given by the Fourier series of the form

$$u(x,t) = \sum_{n=0}^{\infty} A_n \sin(\lambda_n x) T(t). \tag{45}$$

To compute the Fourier coefficients A_n the initial condition $u(x,0)$ is used:

$$\begin{aligned} A_n &= \frac{2}{L}\int_0^L u(x,0)\sin(\lambda_n x)dx = \frac{2}{L}\int_0^L \left(-\frac{a}{L}x^2 + ax\right)\sin(\lambda_n x)dx = \\ &= \frac{2}{L}\left[\left(-\frac{a}{L}x^2 + ax\right)\frac{1}{\lambda_n}(-\cos(\lambda_n x))\right]_0^L + \frac{2}{L}\int_0^L \left(-\frac{2a}{L}x + a\right)\frac{1}{\lambda_n}\cos(\lambda_n x)dx = \\ &= \frac{2}{L}\left[\left(-\frac{2a}{L}x + a\right)\frac{1}{\lambda_n^2}\sin(\lambda_n x)\right]_0^L + \frac{2}{L}\int_0^L \frac{2a}{L}\frac{1}{\lambda_n^2}\sin(\lambda_n x)dx = \\ &= \frac{2}{L}\left[\frac{2a}{L\lambda_n^2}\frac{1}{\lambda_n}(-\cos(\lambda_n x))\right]_0^L = \frac{2}{L}\frac{2aL^2}{n^3\pi^3}(1-\cos(n\pi)). \end{aligned}$$

The Fourier coefficients are therefore

$$A_n = \begin{cases} 0, & \text{if } n \text{ is even,} \\ \dfrac{8aL}{n^3\pi^3}, & \text{if } n \text{ is odd.} \end{cases} \tag{46}$$

We can ignore the even-indexed coefficients in the Fourier series and receive

$$u(x,t) = \sum_{n\in\mathbb{N}\text{, odd}} \frac{8aL}{n^3\pi^3}\sin(\lambda_n x)T(t). \tag{47}$$

To get $T(t)$ we have to solve the second differential equation using the Laplace transform:

$$\begin{aligned} D_t^\alpha T(t) &= -\lambda^2 T(t) \qquad / \, \mathcal{L}[\cdot](s) \\ \mathcal{L}[D_t^\alpha T(t)](s) &= -\lambda^2\,\mathcal{L}[T(t)](s) \end{aligned}$$

At this point we have to distinguish between two cases to be able to give the Laplace transform of the Caputo fractional derivative according to (14). The first case is for $\alpha \in (0,1]$:

$$\begin{aligned} s^\alpha\,\mathcal{L}[T(t)](s) - \frac{1}{s^{1-\alpha}}T(0) &= -\lambda^2\,\mathcal{L}[T(t)](s), \qquad (48) \\ (s^\alpha + \lambda^2)\,\mathcal{L}[T(t)](s) &= \frac{T(0)}{s^{1-\alpha}}, \\ \mathcal{L}[T(t)](s) &= \frac{T(0)}{s^{1-\alpha}(s^\alpha+\lambda^2)}, \\ T(t) &= \mathcal{L}^{-1}\left[T(0)\frac{s^\alpha}{s(s^\alpha+\lambda^2)}\right](t). \end{aligned}$$

$T(0)$ is a constant, w. l. o. g. we can choose $T(0) = 1$, because it is a part of the initial condition, which was already used to compute the Fourier coefficients (46). The inverse Laplace transform of the function above is than according to [Miller, Ross (1993), p.143] a Mittag-Leffler function:

$$T(t) = E_\alpha(-\lambda^2 t^\alpha) = \sum_{k=0}^{\infty}\frac{(-\lambda^2 t^\alpha)^k}{\Gamma(\alpha k+1)}. \tag{49}$$

The other case is for $\alpha \in (1,2)$. As $1 < \alpha < 2 = n$, we try to solve the following equation:

$$s^\alpha\,\mathcal{L}[T(t)](s) - \frac{1}{s^{1-\alpha}}T(0) - \frac{1}{s^{2-\alpha}}T'(0) = -\lambda^2\,\mathcal{L}[T(t)](s).$$

The condition $T'(0) = 0$ leads to the same equation as in (48) and yields therefore the same solution for $T(t)$. This assumption can be rectified by adding another initial condition $u_t(x,0) = 0$.

As we can see, for $\alpha = 1$

$$T(t) = \sum_{k=0}^{\infty} \frac{(-\lambda^2 t)^k}{\Gamma(k+1)} = \mathrm{e}^{-\lambda^2 t},$$

which is exactly the solution we would expect in the second equation of (43) for $\alpha = 1$. Combining the function $T(t)$ from (49) with the Fourier series (47) leads to the solution of the time-fractional boundary value problem (39)-(40) satisfying the initial condition (41) and $u_t(x,0) = 0$

$$\begin{aligned} u(x,t) &= \sum_{n\in\mathbb{N}\,,\ \text{odd}} \frac{8aL}{n^3\pi^3} \sin(\lambda_n x) E_\alpha(-\lambda_n^2 t^\alpha) \\ &= \sum_{n\in\mathbb{N}\,,\ \text{odd}} \frac{8aL}{n^3\pi^3} \sin(\lambda_n x) \left[\sum_{k=0}^{\infty} \frac{(-\lambda_n^2 t^\alpha)^k}{\Gamma(\alpha k+1)}\right], \end{aligned} \tag{50}$$

where $\lambda_n = \dfrac{n\pi}{L}$.

Let us solve the case $\alpha \in (1,2)$ for other initial conditions than $u_t(x,0) = 0$, specifically for the initial condition given in (42). Once again we try to solve the following equation:

$$s^\alpha\, \mathcal{L}[T(t)](s) - \frac{1}{s^{1-\alpha}} T(0) - \frac{1}{s^{2-\alpha}} T'(0) = -\lambda^2\, \mathcal{L}[T(t)](s),$$

but we do not set $T'(0)$ to be equal zero. Instead we choose w. l. o. g. $T(0) = A$ and $T'(0) = B$, $A, B \in \mathbb{R}$:

$$\begin{aligned} (s^\alpha + \lambda^2)\, \mathcal{L}[T(t)](s) &= \frac{A}{s^{1-\alpha}} + \frac{B}{s^{2-\alpha}} \\ \mathcal{L}[T(t)](s) &= A\frac{s^{\alpha-1}}{s^\alpha + \lambda^2} + B\frac{s^{\alpha-2}}{s^\alpha+\lambda^2} \\ T(t) = A\cdot T_1(t) + B\cdot T_2(t) &= A\cdot \mathcal{L}^{-1}\left[\frac{s^{\alpha-1}}{s^\alpha+\lambda^2}\right](t) + B\cdot \mathcal{L}^{-1}\left[\frac{s^{\alpha-2}}{s^\alpha+\lambda^2}\right](t). \end{aligned}$$

We have to find two linearly independent solutions $T_1(t)$ and $T_2(t)$. $T_1(t)$ is the same as the previous solution (49) and using the property (16) of Laplace transform the solution for $T_2(t)$ can be easily derived from $T_1(t)$:

$$\begin{aligned}
T_1(t) &= \mathcal{L}^{-1}\left[\frac{s^{\alpha-1}}{s^\alpha+\lambda^2}\right] = E_\alpha(-\lambda^2 t^\alpha) = \sum_{k=0}^{\infty}\frac{(-\lambda^2 t^\alpha)^k}{\Gamma(\alpha k+1)},\\
T_2(t) &= \mathcal{L}^{-1}\left[\frac{s^{\alpha-2}}{s^\alpha+\lambda^2}\right] = \mathcal{L}^{-1}\left[\frac{1}{s}\frac{s^{\alpha-1}}{s^\alpha+\lambda^2}\right] = \int_0^t E_\alpha(-\lambda^2\tau^\alpha)d\tau =\\
&= \int_0^t \sum_{k=0}^{\infty}\frac{(-\lambda^2\tau^\alpha)^k}{\Gamma(\alpha k+1)}d\tau = \left[\sum_{k=0}^{\infty}\frac{(-\lambda^2)^k\tau^{\alpha k+1}}{\Gamma(\alpha k+1)}\cdot\frac{1}{\alpha k+1}\right]_{\tau=0}^{t}\\
&= t\cdot\sum_{k=0}^{\infty}\frac{(-\lambda^2 t^\alpha)^k}{\Gamma(\alpha k+2)} = t\cdot E_{\alpha,2}(-\lambda^2 t^\alpha).
\end{aligned}$$

The solution of the initial boundary value problem (39), (40) is the Fourier series

$$\begin{aligned}
u(x,t) &= \sum_{n=0}^{\infty} C_n\sin(\lambda_n x)T(t) = \sum_{n=0}^{\infty} C_n\sin(\lambda_n x)(A\cdot E_\alpha(-\lambda_n^2 t^\alpha) + B\cdot t\cdot E_{\alpha,2}(-\lambda_n^2 t^\alpha))\\
&= \sum_{n=0}^{\infty}\left[A_n\sin(\lambda_n x)E_\alpha(-\lambda_n^2 t^\alpha) + B_n\sin(\lambda_n x)tE_{\alpha,2}(-\lambda_n^2 t^\alpha))\right]. \qquad (51)
\end{aligned}$$

We have to find the Fourier coefficients A_n and B_n from the initial conditions $u(x,0)$ and $u_t(x,0)$. The coefficients A_n are equal to (46), so we only have to find the coefficients B_n. They can be obtained similarly to A_n, but instead of the initial condition $u(x,0)$ we will use the second (added) initial condition $u_t(x,0) = -\frac{b}{L}x^2 + bx$:

$$\begin{aligned}
B_n &= \frac{2}{L}\int_0^L u_t(x,0)\sin(\lambda_n x)dx = \frac{2}{L}\int_0^L\left(-\frac{b}{L}x^2+bx\right)\sin(\lambda_n x)dx\\
&= \frac{4bL}{n^3\pi^3}(1-\cos(n\pi))
\end{aligned}$$

Therefore

$$B_n = \begin{cases} 0, & \text{if } n \text{ is even},\\ \dfrac{8bL}{n^3\pi^3}, & \text{if } n \text{ is odd}, \end{cases} \qquad (52)$$

and the complete solution for the problem (39)-(42) in the case, when $\alpha \in (1,2)$ is

$$\begin{aligned} u(x,t) = & \sum_{n\in\mathbb{N},\ \text{odd}} \frac{8aL}{n^3\pi^3} \sin(\lambda_n x) E_\alpha(-\lambda_n^2 t^\alpha) \\ & + \sum_{n\in\mathbb{N},\ \text{odd}} \frac{8bL}{n^3\pi^3} \sin(\lambda_n x) t E_{\alpha,2}(-\lambda_n^2 t^\alpha), \end{aligned} \tag{53}$$

where $\lambda_n = \dfrac{n\pi}{L}$.

For $\alpha = 2$ the equation (39) would be the wave equation. If we extend our solution also for this case we will receive

$$\begin{aligned} u(x,t) &= \sum_{n\in\mathbb{N},\ \text{odd}} \frac{8aL}{n^3\pi^3} \sin(\lambda_n x) E_2(-\lambda_n^2 t^2) + \sum_{n\in\mathbb{N},\ \text{odd}} \frac{8bL}{n^3\pi^3} \sin(\lambda_n x) t E_{\alpha,2}(-\lambda_n^2 t^2)) \\ &= \left[\begin{smallmatrix} n=2j+1, \\ \lambda_j = \frac{(2j+1)\pi}{L} \end{smallmatrix}\right] = \sum_{j=0}^{\infty} \frac{8aL}{(2j+1)^3\pi^3} \sin(\lambda_j x) \sum_{k=0}^{\infty} \frac{(-\lambda_j^2 t^2)^k}{\Gamma(2k+1)} \\ &\quad + \sum_{j=0}^{\infty} \frac{8bL}{(2j+1)^3\pi^3} \sin(\lambda_j x) t \sum_{k=0}^{\infty} \frac{(-\lambda_j^2 t^2)^k}{\Gamma(2k+2)} \\ &= \sum_{j=0}^{\infty} \frac{8aL}{(2j+1)^3\pi^3} \sin(\lambda_j x) \sum_{k=0}^{\infty} \frac{(-1)^k (\lambda_j t)^{2k}}{(2k)!} \\ &\quad + \sum_{j=0}^{\infty} \frac{8bL}{(2j+1)^3\pi^3} \sin(\lambda_j x) \frac{1}{\lambda_j} \sum_{k=0}^{\infty} \frac{(-1)^k (\lambda_j t)^{2k+1}}{(2k+1)!} \\ &= \sum_{j=0}^{\infty} \frac{8aL}{(2j+1)^3\pi^3} \sin(\lambda_j x) cos(\lambda_j t) + \sum_{j=0}^{\infty} \frac{8bL^2}{(2j+1)^4\pi^4} \sin(\lambda_j x) \sin(\lambda_j t). \end{aligned}$$

This function $u(x,t)$ solves indeed the wave equation

$$u_{tt}(x,t) = u_{xx}(x,t)$$

with the boundary conditions

$$u(0,t) = u(L,t) = 0, \quad t \geq 0$$

and the initial conditions given by

$$u(x,0) = u_0(x) = -\frac{a}{L}x^2 + ax,$$
$$u_t(x,0) = u_1(x) = -\frac{b}{L}x^2 + bx.$$

Thus we see, that the time-fractional diffusion equation for $\alpha \in (1,2)$ is solved by a linear combination of two Fourier series, which reminds us more of the solution of the wave equation than of the diffusion equation.

The last step in this section is to prove, that the Fourier series in the solutions (50) and (53) of the time-fractional heat equation on an interval $x \in [0,L]$ for $\alpha \in (0,1]$ and $\alpha \in (1,2)$ respectively converge.

To prove this, we will use the asymptotic expansions of the one-parameter and two-parameter Mittag-Leffler functions given in [Haubold, Mathai, Saxena (2011), p. 7].

Theorem 2.1

Let the one-parameter Mittag-Leffler function be defined as in (4) and the two-parameter Mittag-Leffler function as in (5). If $0 < \alpha < 2$ *and* μ *is a real number such that*

$$\frac{\pi\alpha}{2} < \mu < \min\{\pi, \pi\alpha\},$$

then for $N^* \in \mathbb{N}$, $N^* \neq 1$ *the following asymptotic expansion holds for the one-parameter Mittag-Leffler function*

$$E_\alpha(z) = -\sum_{k=1}^{N^*} \frac{1}{\Gamma(1-\alpha k)} \frac{1}{z^k} + O\left[\frac{1}{z^{N*+1}}\right], \tag{54}$$

as $|z| \to \infty$, $\mu|\arg z| \leq \pi$ *and the following asymptotic expansion holds for the two-parameter Mittag-Leffler function*

$$E_{\alpha,\beta}(z) = -\sum_{k=1}^{N^*} \frac{1}{\Gamma(\beta-\alpha k)} \frac{1}{z^k} + O\left[\frac{1}{z^{N*+1}}\right], \tag{55}$$

as $|z| \to \infty$, $\mu|\arg z| \leq \pi$.

Let us first consider the case $\alpha \in (0,1]$, for which the solution is given by

$$\begin{aligned} u(x,t) &= \sum_{n\in\mathbb{N}\text{, odd}} \frac{8aL}{n^3\pi^3}\sin(\lambda_n x)E_\alpha(-\lambda_n^2 t^\alpha) \\ &= \left[\begin{smallmatrix} n=2j+1, \\ \lambda_j=\frac{(2j+1)\pi}{L}\end{smallmatrix}\right] = \sum_{j=0}^{\infty} \frac{8aL}{(2j+1)^3\pi^3}\sin(\lambda_j x)E_\alpha\left(-\left[\frac{(2j+1)\pi}{L}\right]^2 t^\alpha\right). \end{aligned}$$

The argument of the Mittag-Leffler function in the solution above is a negative real number, therefore $\left|\arg(-\left[\frac{(2j+1)\pi}{L}\right]^2 t^\alpha)\right| = \pi$ and the asymptotic expansion (54) holds as $j \to \infty$. For $\alpha \in (1,2)$ the solution is given by

$$\begin{aligned} u(x,t) &= \sum_{n\in\mathbb{N}\text{, odd}} \frac{8aL}{n^3\pi^3}\sin(\lambda_n x)E_\alpha(-\lambda_n^2 t^\alpha) \\ &\quad + \sum_{n\in\mathbb{N}\text{, odd}} \frac{8bL}{n^3\pi^3}\sin(\lambda_n x)tE_{\alpha,2}(-\lambda_n^2 t^\alpha) \\ &= \left[\begin{smallmatrix} n=2j+1, \\ \lambda_j=\frac{(2j+1)\pi}{L}\end{smallmatrix}\right] = \sum_{j=0}^{\infty} \frac{8aL}{(2j+1)^3\pi^3}\sin(\lambda_j x)E_\alpha\left(-\left[\frac{(2j+1)\pi}{L}\right]^2 t^\alpha\right) \\ &\quad + \sum_{j=0}^{\infty} \frac{8bL}{(2j+1)^3\pi^3}\sin(\lambda_j x)tE_{\alpha,2}\left(-\left[\frac{(2j+1)\pi}{L}\right]^2 t^\alpha\right). \end{aligned}$$

Also in this case, the argument of the two-parameter Mittag-Leffler function is a negative real number, therefore the asymptotic expansion (55) holds as $j \to \infty$. Given the asymptotic behaviour of both Mittag-Leffler functions, as well as the fact, that the sine function is bounded on the interval $[-1,1]$, it is clear, that the Fourier series given in (50) and (53) converge for $\forall\alpha \in (0,1]$ or $\forall\alpha \in (1,2)$ respectively and as previously shown, the solution (53) can be even extended for $\alpha = 2$.

At last, we would like to compare our solution of the boundary value problem (39), (40) with the solutions given in [Kelow, Hayden (2013)]. The authors of the article solved the same boundary value problem using similar initial condition

$$u(x,0) = -\frac{4\tilde{a}}{L^2}x^2 + \frac{4\tilde{a}}{L}x, \qquad \tilde{a} \in \mathbb{R}\,.$$

It is obvious, that this initial condition is equal to the initial equation (41) for $a = \dfrac{4\tilde{a}}{L}$. Slight difference is in the order α of the fractional derivative with respect to time in the time-fractional equation. We solved the boundary value problem for $\alpha \in (0,2]$, but in

[Kelow, Hayden (2013)] α was from a not clearly defined interval $[1-\delta, 1+\delta] \subset \mathbb{R}$ with $\delta > 0$ "relatively small". It is obvious from the form of the interval, that the authors of the article wanted to solve the boundary value problem also for $\alpha > 1$, but they did not mention, that for this case another initial condition $u_t(x, 0)$ has to be used. This can be of course easily rectified by assuming $u_t(x, 0) = 0$ for all $x \in [0, L]$. The particular solution given in the article is

$$u(t, x) = \sum_{n \in \mathbb{N},\ \text{odd}} \left[\frac{32\tilde{a}}{n^3 \pi^3} sin(\lambda_n x) \sum_{k=0}^{\infty} \frac{(-\lambda_n^2 t^\alpha)^k}{\Gamma(\alpha k + 1)} \right], \tag{56}$$

which is equal to the solution (50), we obtained using the Laplace transform. To be able to plot some solutions of the time-fractional diffusion equation, the authors of the article used also other approach to find a solution of the fractional order differential equation with respect to time in (43). They used the rule for standard derivative of the exponential function $D_t^n[\mathrm{e}^{rt}] = r^n\, \mathrm{e}^{rt}$, $n \in \mathbb{N}$, generalized for fractional derivative of order $\alpha \in \mathbb{R}$:

$$D_t^\alpha[\mathrm{e}^{rt}] = r^\alpha\, \mathrm{e}^{rt}\,.$$

The authors used this property to gain the solution of the time-fractional differential equation $D_t^\alpha T(t) = -\lambda^2 T(t)$ and gave the following solution:

$$T(t) = \mathrm{e}^{\sqrt[\alpha]{-\lambda^2} t}\,.$$

They substituted the Mittag-Leffler function in their solution (56) with the new function $T(t)$ and received the alternative solution

$$u(t, x) = \sum_{n \in \mathbb{N},\ \text{odd}} \frac{32\tilde{a}}{n^3 \pi^3} sin(\lambda_n x)\, \mathrm{e}^{\sqrt[\alpha]{-\lambda_n^2} t}, \tag{57}$$

which was used to plot some graphs of the solution for multiple values of α. As we can see, the function above is complex valued, but to be able to plot the graphs the authors used only the real parts of the function values.

They received the following plots of the function (57) at the middle point of the interval

$x = L/2$ for $\tilde{a} = L = 1$ for different orders α of the fractional derivative with respect to time, which they call "physically realistic":

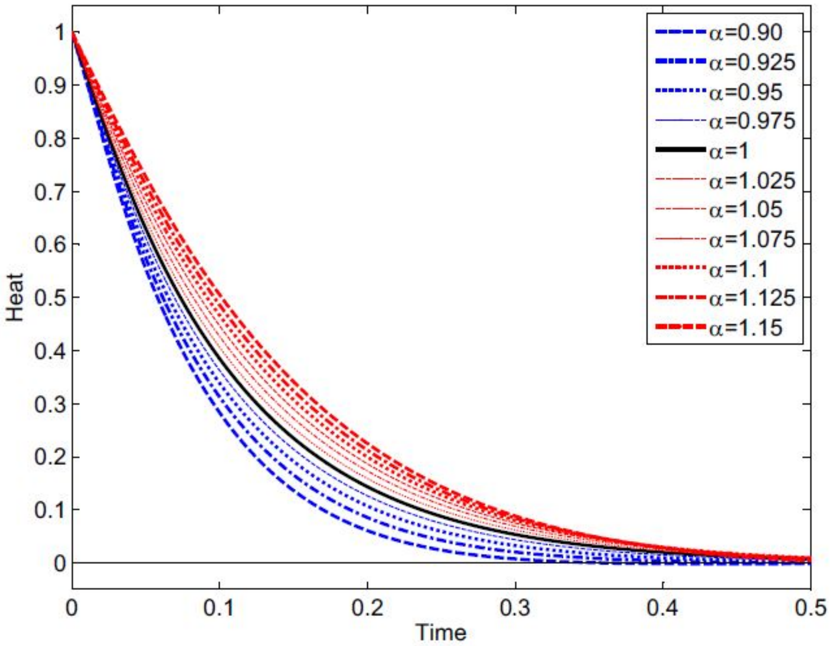

Figure 3: Plots of function (57) for several values of α at $x = L/2$ with $\tilde{a} = L = 1$.

We plotted our solution (50) at the middle point of the interval $x = L/2$ for $L = 1$ and $a = 4$ for the same orders α as in the previous figure. The value of parameter a was chosen, so that our solution would be equal to (56) for $\tilde{a} = 1$. To compute the values of the Mittag-Leffler function, we used the Matlab function **ml**, which was implemented by Roberto Garrappa using the optimal parabolic contour algorithm described in his article [Garrappa (2015)].

If we compare the figures 3 and 4, we can see that although the plots of the alternative solutions have similar decay as the exact solutions, they are not showing the most important properties of the exact solutions. From figure 4 it is obvious, that the decay of the function for $\alpha < 1$ becomes slower than the exponential decay of the solution of the standard diffusion equation. On the other hand, for $\alpha > 1$ the decay becomes faster and the function reaches relatively fast also negative values, which seems unrealistic, if we try to interpret this function as a solution to heat equation, but is understandable, if we expect it to be the solution of a time-fractional wave equation.

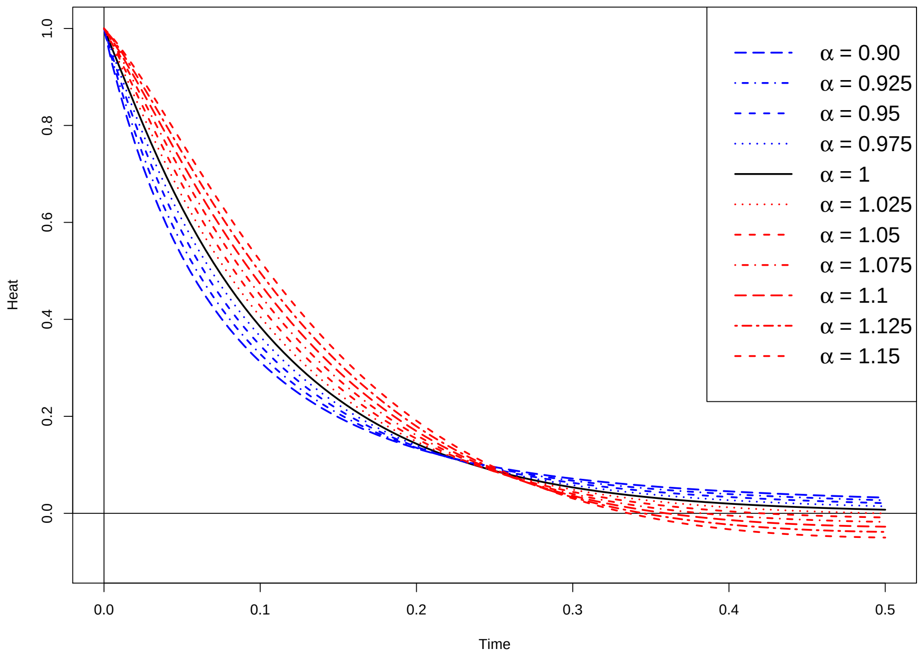

Figure 4: Plots of function (56) for several values of α at $x = L/2$ with $\tilde{a} = L = 1$.

The following figure shows again plots of the alternative solution (57) for other values of α.

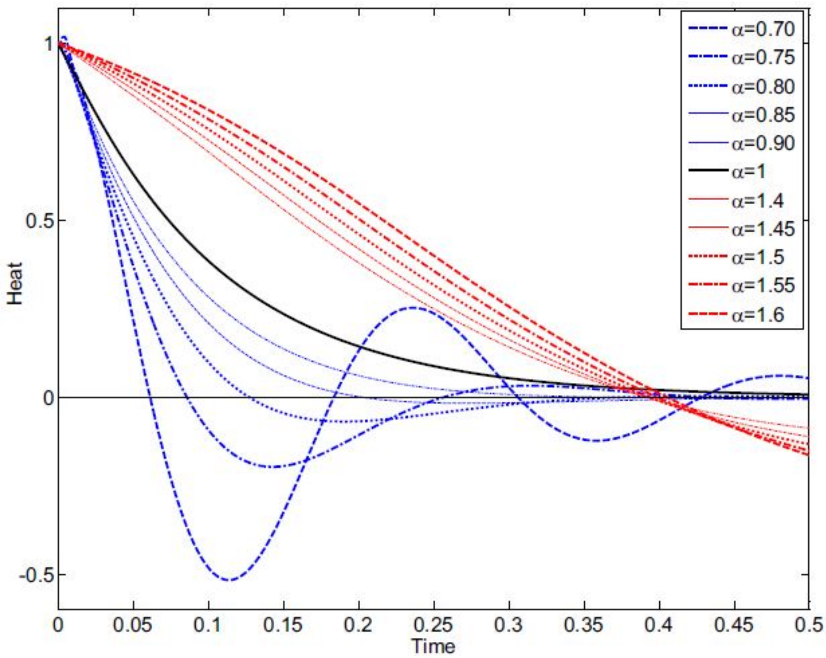

Figure 5: Plots of function (57) for several values of α at $x = L/2$ with $\tilde{a} = L = 1$.

This time, the authors of the article [Kelow, Hayden (2013)] chose those values of the order α of the time-fractional derivative, for which the solution shows "unrealistic" values, if interpreted as heat. For example, cases in which the temperature is negative or the plot is showing an increase of heat without any external heating factors. In figure 6, we plotted again the exact solution (56) for the same values of α and as we can see below, in this case the plots for $\alpha > 1$ are still fairly similar in both figures, but the plots of the solutions for $\alpha < 1$, do not show any "physically unrealistic" behaviour in the second figure. If we compare the plots for $\alpha = 0.7$, it becomes obvious, that the alternative solution (57) given by the authors, might not be very useful, not even as an illustration of the behaviour of the real solution. This is naturally given also by the fact, that the authors transformed this complex-valued function given by (57) to a real-valued function, which could be easily plotted, merely by ignoring the imaginary part of the function.

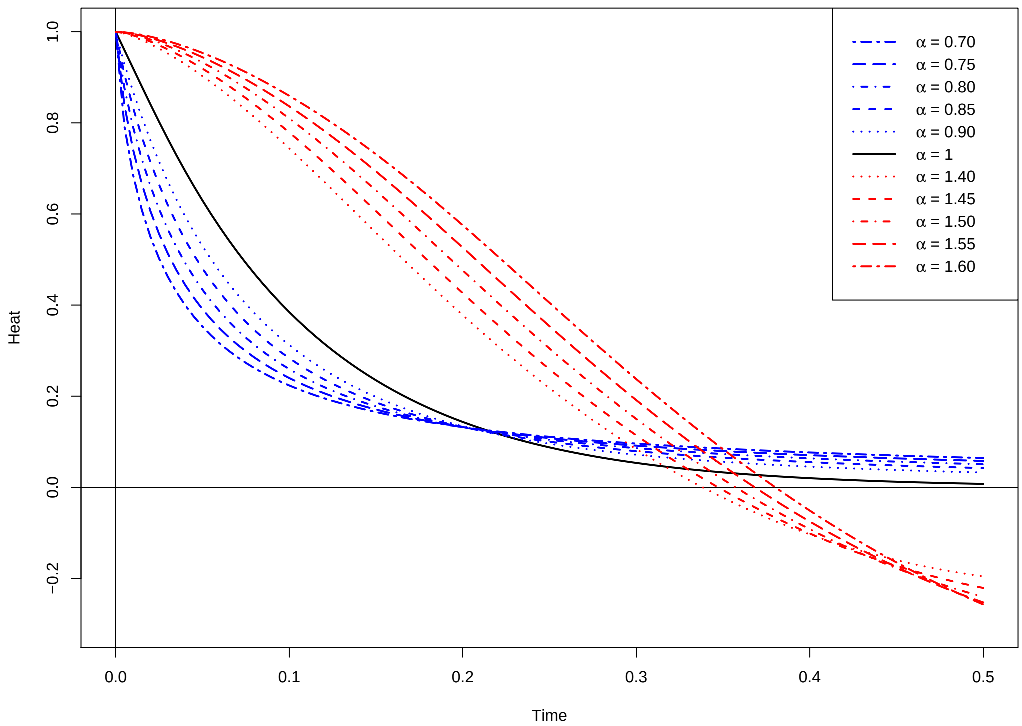

Figure 6: Plots of function (56) for several values of α at $x = L/2$ with $\tilde{a} = L = 1$.

The last figure shows plots of the solution of the boundary value problem (39), (40) for several values of α, which satisfies the initial conditions (41) and (42). The plots are only for several values of $\alpha > 1$, as the initial condition (42) is useful only in these cases. The values of the parameters a, b and L are chosen similar to the previous plots, $a = b = 4$ and $L = 1$ and the plots give the value of the solution at $x = L/2 = 1/2$.

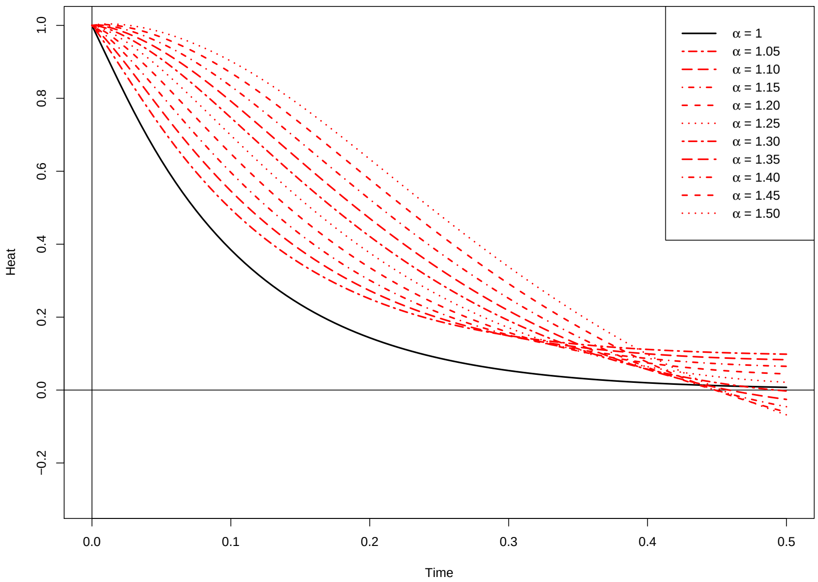

Figure 7: Plots of function (53) for several values of $\alpha \geq 1$ at $x = L/2$ with $a = b = 4$ and $L = 1$.

From the figure above, we can see, that with growing value of the order of the time fractional derivative α, the function (53) looks more and more like a solution of the wave equation.

2.2 Time-Fractional Diffusion Equation on $\mathbb{R}$

Let us now consider the equation (39)

$$ {}_0^C D_t^\alpha u(x,t) = D_x^2 u(x,t), \tag{58}$$

for $t \geq 0$ on an infinite rod $x \in R$, where the order of the Caputo fractional derivative is $\alpha \in (0,2)$. We will search for a solution, which satisfies the following initial and boundary conditions:

$$ u(x,0) = \delta(x), \quad x \in \mathbb{R}, \qquad u(\pm\infty, t) = 0, \quad t > 0, \tag{59}$$

where $\delta(x)$ is the Dirac delta function. For $1 < \alpha < 2$ we have to add additional initial condition $u_t(x,0) = 0$. To find the solution, we will use the Fourier and Laplace integral transforms defined in section **1.2** :

$$\begin{aligned}
{}_0^C D_t^\alpha u(x,t) &= D_x^2 u(x,t), \quad / \mathcal{F} \\
\mathcal{F}\left[{}_0^C D_t^\alpha u(x,t)\right](\kappa) &= \mathcal{F}\left[D_x^2 u(x,t)\right](\kappa), \\
{}_0^C D_t^\alpha\, \mathcal{F}\left[u(x,t)\right](\kappa) &= -\kappa^2\, \mathcal{F}\left[u(x,t)\right](\kappa),
\end{aligned} \tag{60}$$

The equality of the terms on the right side can be proven using the properties of the Fourier transform. We will now show that $\mathcal{F}\left[{}_0^C D_t^\alpha u(x,t)\right](\kappa)$ is indeed equal to ${}_0^C D_t^\alpha\, \mathcal{F}\left[u(x,t)\right](\kappa)$:

$$\begin{aligned}
\mathcal{F}\left[{}_0^C D_t^\alpha u(x,t)\right](\kappa) &= \int_{-\infty}^{\infty} {}_0^C D_t^\alpha u(x,t)\, \mathrm{e}^{i\kappa x}\, dx \\
&= \int_{-\infty}^{\infty} \left[\frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1} \frac{\partial^n}{\partial \tau^n} u(x,\tau) d\tau\right] \mathrm{e}^{i\kappa x}\, dx \\
&= \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1} \left[\int_{-\infty}^{\infty} \frac{\partial^n}{\partial \tau^n} u(x,\tau)\, \mathrm{e}^{i\kappa x}\, dx\right] d\tau \\
&= \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1} \frac{\partial^n}{\partial \tau^n} \left[\int_{-\infty}^{\infty} u(x,\tau)\, \mathrm{e}^{i\kappa x}\, dx\right] d\tau \\
&= {}_0^C D_t^\alpha\, \mathcal{F}\left[u(x,t)\right](\kappa).
\end{aligned} \tag{61}$$

Presuming that the function $\mathcal{F}\{u(x,t)\}(\kappa) = F(\kappa,t)$ is a function of t with a parameter κ, we use the Laplace transform to find the solution of the following equation:

$$\begin{aligned} {}_0^C D_t^\alpha F(\kappa,t) &= -\kappa^2 F(\kappa,t) \quad / \mathcal{L} \\ \mathcal{L}\left[{}_0^C D_t^\alpha F(\kappa,t)\right](s) &= \mathcal{L}\left[-\kappa^2 F(\kappa,t)\right](s). \end{aligned}$$

Using the property (35) of the Caputo fractional derivative, we receive

$$s^\alpha \, \mathcal{L}[F(\kappa,t)](s) - \sum_{k=1}^{n} s^{\alpha-k} \frac{\partial^{k-1}}{\partial t^{k-1}} F(\kappa,t)\Big|_{t=0} = -\kappa^2 \, \mathcal{L}[F(\kappa,t)](s). \tag{62}$$

For $0 < \alpha \leq 1$ is $n = 1$ and we use the initial condition $u(x,0) = \delta(x)$ in the equation (62):

$$\begin{aligned} s^\alpha \, \mathcal{L}[F(\kappa,t)](s) - s^{\alpha-1} F(\kappa,t)\Big|_{t=0} &= -\kappa^2 \, \mathcal{L}[F(\kappa,t)](s), \\ s^\alpha \, \mathcal{L}[F(\kappa,t)](s) - s^{\alpha-1} \, \mathcal{F}[u(x,0)](\kappa) &= -\kappa^2 \, \mathcal{L}[F(\kappa,t)](s), \end{aligned}$$

where

$$\mathcal{F}[u(x,0)](\kappa) = \mathcal{F}[\delta(x)](\kappa) = \int_{-\infty}^{\infty} \delta(x) \, \mathrm{e}^{i\kappa x} \, dx = \mathrm{e}^{i\kappa 0} = 1. \tag{63}$$

For $1 < \alpha < 2$ is $n = 2$ and we have to use also the second initial condition $u_t(x,0) = 0$:

$$s^\alpha \, \mathcal{L}[F(\kappa,t)](s) - s^{\alpha-1} F(\kappa,t)\Big|_{t=0} - s^{\alpha-2} \frac{\partial}{\partial t} F(\kappa,t)\Big|_{t=0} = -\kappa^2 \, \mathcal{L}[F(\kappa,t)](s),$$

where

$$\frac{\partial}{\partial t} F(\kappa,t)\Big|_{t=0} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} u(x,t) \, \mathrm{e}^{i\kappa x} \, dx \Big|_{t=0} = \int_{-\infty}^{\infty} u_t(x,0) \, \mathrm{e}^{i\kappa x} \, dx = 0. \tag{64}$$

Therefore the equation (62) is the same for $\alpha \in (0,1]$ and $\alpha \in (1,2)$ and can be written as

$$\begin{aligned}
s^{\alpha}\,\mathcal{L}[F(\kappa,t)](s) - s^{\alpha-1} &= -\kappa^2\,\mathcal{L}[F(\kappa,t)](s),\\
(s^{\alpha}+\kappa^2)\,\mathcal{L}[F(\kappa,t)](s) &= s^{\alpha-1},\\
\mathcal{L}[F(\kappa,t)](s) &= \frac{s^{\alpha-1}}{s^{\alpha}+\kappa^2},\\
F(\kappa,t) &= \mathcal{L}^{-1}\left[\frac{s^{\alpha-1}}{s^{\alpha}+\kappa^2}\right](t).
\end{aligned}$$

The inverse Laplace transform of a function similar to the one above, was already given in the previous section and is equal to the Mittag-Leffler function introduced in subsection 1.1.2

$$\begin{aligned}
F(\kappa,t) &= E_{\alpha}(-\kappa^2 t^{\alpha}),\\
u(x,t) &= \mathcal{F}^{-1}[E_{\alpha}(-(\kappa t^{\alpha/2})^2)](x).
\end{aligned}$$

Using the already proven Fourier transform (23) of the M-Wright function, as well as the property (19) of the Fourier transform, the fundamental solution of the initial-boundary value problem (58)-(59) can be given as

$$\begin{aligned}
u(x,t) &= \frac{1}{2}\frac{1}{t^{\alpha/2}}M_{\alpha/2}\left(\frac{|x|}{t^{\alpha/2}}\right) \qquad (65)\\
&= \frac{1}{2\pi}\frac{1}{t^{\alpha/2}}\sum_{n=1}^{\infty}\frac{(-|x|)^{n-1}}{(t^{\alpha/2})^{n-1}(n-1)!}\Gamma(\alpha/2n)\sin(\pi\alpha/2n).
\end{aligned}$$

To illustrate the behaviour of the above function as a solution of the time-fractional diffusion equation (58) satisfying the initial condition (59), we plot the graphs of the function $u(x,t)$ at $t=1$ for several values of α. To be able to better compare the decay of the functions, we use the logarithmic scale. We will compare the fundamental solution of the standard diffusion equation for $\alpha = 1$ firstly with the fundamental solutions for several values of $\alpha < 1$ and later also for some values of $\alpha > 1$. As the Gaussian function $\dfrac{1}{\sqrt{\pi}}\,\mathrm{e}^{-x^2/4}$ is a special case of the M-Wright function (23) for the order of the function $\nu = 1/2$, as shown in [Mainardi, Mura, Pagnini (2010)], we can now show, that the above function does for $\alpha = 1$ solve the standard heat equation:

$$\begin{aligned} u(x,t) &= \frac{1}{2}\frac{1}{t^{1/2}} M_{1/2}\left(\frac{|x|}{t^{1/2}}\right) = \frac{1}{2\sqrt{\pi t}}\, \mathrm{e}^{-|x|^2/4t} \\ &= \frac{1}{\sqrt{4\pi t}}\, \mathrm{e}^{-x^2/4t}\,. \end{aligned}$$

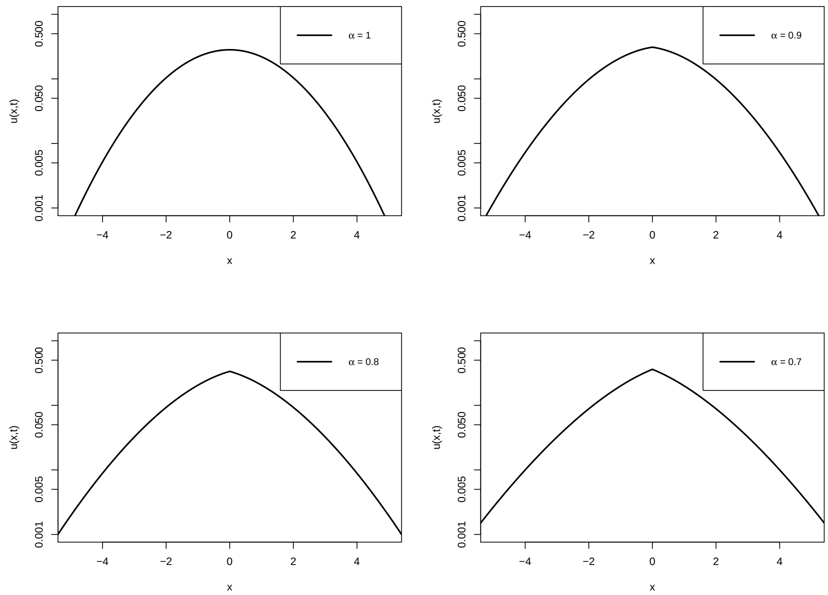

Figure 8: Plots of function (65) at $t = 1$ for several values $\alpha < 1$ compared to the solution of standard diffusion equation with $\alpha = 1$.

In the figure 8 we can see, that the decay of the functions is slower for $\alpha < 1$ than the exponential decay of the solution for $\alpha = 1$ and if we interpret the function $u(x,t)$ as heat, we can also say, that the distribution of heat has fatter tails for $\alpha < 1$.
On the other side, the decay of the function (65) is faster than exponential for $\alpha > 1$ as x tends to $-\infty$ and $+\infty$. Other interesting behaviour of the function is best visible in the last plot for $\alpha = 1.9$. We observe, that the function has two maxima at $x = -1$ and at $x = 1$, so for the two cases when $|x| = t = 1$. This reminds us more of a solution of the wave equation, for which the fundamental solution is given by $u(x,t) = \dfrac{\delta(x+t) + \delta(x-t)}{2}$.

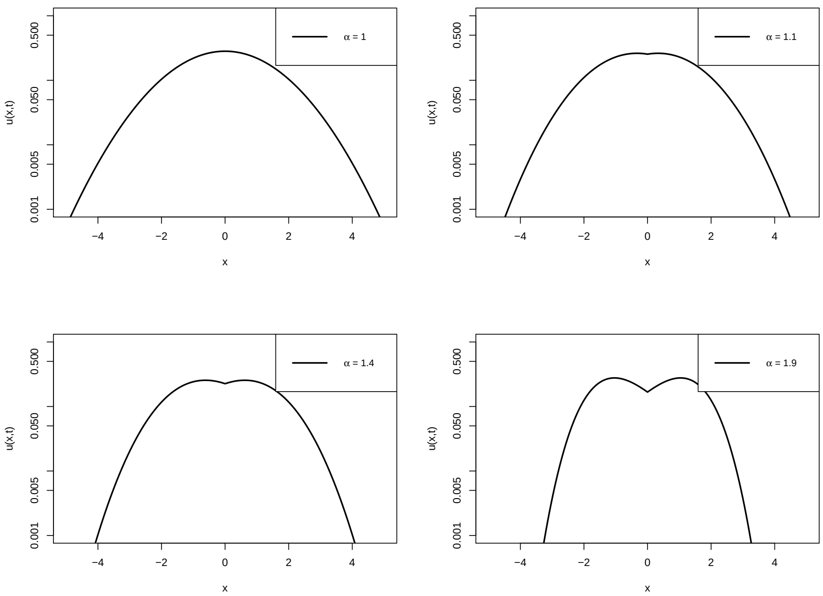

Figure 9: Plots of function (65) at $t = 1$ for several values $\alpha > 1$ compared to the solution of standard diffusion equation with $\alpha = 1$.

3 Space-Time Fractional Diffusion Equation

In this chapter, we would like to study the solution of the space-time fractional diffusion equation, the diffusion equation we receive, when we replace the first derivative with respect to time with a Caputo derivative of fractional order $\alpha \in (0,2] \subset \mathbb{R}$ and the second derivative with respect to space with the Riesz derivative of fractional order $\beta \in (0,2] \subset \mathbb{R}$:

$$ {}_0^C D_t^{\alpha} u(x,t) = {}^{RZ}D_x^{\beta} u(x,t). \tag{66} $$

Similar equation was solved also in [Mainardi, Luchko, Pagnini (2001)], although they used more generalized version of the Riesz fractional derivative with respect to space, the so called Riesz-Feller fractional derivative, which includes also an asymmetry parameter θ. We will search for the solution of this equation for $t \geq 0$ on a one dimensional infinite rod $x \in \mathbb{R}$ for the boundary condition

$$ u(\pm\infty, t) = 0, \quad t > 0, \tag{67} $$

and the initial condition

$$ u(x,0) = \delta(x), \quad x \in \mathbb{R}, \tag{68} $$

where $\delta(x)$ is the Dirac delta function. We add an additional initial condition $u_t(x,0) = 0$ for $\alpha \in (1,2]$. Once again we will use the Fourier transform first and than the Laplace transform:

$$ \begin{aligned} {}_0^C D_t^{\alpha} u(x,t) &= {}^{RZ}D_x^{\beta} u(x,t), \quad / \mathcal{F} \\ \mathcal{F}\left[{}_0^C D_t^{\alpha} u(x,t)\right](\kappa) &= \mathcal{F}\left[{}^{RZ}D_x^{\beta} u(x,t)\right](\kappa). \end{aligned} $$

Using the already proven relationship between the Fourier transform and the Caputo fractional derivative (61) and the Fourier transform of the Riesz fractional derivative

(38), we obtain the following equation, on which we apply the Laplace transform:

$$\begin{aligned} {}_0^C D_t^\alpha F(\kappa, t) &= -|\kappa|^\alpha F(\kappa, t), \quad / \mathcal{L} \\ \mathcal{L}\left[{}_0^C D_t^\alpha F(\kappa, t)\right](s) &= \mathcal{L}\left[-|\kappa|^\beta F(\kappa, t)\right](s). \end{aligned} \tag{69}$$

We have to distinguish between the two cases for the order of the Caputo fractional derivative with respect to time, to compute the Laplace transform of the left side of the previous equation using also the respective initial conditions. For $0 < \alpha \leq 1$, we use the first initial condition $u(x, 0) = \delta(x)$, as well as its already proven Fourier transform (63) :

$$\begin{aligned} \mathcal{L}\left[{}_0^C D_t^\alpha F(\kappa, t)\right](s) &= s^\alpha \, \mathcal{L}[F(\kappa, t)](s) - s^{\alpha-1} F(\kappa, t)\Big|_{t=0} \\ &= s^\alpha \, \mathcal{L}[F(\kappa, t)](s) - s^{\alpha-1}. \end{aligned}$$

For $1 < \alpha \leq 2$, the second initial condition $u_t(x, 0) = 0$ and its Fourier transform (64) is needed as well:

$$\begin{aligned} \mathcal{L}\left[{}_0^C D_t^\alpha F(\kappa, t)\right](s) &= s^\alpha \, \mathcal{L}[F(\kappa, t)](s) - s^{\alpha-1} F(\kappa, t)\Big|_{t=0} - s^{\alpha-2} \frac{\partial}{\partial t} F(\kappa, t)\Big|_{t=0} \\ &= s^\alpha \, \mathcal{L}[F(\kappa, t)](s) - s^{\alpha-1}. \end{aligned}$$

The equation (69) can be therefore written as

$$\begin{aligned} s^\alpha \, \mathcal{L}[F(\kappa, t)](s) - s^{\alpha-1} &= -|\kappa|^\beta \, \mathcal{L}\left[F(\kappa, t)\right](s), \\ \mathcal{L}[F(\kappa, t)](s) &= \frac{s^{\alpha-1}}{s^\alpha + |\kappa|^\beta}, \end{aligned}$$

in both cases, for $\alpha \in (0, 1]$ as well as for $\alpha \in (1, 2]$. We solve this equation for $F(\kappa, t)$ as a function of the variable t with the parameter κ:

$$\begin{aligned} F(\kappa, t) &= \mathcal{L}^{-1}\left[\frac{s^{\alpha-1}}{s^\alpha + |\kappa|^\beta}\right](t), \\ F(\kappa, t) &= E_\alpha(-|\kappa|^\beta t^\alpha). \end{aligned}$$

The last step to find the solution of the space-time fractional initial boundary value problem (66)-(68) would be finding of the inverse Fourier transform of the Mittag-Leffler function above:

$$u(x,t) = \mathcal{F}^{-1}\left[E_\alpha(-|\kappa|^\beta t^\alpha)\right](x).$$

We try to use the inverse Fourier transform defined by (18):

$$\begin{aligned} u(x,t) &= \mathcal{F}^{-1}\left[E_\alpha(-|\kappa|^\beta t^\alpha)\right](x) \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} E_\alpha(-|\kappa|^\beta t^\alpha)\,\mathrm{e}^{-i\kappa x}\,d\kappa \\ &= \frac{2}{2\pi}\int_0^{\infty} E_\alpha(-\kappa^\beta t^\alpha)\cos(\kappa x)d\kappa \\ &= \frac{1}{\pi}\int_0^{\infty}\sum_{j=0}^{\infty}\frac{(-1)^j\kappa^{\beta j}t^{\alpha j}}{\Gamma(\alpha j+1)}\cos(\kappa x)d\kappa. \end{aligned} \tag{70}$$

The problem in finding the integral above lies in the Mittag-Leffler function. The most properties and integrals of the Mittag-Leffler functions are proven using its integral representation and requires use of complex analysis and contour integrals. Finding the solution would therefore be out of the scope of this thesis.

Nowadays, there are many works dedicated to the application of the fractional calculus on many differential equations. As the Mittag-Leffler function seems to be one of the key tools in finding the solutions of the fractional diffusion equations, it is still studied by many authors and new properties are given and proven in their works, but it is not always easy to determine the validity of the statements given in the articles, as they often refer to other works or use techniques, that are not comprehensible to students without any theoretical background in complex analysis. Nevertheless, to find out more about the Mittag-Leffler functions and their properties, we would like to refer the reader to [Haubold, Mathai, Saxena (2011)] and the references therein. If the reader is interested in the applications of the fractional calculus also on other fractional differential equations, we recommend [Podlubny (1999)], which is devoted not only to the analytical but also to numerical ways of finding the solutions of the fractional differential equations.

Conclusion

In this work, we have focused on the fractional diffusion equation and its solutions for several cases. To do so, we began with an overview of special functions, integral transforms and fractional integrals and derivatives. We listed their definitions and attributes and gave proofs to some of them, combining several sources to create a consolidated toolbox, which could be useful also for other students as an introduction to the field of fractional differential equations.

For the case of the time fractional diffusion equation on an interval, we tried to find the solution and compare it to the one given in [Kelow, Hayden (2013)]. We were able to complete this goal and moreover, we corrected the solution given in the article by adding clearer restrictions for the order of the time fractional derivative and additional initial condition, as the authors omitted the fact, that for the case, when the order of the time fractional derivative α is greater than 1, there is also an initial condition for $u_t(x, 0)$ needed to obtain a particular solution of the problem.

The study of the time fractional and space-time fractional diffusion equation on the infinite one-dimensional rod showed, that the methods used to obtain the fundamental solution of the standard diffusion equation can be used in this cases as well, but to successfully find a solution, some special functions have to be introduced. The plots of the solutions in the case of the time-fractional diffusion equation also illustrated the slower decay of the functions with growing $|x|$ than in the case of standard diffusion equation for $\alpha \in (0, 1)$ and faster decay for $\alpha \in (1, 2)$.

In conclusion, we are convinced, that the aims defined in the thesis assignment were fulfilled and we were also able to sum up the definitions, functions and basic methods to solve the fractional diffusion equations.

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