

### Theory and application of numerical methods for fractional diffusion equations

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## *Declaration of Authorship*

I, Thomas Camminady, hereby certify that this thesis has been composed by me and is based on my own work, unless stated otherwise. No other person's work has been used without due acknowledgement in this thesis. All references and verbatim extracts have been quoted, and all sources of information, including graphs and data sets, have been specifically acknowledged.

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## *Abstract*

In random processes where the memorylessness assumption is no longer valid and the mean square displacements scales like  $\langle x^2 \rangle \propto t^\alpha$ , fractional differential operators can be used to model the underlying microscopic behavior by fractional partial differential equations on a macroscopic level.

Starting from a random walk approach, we use algebraic decaying waiting time and path length distributions to derive diffusion equations that are fractional in space and time. The theoretical setting, necessary for the understanding of fractional calculus, is outlined.

Afterwards, we implement, analyze and partially extend recent numerical methods for the solution of fractional diffusion equations. The derivation shows, how classical algorithms like the finite difference method, pseudo spectral collocation methods and fully spectral methods can be applied in the fractional context. Since fractional differential operators are global operators, we encounter non sparsity in the involved differentiation matrices. For the pseudo spectral and fully spectral method, the choice of the basis functions which we use to expand the solution is essential as it has to consist of eigenfunctions of the differential operators, if we want to compute the involved projections with acceptable effort.

Numerical simulations are performed to verify the theoretical predicted convergence behavior for the three different approaches.



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# 1

## From random walks to classical diffusion

The concept of diffusive processes plays a key role in the modelling and understanding of time dependent processes in biology, chemistry, physics, finance, psychology and a variety of other disciplines. Quoting the Encyclopædia Britannica, diffusion is defined as the

“process resulting from random motion of molecules by which there is a net flow of matter from a region of high concentration to a region of low concentration.”

This definition is given in the context of physics, however by replacing the quantity of interest that spreads over the domain from high to low concentration, the construct can be applied to different disciplines. In psychology or sociology, diffusion can describe the spreading out of ideas from an initial group of individuals over time. In finance, jump-diffusion processes can model returns from stock indices or to describe the diffusion of price values.

The above definition implies, that the underlying concept of diffusion is the idea of a random motion on the microscopic level. That this random motion can be used, to derive macroscopic and deterministic quantities has been shown by a variety of scientists throughout the history.

Robert Brown discovered the random motion of non-living particles due to collisions on an atomic level in 1827. This process was later called Brownian motion. Further contributors were Adolf Fick and Thomas Graham. In 1905, Albert Einstein made significant contributions to the topic in his paper “Investigations on the theory of the Brownian movement”, where Einstein derives the diffusion equation from a molecular point of view. For a detailed overview of the history of diffusion during the last 150 years, the reader may refer to the very detailed historical survey by Mehrer and Stolwijk<sup>[1]</sup> and Philbert<sup>[2]</sup>.

In this chapter, we will derive different equations for the description of diffusive processes as well as the kinetic equations in this context. We will do so, by using the atomic or microscopic point of view where we derive quantities of interest on the macroscopic level from the microscopic random motion. We will show, that deterministic quantities of interest can be derived from independent assumptions or concepts. This results can even be generalized to higher dimensions and explicit solutions for the arising equations can be given analytically.

## 1.1 Random walk on an integer lattice $\mathbb{Z}$ in one dimension

For simplicity, we start with the plain vanilla case in the derivation of the classical diffusion. Assume, that all particles are positioned on an integer lattice. That is, the position at time  $t = n$  is  $S_n = i$  with  $i \in \mathbb{Z}$ . Then assume further, that particles move only at fixed time intervals, and simplify  $\Delta t = 1$ . A particle has to move at each time step, and under the assumption of an unbiased random walk, a particle moves with probability  $1/2$  to the left and probability  $1/2$  to the right. We introduce the variable  $X_i \in \{-1, 1\}$ . At time  $t = n$  a particle then either moves to the left, i.e.  $X_n = -1$  or for  $X_n = 1$  the particle moves to the right, respectively. Since the random walk is unbiased, we have  $P\{X_n = -1\} = P\{X_n = 1\} = 1/2$ . Furthermore, let  $P_i^n$  denote the probability of a particle to be at position  $i$  in space at time  $t = n$ . A random walk is then defined as a sequence of random steps  $\{X_1, X_2, \dots, X_n\}$ , where we can compute the distance from the origin  $S_0$  as  $S_n = S_0 + \sum_{i=1}^n X_i$ . For further computation, assume  $S_0 = 0$ , i.e. we start at the origin of the lattice. Given this basic assumptions, we can derive several probabilistic quantities of the underlying process.

1. The maximal distance from the origin after  $n$  steps is  $n$ .
2. The expected position at a given time is zero, i.e.  $\mathbb{E}(S_n) = \sum_{i=1}^n \mathbb{E}(X_i) = 0$  due to the additivity of the expectation operator.

3. Similar, we can compute the variance as

$\mathbb{E}(S_n^2) = \sum_{i=1}^n \sum_{j=1}^n \mathbb{E}(X_i X_j) = \sum_{i=1}^n \mathbb{E}(X_i^2) = \sum_{i=1}^n 1 = n$  since the  $X_i$  and  $X_j$  are independent from each other.

4. The mean absolute deviation can be computed by making use of Pascal's triangle, the Binomial distribution and Stirling's formula for the approximation of the factorial. By induction, one derives<sup>[3]</sup>

$$\mathbb{E}(|S_n|) \rightarrow \sqrt{\frac{2n}{\pi}}, \quad (1.1)$$

as  $n \rightarrow \infty$ .

5. The probability of finding a particle at position  $i$  at time  $n+1$  is composed of the probability of finding a particle on its adjacent nodes at the prior time step, i.e.

$$P_i^{n+1} = 1/2P_{i-1}^n + 1/2P_{i+1}^n, \quad (1.2)$$

which can be used to derive the diffusion equation. Therefore, we subtract  $P_i^n$  on both sides to get

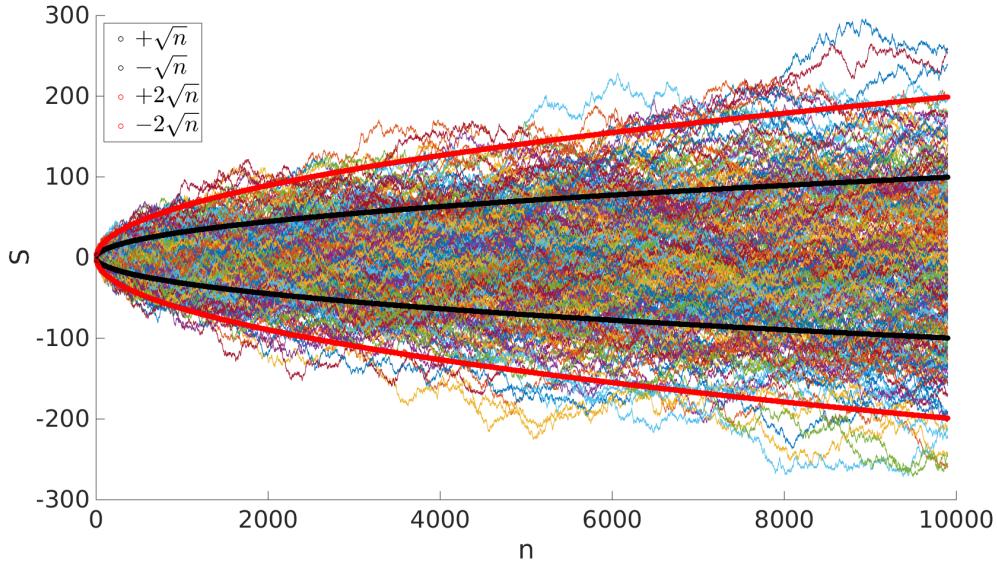
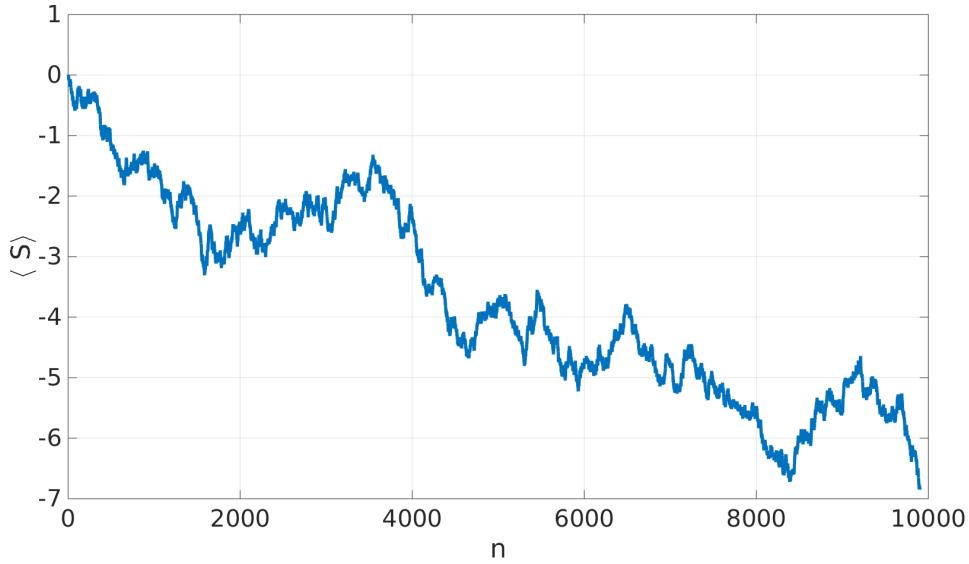
$$P_i^{n+1} - P_i^n = 1/2 [P_{i-1}^n - 2P_i^n + P_{i+1}^n]. \quad (1.3)$$

Up to scaling, this yields

$$\frac{\partial}{\partial t} P_n^i = \frac{\Delta x^2}{2\Delta t} \frac{\partial^2}{\partial x^2} P_n^i = D \frac{\partial^2}{\partial x^2} P_n^i, \quad (1.4)$$

where  $D = \frac{\Delta x^2}{2\Delta t}$  is the diffusion coefficient. The derived equation is a partial differential equation for the probability  $P$  of finding particles at a certain position in time and space and can be seen as a measure of the concentration or density of the particle distribution.

In Figure 1.1a, the above described process is simulated for  $N_{particles} = 1000$  over a time span of 10000 iterations. Figure 1.1b shows the expected value of  $S_i$  which does not converge. However, as derived above, the mean absolute displacement behaves like  $\sqrt{n}$ , which can be seen in Figure 1.1c. We also observe the linear scaling of the mean square displacement in Figure 1.1d as postulated.

(A) Position of particle with  $\pm\sqrt{n}$  and  $\pm 2\sqrt{n}$  for comparison.(B) Mean displacement  $\langle S \rangle$ 

## 1.2 Random walk on an integer lattice $\mathbb{Z}^d$ in multiple dimensions

The random process for the one dimensional case can easily be extended to multiple dimensions. Instead of allowing a particle to move to the left or right, we allow movements to each face of a  $d$  dimensional hypercube. For the case of  $d = 2$ , valid movements are up, down, left and right and for  $d = 3$ , we add the directions top and bottom. Movements in all directions happen with equal probability when assuming an unbiased walk. The derived properties for the one dimensional random walk in section 1.1 can easily be adapted. Properties 1 to 4 remain unchanged for multiple dimensions, except that

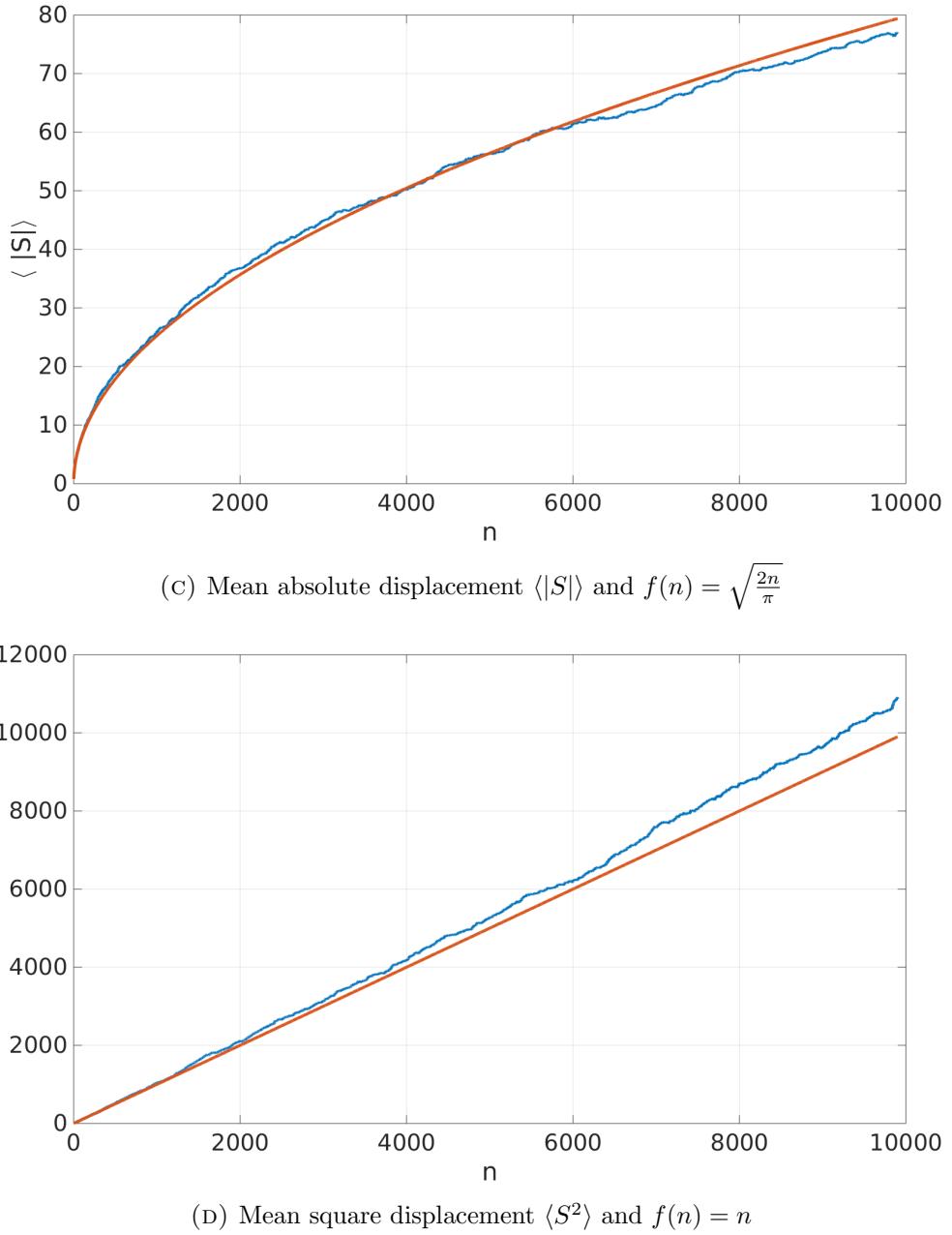


FIGURE 1.1: 1000 particles simulated over 10.000 iterations.

we have to understand the first point component wise. For  $d$  dimension, equation (1.3) reads

$$P_I^{n+1} - P_I^n = -P_I^n + \frac{1}{2d} \sum_{j \in J_I} P_J^n, \quad (1.5)$$

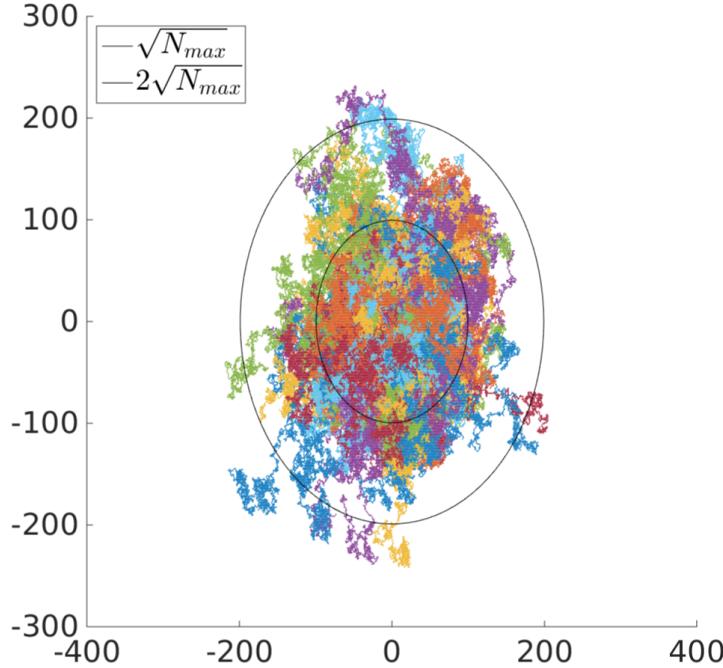


FIGURE 1.2: Position of particle with circle of radius  $\sqrt{N_{max}}$  and  $2\sqrt{N_{max}}$  for comparison.

where  $I$  is the multiindex that describes the position on the  $d$  dimensional lattice and  $J_I$  is the set of adjacent nodes, i.e.  $|I - J| = 1 \quad \forall J \in J_I$ . In two dimensions, this yields

$$P_I^{n+1} - P_I^n = -P_I^n + \frac{1}{4} [P_{I+e_1}^n + P_{I-e_1}^n + P_{I+e_2}^n + P_{I-e_2}^n], \quad (1.6)$$

with the unit vectors  $e_1$  and  $e_2$ . Which gives exactly the discretization of the two dimensional Laplace Operator. Consequently, we end up with an approximation of

$$\frac{\partial}{\partial t} P_I^n = D \Delta P_I^n. \quad (1.7)$$

This is the extension of (1.4) to two dimensions. Figure 1.2 shows the random walk on a two dimensional lattice together with circles of radius  $\sqrt{N_{max}}$  and  $2\sqrt{N_{max}}$  and in Figure 1.3 we see the three dimensional case.

### 1.3 Master equation and Fokker-Planck equation

Another way to derive the diffusion equation from a microscopic viewpoint was presented by Einstein in 1905 in his paper on the movement of small particles in a stationary liquid<sup>[4]</sup>. Consider therefore the probability density function  $P(x, t)$  for random walkers, that take jumps at discrete intervals in time, namely  $\Delta t$  with a jump length, sampled according to some density function  $\lambda(\Delta x)$ . One can then derive<sup>[5]</sup> the probability density

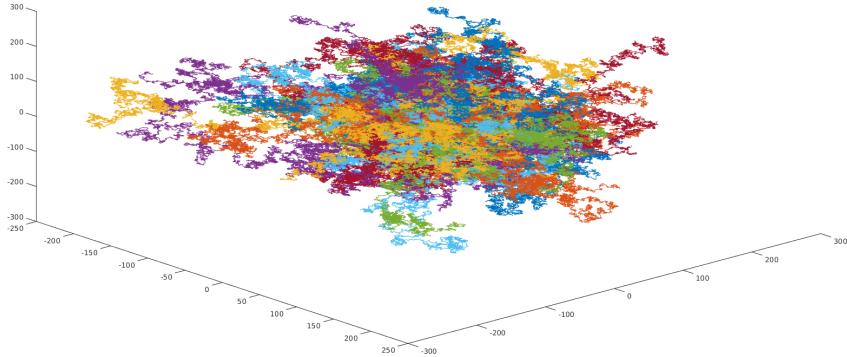


FIGURE 1.3: 3D random walk.

of a given point  $(x, t)$  in dependency of the probability at the prior time step  $t - \Delta t$  and all positions in space that can be reached during one time step with the given jump length distribution. This yields

$$P(x, t) = \int_{-\infty}^{\infty} \lambda(\Delta x) P(x - \Delta x, t - \Delta t) d\Delta x. \quad (1.8)$$

We sample the probabilities of particles jumping from any point in space at the last time step. Now we can use Taylor expansion to express  $P(x, t)$  and  $P(x - \Delta x, t - \Delta t)$  in terms of  $P_{x, t - \Delta t}$  under the assumption that  $\Delta x$  and  $\Delta t$  are small. A simple computation yields

$$P(x, t) \approx P|_{x, t - \Delta t} + \Delta t \frac{\partial}{\partial t} P|_{x, t - \Delta t}, \quad (1.9)$$

for the left-hand side and

$$P(x - \Delta x, t - \Delta t) \approx P|_{x, t - \Delta t} - \Delta x \frac{\partial}{\partial x} P|_{x, t - \Delta t} + \frac{\Delta x^2}{2} \frac{\partial^2}{\partial x^2} P|_{x, t - \Delta t}, \quad (1.10)$$

for the right-hand side, respectively. Plugging this into the master equation (1.8) we obtain

$$\begin{aligned} P|_{x, t - \Delta t} + \Delta t \frac{\partial}{\partial t} P|_{x, t - \Delta t} &\approx \\ \int_{-\infty}^{\infty} \lambda(\Delta x) P|_{x, t - \Delta t} - \Delta x \frac{\partial}{\partial x} P|_{x, t - \Delta t} + \frac{\Delta x^2}{2} \frac{\partial^2}{\partial x^2} P|_{x, t - \Delta t} d\Delta x. \end{aligned} \quad (1.11)$$

Integrating  $\lambda(\Delta x)$  against  $\Delta x^n$  just gives the  $n$ th moment  $\langle \Delta x^n \rangle$ . Furthermore, the density  $\lambda(\Delta x)$  integrates to unity. Omitting the location of the Taylor expansion, we

can simplify the above expression to

$$\frac{\partial}{\partial t} P \approx -\frac{\langle \Delta x \rangle}{\Delta t} \frac{\partial}{\partial x} P + \frac{\langle \Delta x^2 \rangle}{2\Delta t} \frac{\partial^2}{\partial x^2} P, \quad (1.12)$$

where we define the diffusion coefficient as

$$D = \lim_{\Delta x, \Delta t \rightarrow 0} \frac{\langle \Delta x^2 \rangle - \langle \Delta x \rangle^2}{2\Delta t} = \lim_{\Delta x, \Delta t \rightarrow 0} \frac{\langle \Delta x^2 \rangle}{2\Delta t} + \mathcal{O}\left(\frac{\langle \Delta x \rangle^2}{\Delta t}\right), \quad (1.13)$$

and

$$v = \lim_{\Delta x, \Delta t \rightarrow 0} \frac{\langle \Delta x \rangle}{\Delta t}, \quad (1.14)$$

as the drift velocity, respectively. In the same manner as for the random walk on a lattice, we assume an unbiased walk, meaning that the density for the step length distribution is symmetric, i.e.  $\lambda(\Delta x) = \lambda(-\Delta x)$ , which yields  $\langle \Delta x \rangle = 0$  and therefore, the drift velocity is zero. Summarizing this, we obtain, up to an approximation error,

$$\frac{\partial}{\partial t} P(t, x) = D \frac{\partial^2}{\partial x^2} P(t, x), \quad (1.15)$$

which is again the diffusion equation with quantity  $P(t, x)$ .

*Remark 1.1.* Under the assumption of a step length distribution that is depending on the position as well, i.e.  $\lambda = \lambda(\Delta x, x)$  we can perform the same computation and end up with the same results as in equation (1.15), but the diffusion coefficient (and for non symmetric distributions the drift velocity as well) is now also depending on  $x$ . This is then expressed in the generalized Fokker-Planck equation

$$\frac{\partial}{\partial t} P(x, t) = \frac{\partial^2}{\partial x^2} (D(x)P(x, t)) - \frac{\partial}{\partial x} (v(x)P(x, t)), \quad (1.16)$$

where  $v(x) = 0$  if  $\lambda(\Delta x)$  is symmetric.

## 1.4 Fundamental solution

By analysis of simple diffusion processes, it is possible to derive a fundamental solution of the corresponding differential equations. Fundamental solutions are not only helpful for the concrete simplified equation they rely on, but also give insight in the general structure of the underlying problem. Let us consider the simple equation

$$\frac{\partial}{\partial t} G(t, x) = D \frac{\partial^2}{\partial x^2} G(t, x), \quad (1.17)$$

$$G(0, x) = \delta(x). \quad (1.18)$$

Here,  $\delta(x)$  denotes the Kronecker delta. This equation corresponds to a diffusion process where initially, the whole quantity of interest is located at the origin. Applying Fourier transform in space yields

$$\frac{\partial}{\partial t} \hat{G}(s, t) = -Ds^2 \hat{G}(s, t), \quad (1.19)$$

$$\hat{G}(s, t) = \hat{\delta}(s) = 1, \quad (1.20)$$

which has the solution

$$\hat{G}(s, t) = e^{-Ds^2 t}. \quad (1.21)$$

By applying the inverse Fourier transform, we derive

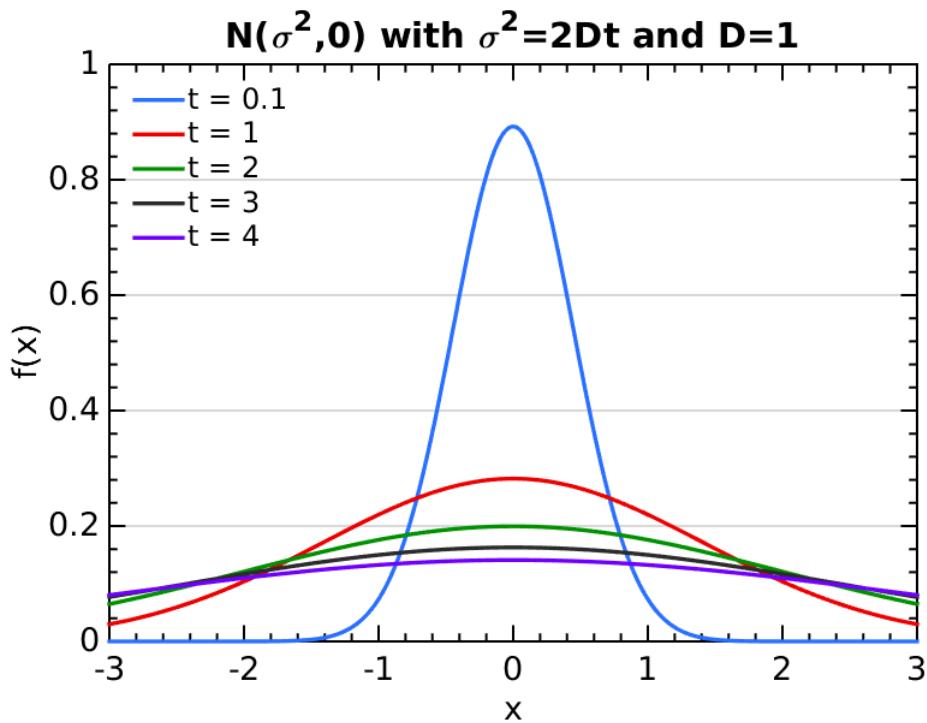
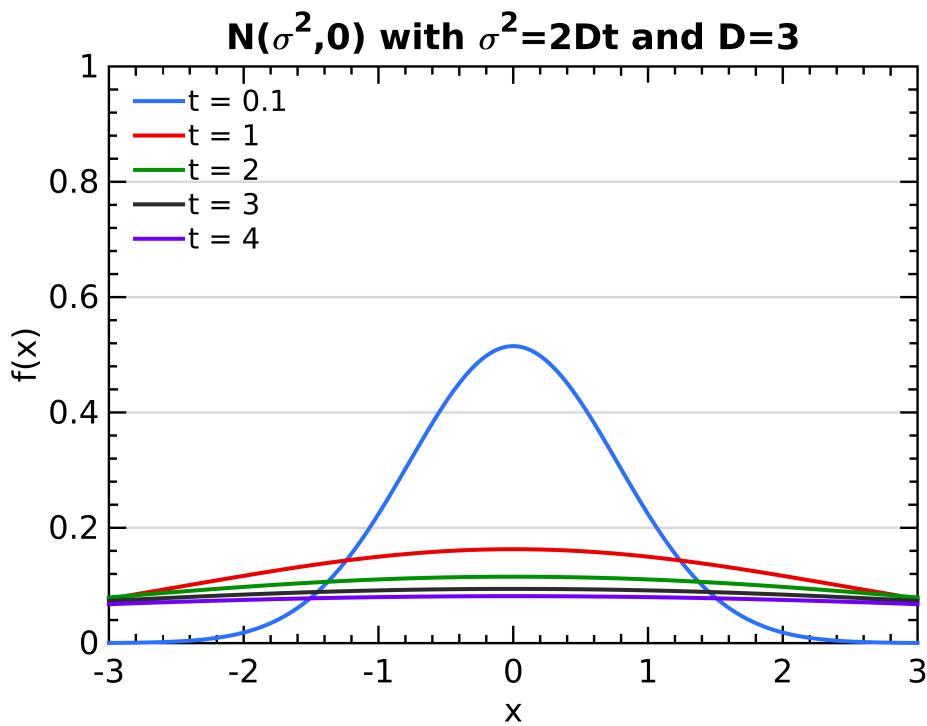
$$G(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}, \quad (1.22)$$

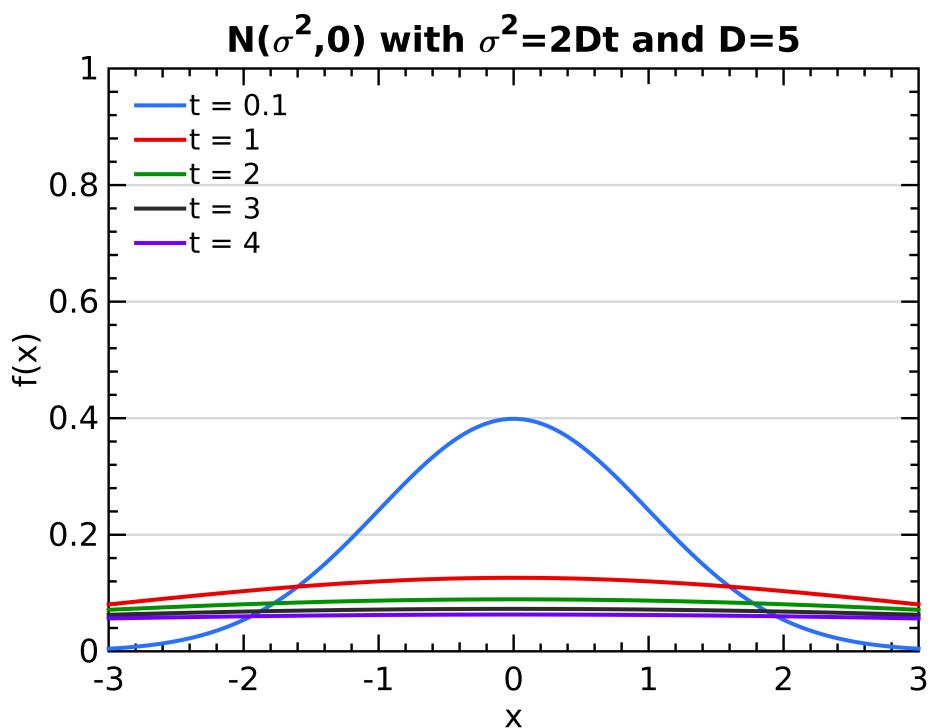
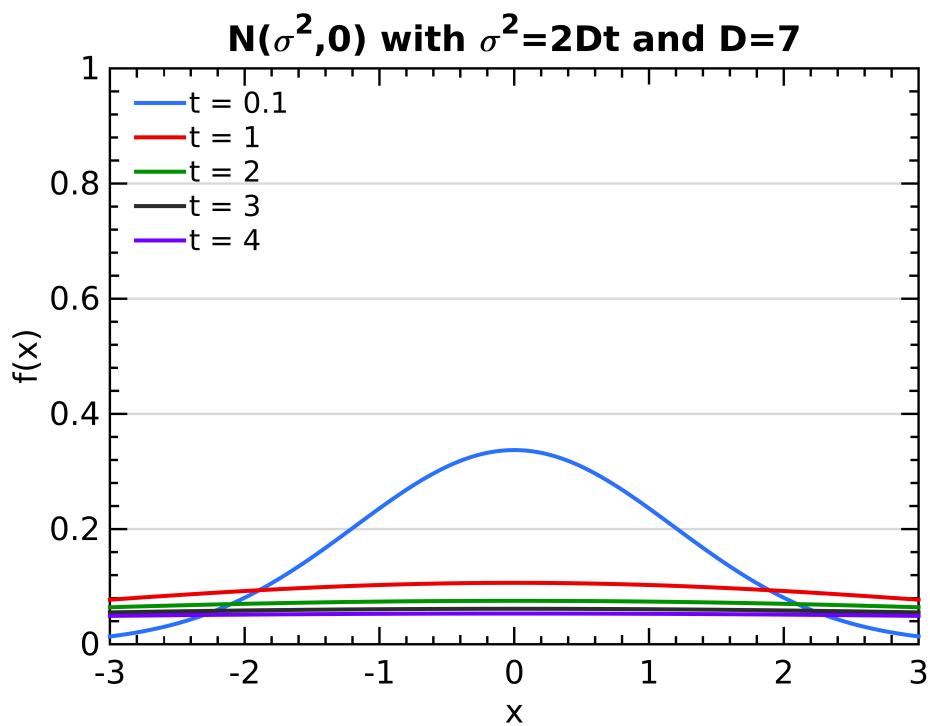
which coincides with the density function of the Normal distribution, that is

$$N(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \quad (1.23)$$

for  $\sigma^2 = 2Dt$  and  $\mu = 0$ . Since  $\sigma^2$  corresponds to the variance, which is the second moment and therefore identically with the mean squared displacement, we verify that  $\langle x^2 \rangle \propto \sqrt{t}$ , as well as  $\mu = 0$ , which corresponds to the symmetric initial condition.

The diffusion process for equation (1.19) is visualized in Figures 1.4, 1.5, 1.6 and 1.7 for different values of the diffusion coefficient  $D$  at different time steps  $t$ . We can see, that the higher the value of  $D$  the faster the quantity of interest spreads over the domain. Each of the illustrated functions itself is a Normal distribution with different values of  $\sigma$  and no mean displacement, i.e.  $\mu = 0$ . In agreement with physical intuition, for increasing time  $t$  the function reaches a constant level, which corresponds to an equal distribution of the initial quantity.

FIGURE 1.4: Normal distribution with diffusion coefficient  $D = 1$ .FIGURE 1.5: Normal distribution with diffusion coefficient  $D = 3$ .

FIGURE 1.6: Normal distribution with diffusion coefficient  $D = 5$ .FIGURE 1.7: Normal distribution with diffusion coefficient  $D = 7$ .



“What if  $n = 1/2$  in  $\frac{d^n f(x)}{dx^n}$  ?”  
L’Hospital to Leibniz, 1695

“This is an apparent paradox from which, one day,  
useful consequences will be drawn.”

Leibniz to L’Hospital, 1695

# 2

## Fractional calculus

As already mentioned in letters between Leibniz and L’Hospital at the end of the 17th century, fractional calculus defines the mathematical branch, that tries to generalize the differential operator  $D = d/dx$  and the integral operator  $I$  to orders that are no longer restricted to the natural numbers, but also allow for the order to be any real number or even complex valued. The term fractional calculus might be misleading, since the order is not restricted to fractions, therefore the term “differentiation and integration of fractional order” might be more suitable. However, in the historic context and current literature, the topic is almost always referenced as fractional calculus.

### 2.1 Historical survey

To outline the progress in fractional calculus over the past centuries, we will summarize the comprehensive work of Ross<sup>[6]</sup> and Mendes<sup>[7]</sup> below.

In the historical context, Leibniz and L’Hospital provide the first documented thoughts about a generalization of the  $n$ th derivative to non integer order. Even though the first thoughts about fractional calculus were purely theoretical, physical examples and a more intuitive understanding have followed soon after.

L'Hospital noticed in 1665 in his correspondence with Leibniz, that “ $d^{1/2}x$  will be equal to  $x\sqrt{dx : x}$ ” from which “one day, useful consequences will be drawn”. However, it weren't Leibniz or L'Hospital who went into further details regarding the topic of fractional calculus.

Another famous mathematician who dealt with the topic was Euler, who noticed in 1730, that “the ratio  $d^n p$  to  $dx^n$  can always be expressed algebraically” and asked for a generalization for  $n$  being arbitrary<sup>1</sup>.

In 1819, Lacroix explicitly stated, that for  $y = x^m$  one can easily derive

$$\frac{d^n y}{dx^n} = \frac{m!}{(m-n)!} x^{m-n} \quad \text{for } m \geq n. \quad (2.1)$$

This can extend to arbitrary order with the use of the Gamma function, yielding

$$\frac{d^n y}{dx^n} = \frac{\Gamma(m+1)}{\Gamma(m-n+1)} x^{m-n}. \quad (2.2)$$

Lacroix then furthermore gives the example for  $y = x$  and  $n = 1/2$ ,

$$\frac{d^{1/2} x}{dx^{1/2}} = 2\sqrt{\frac{x}{\pi}}. \quad (2.3)$$

It is worth mentioning, that this is exactly the result, one would obtain with the use of the Riemann-Liouville derivative, which we will define later on.

Further contributions were provided by Fourier, by expressing a function in its Fourier series. Fourier used the expansion of  $f(x)$  as

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\alpha) \int_{-\infty}^{\infty} \cos(p(x-\alpha)) dp d\alpha. \quad (2.4)$$

Using the following identity

$$\frac{d^n}{dx^n} \cos(p(x-\alpha)) = p^n \cos(p(x-\alpha)) + \frac{1}{2} n\pi, \quad (2.5)$$

one can give meaning to

$$\frac{d^u}{dx^u} f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\alpha) \int_{-\infty}^{\infty} p^n \cos(p(x-\alpha) + \frac{1}{2} n\pi) dp d\alpha, \quad (2.6)$$

where “The number  $u$  [...] will be regarded as any quantity whatsoever”.

It was then Liouville, who provided major contributions in the second half of the 19th century. Inspired by Fourier, he started with functions that could be expressed as an

---

<sup>1</sup>  $d^n p$  denotes the  $n$ th derivative of a polynomial  $p(x)$ .

infinite sum, namely

$$f(x) = \sum_{n=0}^{\infty} c_n \exp(a_n x), \quad \operatorname{Re}(a_n) > 0. \quad (2.7)$$

Together with the fact, that

$$\frac{d^\nu}{dx^\nu} \exp(ax) = a^\nu \exp(ax), \quad (2.8)$$

is a logical extension of the integer case, he then derived

$$\frac{d^\nu}{dx^\nu} f(x) = \sum_{n=0}^{\infty} c_n a_n^\nu \exp(a_n x) \quad \operatorname{Re}(a_n) > 0. \quad (2.9)$$

Disadvantageous is the fact, that this formula is only applicable to functions that can be expanded as presented in (2.7). Liouville's second case considered functions of the type  $y = x^{-a}$  with  $a > 0$ . Using the definition of the Gamma function and substitution, he obtained

$$D^\nu x^{-a} = \frac{(-1)^\nu \Gamma(a + \nu)}{\Gamma(a)} x^{-a - \nu}. \quad (2.10)$$

However, all these calculations were only applicable to a small class of functions.

A more versatile approach and the starting point for today's definition of Riemann and Liouville was inspired by Cauchy's integral formula, according to which the  $n$ th derivative can be expressed as

$$D^n f(z) = \frac{n!}{2\pi i} \int_C \frac{f(\xi)}{(\xi - z)^{n+1}} d\xi. \quad (2.11)$$

Where it is possible to generalize the definition to non integer values using the Gamma function. However, there are technical problems regarding the contour  $C$  when  $n$  is not an integer<sup>[8]</sup>. Based on Cauchy's integral formula, Laurent was able to derive the fractional integral operator, which for  $c = 0$  gives the Riemann-Liouville fractional integral

$${}_c D_x^{-\nu} f(x) = \frac{1}{\Gamma(\nu)} \int_c^x (x - t)^{\nu-1} f(t) dt. \quad (2.12)$$

Functions for which (2.12) converges are said to be of Riemann class. Another choice for the lower bound of the integration is  $c = -\infty$ , which converges for functions of Liouville class.

At the end of the nineteenth century, there were several definitions and different opinions on the topic of fractional calculus. During the twentieth century, the concept of

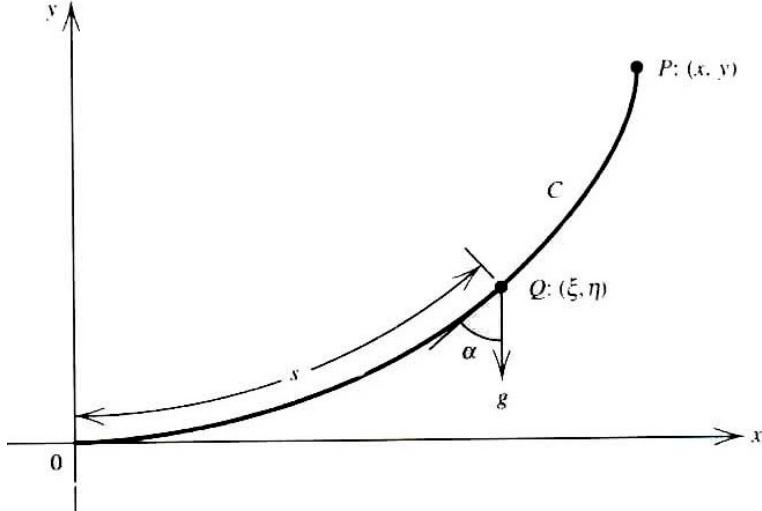


FIGURE 2.1: The tautochrone problem. Figure taken from Delkhosh et al. [9].

fractional calculus has found a variety of applications in applied sciences and engineering, where different definitions have been shown to be advantageous.

So far, the derivations have been of rather theoretical nature, but there exist several practical problems that can be related to the concept of fractional calculus. One of these problems was Abel's tautochrone problem (not to be confused with the brachistochrone problem). Abel asked for the form of a curve  $C$  for which, under the influence of gravity and without friction, the time for a particle starting at rest and moving to the lowest point is independent of the starting point  $P$  on the curve  $C$ , shown in Figure (2.1).

The following calculation is taken from Miller & Ross<sup>[8]</sup>. Denote the arc length from the origin to an arbitrary point  $Q$  with coordinates  $(\xi, \eta)$  by  $s$ . Further, let  $\alpha$  denote the slope and  $-g$  the gravitational force, then

$$\frac{d\eta}{ds} = \cos(\alpha). \quad (2.13)$$

Newton's law then yields the differential equation

$$\frac{ds^2}{dt^2} = -g \frac{d\eta}{ds}, \quad (2.14)$$

from which we obtain by integration and application of the initial values

$$\frac{ds}{dt} = -\sqrt{2g(y - \eta)}. \quad (2.15)$$

The time of the descent from  $P$  to the origin can then be calculated as

$$T = -\frac{1}{\sqrt{2g}} \int_P^0 \frac{1}{\sqrt{y - \eta}} ds. \quad (2.16)$$

The arc length  $s$  is a function of  $\eta$ , i.e.  $s = h(\eta)$  and therefore

$$T = -\frac{1}{\sqrt{2g}} \int_y^0 \frac{1}{\sqrt{y-\eta}} h'(\eta) d\eta, \quad (2.17)$$

$$\Leftrightarrow \sqrt{2g}T = \int_0^y \frac{h'(\eta)}{\sqrt{y-\eta}} d\eta, \quad (2.18)$$

and with  $f(y) = h'(y)$  we can write

$$\frac{\sqrt{2g}}{\Gamma(\frac{1}{2})} T = D^{-1/2} f(y). \quad (2.19)$$

That is,  $D^{-1/2} f(y)$  is the Riemann-Liouville fractional integral of order 1/2. To solve the equation (2.19), Abel applied the fractional operator  $D^{1/2}$  to both sides to get

$$D^{1/2} \sqrt{\frac{2g}{\pi}} T = f(y). \quad (2.20)$$

Together with

$$D^{1/2} T = \frac{T}{\sqrt{\pi y}}, \quad (2.21)$$

one obtains

$$f(y) = \frac{\sqrt{2g}}{\pi} T y^{-1/2}. \quad (2.22)$$

Since the function  $f$  that measures the arc length is known and given by

$$f(y) = h'(y) = \sqrt{1 + \left(\frac{dx}{dy}\right)^2}, \quad (2.23)$$

we can derive

$$x = \int_0^y \sqrt{\frac{2gT^2}{\pi^2 \eta} - 1} d\eta + c. \quad (2.24)$$

If we use the initial conditions and a change of variables, further computation yields

$$x = \frac{gT^2}{\pi^2} (\theta + \sin(\theta)), \quad (2.25)$$

$$y = \frac{gT^2}{\pi^2} (1 - \cos(\theta)), \quad (2.26)$$

which is the definition of a cycloid. Even though, this problem has been solved by several mathematicians prior, Abel was the first to tackle this problem with the tools of fractional calculus.

In the remaining part of this chapter, we will present the most common definitions of fractional derivatives in a more mathematical rigorous fashion. Therefore, we will at first recall the definitions of a variety of non elementary functions that will be useful later on. As the historical survey suggests, these definitions are strongly coupled to the field of application and often seem to be gratuitous, inconsistent or even contradictory. However, all the presented definitions have their *raison d'être* and will be used during the theoretical or numerical analysis in the later part of this work.

## 2.2 Special functions in the context of fractional calculus

There are certain functions that occur frequently throughout this thesis. Those functions, that are not elementary or might require some further background are defined in the following, together with some of their basic properties.

### 2.2.1 Gamma function

The Gamma function  $\Gamma(n)$  is an extension of the factorial function for the non integer values with the property

$$\Gamma(n) = (n-1)! , \quad (2.27)$$

for  $n \in \mathbb{N}^+$ . For complex numbers  $t$  with positive real part, Legendre defined the Gamma function as

$$\Gamma(t) = \int_0^\infty x^{t-1} e^{-x} dx, \quad (2.28)$$

which converges absolutely. A recurrence relation can be given by  $\Gamma(t+1) = t\Gamma(t)$ . This relation can be used to extend the definition of the Gamma function to negative non integer values. Further equivalent definitions exist according to Euler, Weierstrass or Laguerre, but aren't used in the following sections. According to Stirling's formula, we can write

$$\Gamma(t+1) \sim \sqrt{2\pi t} \left( \frac{t}{e} \right)^t , \quad (2.29)$$

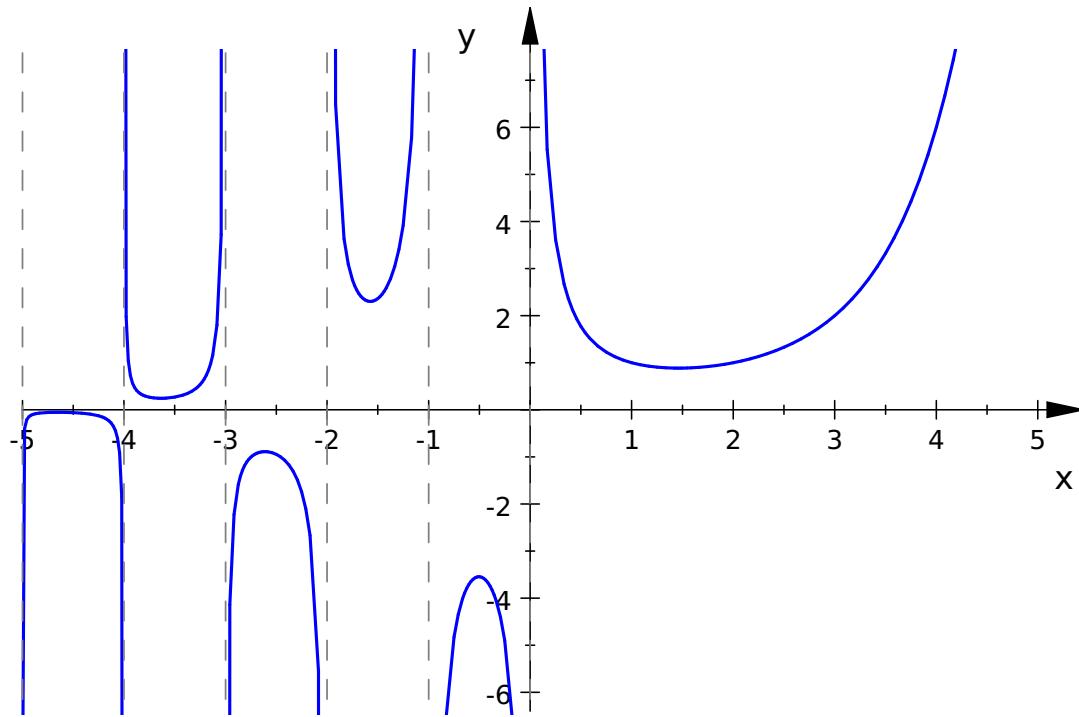


FIGURE 2.2: The gamma function

for  $t \rightarrow \infty$ . Some notable values of the Gamma function are

$$\Gamma(0) = \infty, \quad (2.30)$$

$$\Gamma(1/2) = \sqrt{\pi}, \quad (2.31)$$

$$\Gamma(1) = 1. \quad (2.32)$$

Further note, that  $|\Gamma(-n)|$  diverges for  $n \in \mathbb{N}$ .

### 2.2.2 Mittag-Leffler function

This class of functions has been defined and studied by Mittag-Leffler<sup>2</sup> in the beginning of the 20th century. In its most general form, it is given by

$$E_{\alpha, \beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\beta + \alpha k)}, \quad (2.33)$$

<sup>2</sup> The rumor that Alfred Nobel didn't offer a Nobel Prize for mathematics because Mittag-Leffler had an affair with Nobel's wife is not true. Nobel was never married. For more gossip, the reader may refer to <http://www.fields.utoronto.ca/aboutus/jcfields/fieldsnobel.html>.

with  $\alpha, \beta \in \mathbb{C}$  with positive real part and  $z \in \mathbb{C}$ . A special case of the Mittag-Leffler, that is often of interest, is

$$E_\alpha(z) := E_{\alpha,1}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+\alpha k)}, \quad (2.34)$$

with  $\alpha$  and  $z$  defined as before.

Another way to define the Mittag-Leffler function is by an integral representation. We can write  $E_\alpha(z)$  as

$$E_\alpha(z) = \frac{1}{2\pi i} \int_{\Omega} \frac{t^{\alpha-1} \exp(t)}{t^\alpha - z} dt, \quad (2.35)$$

with  $\alpha$  and  $z$  defined as before. The path of integration  $\Omega$  is a loop starting and ending at  $-\infty$  around the singularities and branch points of the integrand.

Referring to Haubold, Mathai and Saxena<sup>[10]</sup> we can list some interesting properties and identities of the Mittag-Leffler function.

$$E_0(z) = \frac{1}{1-z} \quad \text{for } |z| < 1, \quad (2.36)$$

$$E_1(z) = e^z, \quad (2.37)$$

$$E_2(z) = \cosh(\sqrt{z}) \quad \text{for } z \in \mathbb{C}, \quad (2.38)$$

$$E_2(-z^2) = \cos(z) \quad \text{for } z \in \mathbb{C}. \quad (2.39)$$

A visualization of the different entities is given in Figure 2.3.

The Mittag-Leffler class of functions is especially relevant due to its relation to fractional calculus. Using the Riemann-Liouville Definition of the fractional derivative, which we will encounter later, we can see, that the solution of the eigenvalue problem

$$\left[ {}_0^{RL} D_t^\alpha \right] f(t) = \lambda f(t), \quad (2.40)$$

can be computed<sup>[11]</sup> to be

$$f(t) = t^{\alpha-1} E_{\alpha,\alpha}(\lambda t^\alpha). \quad (2.41)$$

*Remark 2.1.* For  $\alpha = 1$  this corresponds to the solution of the eigenvalue problem  $f'(t) = \lambda f(t)$  which has the solution  $f(t) = e^{\lambda t}$ . Substituting  $\alpha = 1$  in (2.41) and using (2.37), we see that the generalized problem in (2.40) and its solution coincides with the integer valued problem.

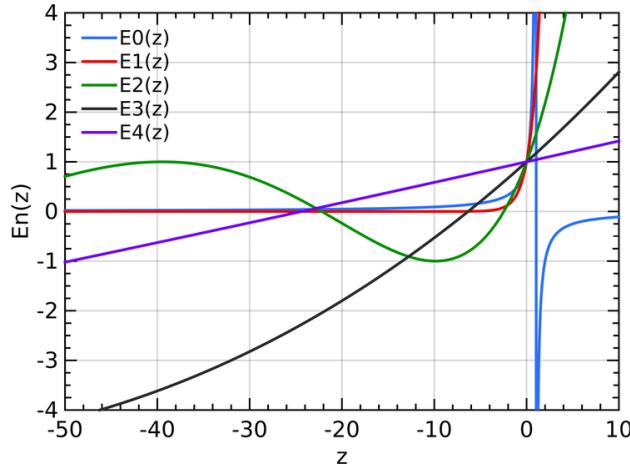


FIGURE 2.3: Entities of the Mittag-Leffler function for  $\beta = 0$  and  $\alpha \in [0, 1, 2, 3, 4]$ .

Furthermore, the Mittag-Leffler function is capable of combining algebraic and exponential decay, which is of importance in the setting of fractional calculus. For small values of  $t$ , i.e.  $0 \leq t \ll 1$  we have the expansion

$$E_{\alpha,1}(-t^\alpha) \simeq 1 - \frac{t^\alpha}{\Gamma(1+\alpha)} \simeq \exp \left[ -\frac{1}{\Gamma(1+\alpha)} t^\alpha \right]. \quad (2.42)$$

On the other hand, for  $t \rightarrow \infty$  one observes algebraic decay, i.e.

$$E_{\alpha,1}(-t^\alpha) \simeq \frac{t^{-\alpha}}{\Gamma(1-\alpha)}. \quad (2.43)$$

This property is visualized in Figure 2.4, where we can see the Mittag-Leffler function in a log-log plot together with the corresponding exponential expansion and the algebraic expansion, respectively.

### 2.2.3 Wright function

Another important function in the context of fractional partial differential equations is the Wright function, named after E.M. Wright. It is given by

$$\phi(\rho, \beta, z) = \sum_{k=0}^{\infty} \frac{z^k}{k! \Gamma(\rho k + \beta)}, \quad (2.44)$$

for  $\rho > -1$  and  $\beta \in \mathbb{C}$ . The interest in this function arises from the fact, that the Green's function of a fractional partial differential equation can be expressed in terms of the Wright function.

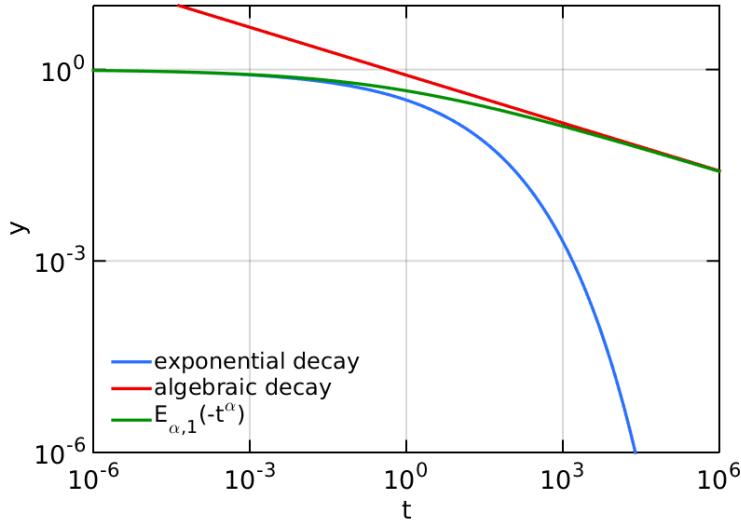


FIGURE 2.4: Log-log plot of the Mittag-Leffler function. We observe exponential decay for small  $t$  and algebraic decay for large  $t$ .

Applying the Laplace transform to the Wright function [12], we derive a relation between the Wright function and the Mittag-Leffler function, namely

$$\mathcal{L}[\phi(\rho, \beta, \pm t)](s) = \frac{1}{s} E_{\rho, \beta} \left( \pm \frac{1}{s} \right), \quad (2.45)$$

with  $\rho > 0$  and  $\mathcal{L}$  denoting the well-known Laplace transform that is also explained in more detail in subsection 2.4.2 and  $E_{\rho, \beta}$  is defined as in (2.33).

A detailed analysis of the Wright function within the context of fractional differential equations can be found in the work of Gorenflo, Luchko and Mainardi [12].

### 2.3 Integrals and derivatives of fractional order

We are now going to present the most common definitions of integrals and derivatives of fractional order. As the history of fractional calculus suggests, different mathematicians came up with different generalizations of the derivative for fractional order. Since the Caputo derivative, as well as the Riemann-Liouville derivative rely on the generalized concept of integration for fractional order, this concept will also be derived here. Additionally to the definition of Caputo and Riemann and Liouville, we will present the definition according to Grünwald and Letnikov, which differs in its derivation, but is of interest when dealing with numerical approximation of fractional derivatives.

### 2.3.1 Cauchy's formula for integration

One of the main contributions to the field of fractional calculus, was the definition of integration according to Cauchy. With the help of this equivalent formulation of repeated integration, it was possible to extend integration of order  $n$  to integration of fractional order.

Let  $I^n f(x)$  denote repeated integration, i.e.

$$I^n f(x) := \underbrace{\int_0^x \int_0^t \int_0^s \dots \int_0^q f(p) dp dq \dots ds dt}_{n \text{ times}}. \quad (2.46)$$

Then, according to Cauchy, the integral can be represented equivalently as a single integral, stated in

*Theorem 2.2. Cauchy's formula for integration.*

$$\frac{1}{(n-1)!} \int_0^x (x-t)^{n-1} f(t) dt = \int_0^x \int_0^t \int_0^s \dots \int_0^q f(p) dp dq \dots ds dt. \quad (2.47)$$

*Proof.* We will use induction to proof the result.

There is nothing to show for  $n = 1$ .

Assume that the result holds for  $n - 1$ . For  $n$  we have

$$I^n f(x) = \int_0^x \int_0^t \int_0^s \dots \int_0^q f(p) dp dq \dots ds dt \quad (2.48)$$

$$\stackrel{IH}{=} \frac{1}{(n-2)!} \int_0^x \int_0^t (t-s)^{n-2} f(s) ds dt \quad (2.49)$$

$$= \frac{1}{(n-2)!} \int_0^x \int_s^x (t-s)^{n-2} f(s) dt ds \quad (2.50)$$

$$= \frac{1}{(n-2)!} \int_0^x \frac{1}{n-1} (x-s)^{n-1} f(s) ds \quad (2.51)$$

$$= \frac{1}{(n-1)!} \int_0^x (x-s)^{n-1} f(s) ds. \quad (2.52)$$

□

This is the initial statement, up to a change of variable names. Note, that we used a change of the integration order from (2.49) to (2.50), thus changing the integration boundaries.

Using this definition of repeated integration, we are no longer restricted to the natural numbers for  $n$ . We have been able to extend the definition of integration to fractional integration. Note, that almost all definitions of fractional derivatives rely on this

mechanism. Instead of a direct generalization of derivatives of fractional order  $\alpha$  with  $n-1 < \alpha \leq n$ , with  $n$  being a natural number, one applies the derivative up to the next higher integer order  $n$ , followed by fractional integration of order  $n-\alpha$ . For example, the Caputo derivative and the Liemann-Riouville derivative only vary in the order of the differential and integral operator.

### 2.3.2 Riemann-Liouville integral

As mentioned during the derivation of Cauchy's formula for derivation, the Riemann-Liouville derivative relies on a definition of a fractional integral.

*Definition 2.3.* Riemann-Liouville fractional integral of  $f$  of order  $\nu$  according to Miller and Ross<sup>[8]</sup>:

Let  $\nu$  have positive real part. Let  $f$  be piecewise continuous on  $J' = (0, \infty)$  and integrable on any finite subinterval of  $J = [0, \infty)$ . Then for  $t > 0$  we define

$${}_0D_t^{-\nu} f(t) = \frac{1}{\Gamma(\nu)} \int_0^t (t-\xi)^{\nu-1} f(\xi) d\xi, \quad (2.53)$$

as the Riemann-Liouville fractional integral.

We will now go through some examples by increasing complexity.

*Example 2.3.1.*  $f(t) = c = \text{const.}$

By definition we have

$${}_0D_t^{-\nu} f(t) = \frac{1}{\Gamma(\nu)} \int_0^t (t-\xi)^{\nu-1} c d\xi \quad (2.54)$$

$$= \frac{c}{\Gamma(\nu)} \int_0^t (t-\xi)^{\nu-1} d\xi \quad (2.55)$$

$$= -\frac{c}{\Gamma(\nu)} \frac{1}{\nu} (t-\xi)^\nu \Big|_{\xi=0}^t \quad (2.56)$$

$$= \frac{c}{\Gamma(\nu)} \frac{1}{\nu} t^\nu \quad (2.57)$$

$$= \frac{c}{\Gamma(\nu+1)} t^\nu. \quad (2.58)$$

For the simple case  $c = 1$  and  $\nu \in [0.2, 0.4, 0.6, 0.8, 1]$  we see the results in Figure 2.5

*Example 2.3.2.*  $f(t) = t^\mu$

By an analogue computation<sup>[8]</sup>, we can derive

$${}_0D_t^{-\nu} f(t) = \frac{\Gamma(\mu+1)}{\Gamma(\mu+\nu+1)} t^{\nu+\mu}, \quad (2.59)$$

with  $\text{Re}(\nu) > 0$ ,  $\text{Re}(\mu) > -1$ , which is plotted for  $\mu = 1$  in Figure 2.6.

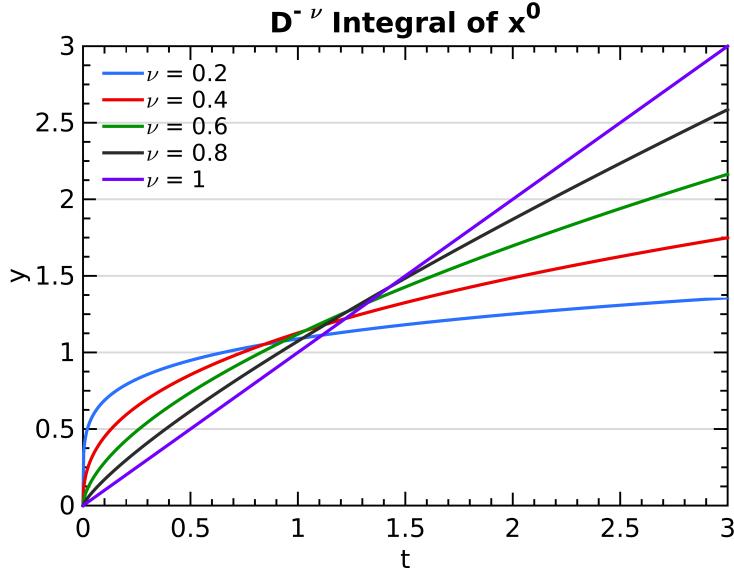
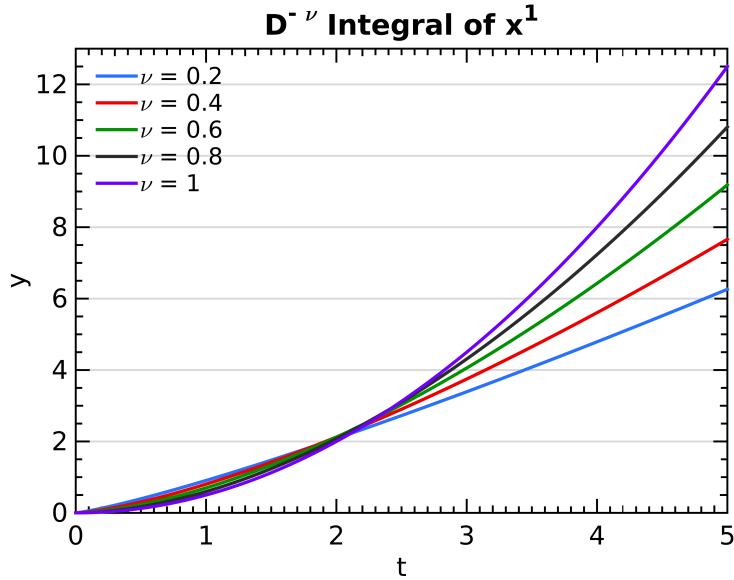


FIGURE 2.5: Fractional integral of a constant.

FIGURE 2.6: Fractional integral of  $x$ .

*Example 2.3.3.*  $f(t) = \exp(at)$  with  $a = \text{const.}$

This seemingly easy example shall demonstrate, that even for simple functions, the integral can become a transcendental function. We want to compute

$${}_0D_t^{-\nu} f(t) = \frac{1}{\Gamma(\nu)} \int_0^t (t-\xi)^{\nu-1} \exp(a\xi) d\xi. \quad (2.60)$$

By substituting  $x = t - \xi$  we obtain

$$\frac{1}{\Gamma(\nu)} \int_0^t (t-\xi)^{\nu-1} \exp(a\xi) d\xi = \frac{\exp(at)}{\Gamma(\nu)} \int_0^t (x)^{\nu-1} \exp(-ax) dx, \quad (2.61)$$

which we can write as

$${}_0D_t^{-\nu} f(t) = t^\nu \exp(at) \gamma^*(\nu, at), \quad (2.62)$$

with the incomplete Gamma function  $\gamma^*$ , defined as

$$\gamma^*(\nu, t) = \frac{1}{\Gamma(\nu)t^\nu} \int_0^t \xi^{\nu-1} \exp(-\xi) d\xi. \quad (2.63)$$

Due to frequent use in the context of fractional calculus, one often defines

$$E_t(\nu, a) = t^\nu \exp(at) \gamma^*(\nu, at). \quad (2.64)$$

Furthermore, we have an important property of the integral operator, namely

*Theorem 2.4.* *Let  $f$  be continuous on  $J$  and let  $\operatorname{Re}(\nu) > 0$  and  $\operatorname{Re}(\mu) > 0$ . We then have the equality*

$${}_0D_t^{-\nu} {}_0D_t^{-\mu} f(t) = {}_0D_t^{-\nu-\mu} f(t) = {}_0D_t^{-\mu} {}_0D_t^{-\nu} f(t). \quad (2.65)$$

*Proof.* We apply the definition of the fractional integral to obtain

$${}_0D_t^{-\nu} {}_0D_t^{-\mu} f(t) = \frac{1}{\Gamma(\nu)\Gamma(\mu)} \int_0^t (t-x)^{\nu-1} \int_0^x (x-y)^{\mu-1} f(y) dy dx \quad (2.66)$$

$$= \frac{1}{\Gamma(\nu)\Gamma(\mu)} \int_0^t \int_y^t (t-x)^{\nu-1} (x-y)^{\mu-1} f(y) dx dy \quad (2.67)$$

$$= \frac{1}{\Gamma(\nu)\Gamma(\mu)} \int_0^t f(y) \int_y^t (t-x)^{\nu-1} (x-y)^{\mu-1} dx dy. \quad (2.68)$$

Using the identity<sup>3</sup>

$$\int_y^t (t-x)^{\nu-1} (x-y)^{\mu-1} dx = \frac{\Gamma(\nu+\mu)}{\Gamma(\nu)\Gamma(\mu)} (t-y)^{\nu+\mu-1}, \quad (2.69)$$

we finally obtain

$${}_0D_t^{-\nu} {}_0D_t^{-\mu} f(t) = \frac{1}{\Gamma(\nu+\mu)} \int_0^t (t-y)^{\nu+\mu-1} f(y) dy = {}_0D_t^{-\nu-\mu} f(t). \quad (2.70)$$

To proof  ${}_0D_t^{-\nu} {}_0D_t^{-\mu} f(t) = {}_0D_t^{-\mu} {}_0D_t^{-\nu} f(t)$ , we can simply reverse the proof for the first part and switch  $\nu$  and  $\mu$ .  $\square$

<sup>3</sup>Substitute  $x = y + z$  and apply the generalized Binomial expansion for fractional order. The result follows immediately.

### 2.3.3 Riemann-Liouville derivative

We now have tools to generalize the integral operator to fractional order. For the generalization of the derivative operator, we simply combine integration of arbitrary order with the classical derivative.

Let  $D^n$  be the derivative operator of order  $n \in \mathbb{N}$ . Then with  ${}_0D_t^{-\nu}f(t)$  defined as above, we have

$$D^n({}_0D_t^{-n}f(t)) = f(t). \quad (2.71)$$

This implies, that the classical derivative operator is a left-inverse of the generalized integral operator. Consequently, we can then extend this concept for arbitrary order of the derivative operator, namely

$$D^\alpha f(t) := D^m({}_0D_t^{-(m-\alpha)}f(t)), \quad (2.72)$$

for  $m-1 < \alpha \leq m$ , which is exactly the definition according to Riemann-Liouville.

*Definition 2.5.* Riemann-Liouville fractional derivative of  $f$  of order  $\nu$ .

Let  $m-1 < \alpha \leq m$ . Then for  $f$  defined on  $(0, \infty)$  we define

$${}_0^{RL}D_t^\alpha f(t) = \begin{cases} \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dt^m} \int_0^t \frac{f(\tau)}{(t-\tau)^{\alpha+1-m}} d\tau & m-1 < \alpha < m, \\ \frac{d^m}{dt^m} f(t) & \alpha = m, \end{cases} \quad (2.73)$$

to be the Riemann-Liouville fractional derivative.

Again, we will apply this definition to some examples.

*Example 2.3.4.*  $f(t) = t^\nu$  where  $\nu > -1$  and  $m-1 < \alpha < m$ . By applying the definition and making use of example (2.3.2) we get

$${}_0^{RL}D_t^\alpha t^\nu = D^m({}_0D_t^{-(m-\alpha)}t^\nu) = D^m({}_0D_t^{-(m-\alpha)}t^\nu) \quad (2.74)$$

$$= D^m\left(\frac{\Gamma(\nu+1)}{\Gamma(\nu+m-\alpha+1)} t^{\nu+m-\alpha}\right) \quad (2.75)$$

$$= \frac{\Gamma(\nu+1)}{\Gamma(\nu+m-\alpha+1)} \frac{\Gamma(\nu+m-\alpha+1)}{\Gamma(\nu+1-\alpha)} t^{\nu-\alpha} \quad (2.76)$$

$$= \frac{\Gamma(\nu+1)}{\Gamma(\nu+1-\alpha)} t^{\nu-\alpha}, \quad (2.77)$$

which generalizes the integer case. The results for different values of  $\alpha$  can be seen in Figure 2.7.

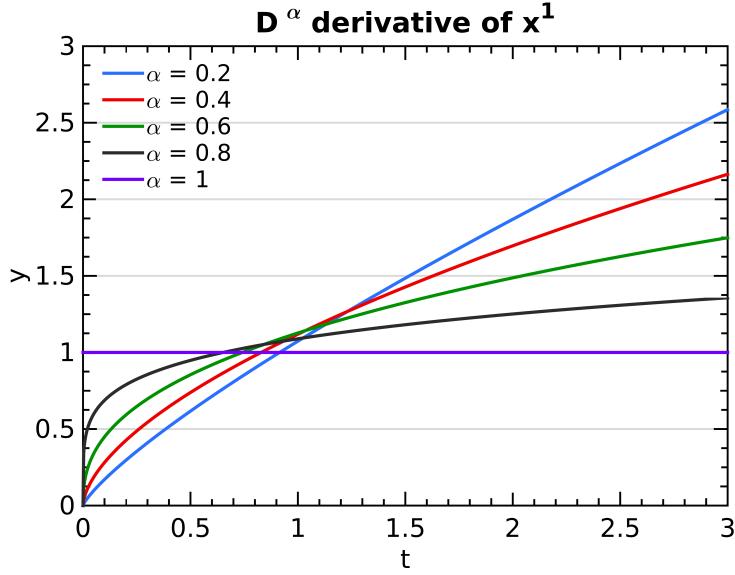
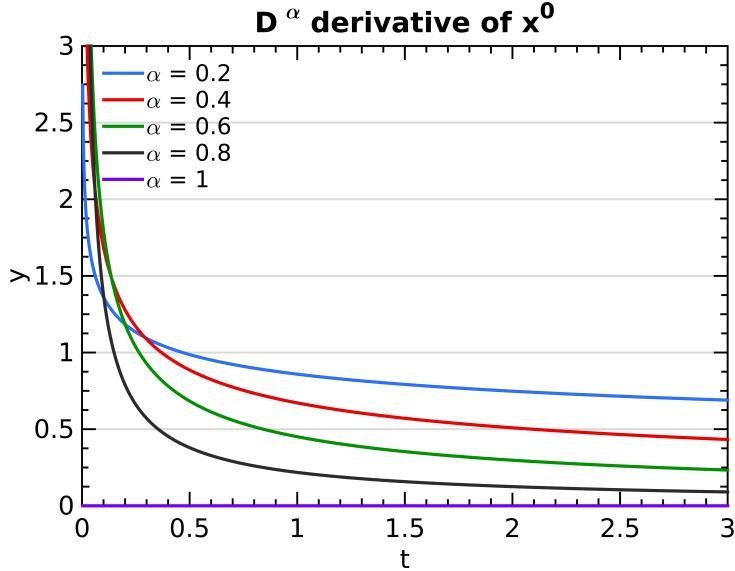
FIGURE 2.7: Fractional derivative of  $x$ .

FIGURE 2.8: Fractional derivative of a constant, which is not necessarily zero.

*Example 2.3.5.*  $f(t) = c = \text{const.}$  can be seen as a special case of the example above for  $\nu = 0$ . Consequently, we obtain

$${}_0^{RL}D_t^\alpha c = \frac{1}{\Gamma(1-\alpha)} t^{-\alpha}. \quad (2.78)$$

This means, that the fractional derivative of a constant is not zero, as long as  $\alpha \notin \mathbb{N}$ . For  $\alpha \in \mathbb{N}$  the expression is zero, as the Gamma function has poles for non positive natural numbers. Again, the results for different values of  $\alpha$  are plotted in Figure 2.8.

### 2.3.4 Caputo derivative

For the Caputo derivative, the order of integration and differentiation is changed with respect to the Riemann-Liouville derivative. Since we perform the differentiation first, this definition is more restrictive than the previous definition [13].

*Definition 2.6.* Caputo fractional derivative of  $f$  of order  $\nu$ .

Let  $m - 1 < \alpha \leq m$ . Then for  $f$  defined on  $(0, \infty)$  we define

$${}_0^C D_t^\alpha f(t) = \begin{cases} \frac{1}{\Gamma(m-\alpha)} \int_0^t \frac{\frac{d^m}{d\tau^m} f(\tau)}{(t-\tau)^{\alpha+1-m}} d\tau & m-1 < \alpha < m, \\ \frac{d^m}{dt^m} f(t) & \alpha = m, \end{cases} \quad (2.79)$$

to be the Caputo fractional derivative.

#### 2.3.4.1 Differences between the Caputo derivative and the Riemann-Liouville derivative

For a general function  $f(t)$  we can not assume, that the Riemann-Liouville and the Caputo derivative yield the same result. For this to be the case, we need  $f(t)$  and  $f^{(k)}(t)$  for  $k = 1, \dots, m$  to vanish at  $t = 0^+$ . For the general case and given that  $f$  fulfils all required assumptions, we have the following relationship between the Riemann-Liouville and the Caputo derivative.

$${}_0^{RL} D_t^\alpha f(t) = {}_0^C D_t^\alpha f(t) + \sum_{k=1}^{m-1} \frac{t^{k-\alpha}}{\Gamma(k-\alpha+1)} f^{(k)}(0^+). \quad (2.80)$$

Which can be rewritten as

$${}_0^C D_t^\alpha f(t) = {}_0^{RL} D_t^\alpha \left[ f(t) - \sum_{k=1}^{m-1} \frac{t^{k-\alpha}}{\Gamma(k-\alpha+1)} f^{(k)}(0^+) \right]. \quad (2.81)$$

This alternate definition shows, that the Caputo derivative includes the initial values of the function and its derivatives [13].

In contrast to the Riemann-Liouville derivative, we then compute  ${}_0^C D_t^\alpha t^{(\alpha-1)} = 0$  for  $\alpha > 0$ . From this calculation, we conclude that for the Caputo derivative, any constant function has a vanishing derivative, i.e.

$${}_0^C D_t^\alpha c \equiv 0 \quad \text{for } \alpha > 0. \quad (2.82)$$

In the context of fractional differential equations, the definitions according to Caputo and Riemann and Liouville differ in the way they treat initial conditions. Using the Caputo derivative, the initial conditions are the same as for non fractional differential equations (i.e. the integer case). This is in contrast to the Riemann-Liouville case, in which the initial condition are also of fractional order<sup>[14]</sup>. However, using the relationship in equation (2.80) it is possible to transform fractional initial conditions into standard initial conditions.

Another difference is the fact, that the Caputo derivative does not coincide with the classical derivative for integer order derivatives, whereas this is the case for the Riemann-Liouville derivative<sup>[14]</sup>, i.e. for  $\alpha \in (m-1, m)$

$$\lim_{\alpha \rightarrow (m-1)^+} {}_0^C D_t^\alpha x(t) = x^{(m-1)}(t) - x^{(m-1)}(0), \quad (2.83)$$

$$\lim_{\alpha \rightarrow m^+} {}_0^C D_t^\alpha x(t) = x^m(t), \quad (2.84)$$

but

$$\lim_{\alpha \rightarrow (m-1)^+} {}_0^{RL} D_t^\alpha x(t) = x^{(m-1)}(t), \quad (2.85)$$

$$\lim_{\alpha \rightarrow m^+} {}_0^{RL} D_t^\alpha x(t) = x^m(t). \quad (2.86)$$

Here, the superscript  $(m)$  and  $(m-1)$  denote the standard derivative. A more detailed comparison of the properties of the two definitions can be found in the work of Li & Deng<sup>[15]</sup>.

### 2.3.5 Grünwald-Letnikov derivative

The definition according to Grünwald and Letnikov follows a different approach than the prior definitions. The basic idea is to generalize the principle of approximating derivatives with finite differences. For simplicity we assume the one dimensional case. The derivative, if it exists, can be defined as

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}, \quad (2.87)$$

which can easily be extended to obtain a definition for second order derivatives, namely

$$f''(x) = \lim_{h \rightarrow 0} \frac{f'(x+h) - f'(x)}{h}, \quad (2.88)$$

$$= \lim_{h \rightarrow 0} \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2}. \quad (2.89)$$

It is an easy task to proof, that the  $n$ th derivative is then

$$f^{(n)}(x) = \lim_{h \rightarrow 0} \frac{1}{h^n} \sum_{m=0}^n (-1)^m \binom{n}{m} f(x + (n-m)h), \quad (2.90)$$

since  $\binom{n}{m} = 0$  for  $n > m$  we can replace the upper limit of the sum by  $+\infty$ . If we now extend the binomial coefficients by making use of the gamma function we can give a definition of the derivative for fractional order.

*Definition 2.7.* Grünwald-Letnikov derivative of  $f$  of order  $\nu$ .

$${}_0^{GL}D_x^\nu f(x) = \lim_{h \rightarrow 0} \frac{1}{h^\nu} \sum_{m=0}^{\infty} (-1)^m \binom{\nu}{m} f(x + mh). \quad (2.91)$$

*Remark 2.8.* This definition is not unique, since there exist different formulations of equation (2.87).

*Remark 2.9.* For a more mathematical rigorous derivation we refer to Ortigueira & Coito<sup>[16]</sup>, Diaz & Osler<sup>[17]</sup> or Néel & Joelson<sup>[18]</sup>.

An obvious advantage of this definition over the prior definitions is the simplicity of evaluating the fractional derivative according to Grünwald and Letnikov numerically. However, actual implementations often encounter numerical instabilities when implemented naively.

### 2.3.6 Riesz fractional derivative

Whereas the Riemann-Liouville, as well as the Caputo definition of the fractional integral are non symmetric definitions, the Riesz fractional integral and derivative present a symmetric variant of the fractional derivative. Recall, that in (2.53), the left-sided integral was defined as

$${}_0 D_t^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \xi)^{\alpha-1} f(\xi) d\xi. \quad (2.92)$$

In the same way, we can define a right-sided fractional integral by

$${}_t D_T^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_t^T (\xi - t)^{\alpha-1} f(\xi) d\xi, \quad (2.93)$$

where we assume, that  $t \in [0, T]$ .

The Riesz fractional integral or Riesz potential is then defined as an average of the right- and left-sided fractional integral, i.e.

$${}^R D_t^{-\alpha} f(t) = \frac{{}^0 D_t^{-\alpha} f(t) + {}_t D_T^{-\alpha} f(t)}{2 \cos(\alpha\pi/2)}, \quad (2.94)$$

with  $\alpha \notin \mathbb{Z}$ .

Similar to the Riemann-Liouville derivative, the Riesz fractional derivative is obtained by differentiating the fractional Riesz integral, yielding the Riesz fractional derivative of a function  $f(t)$  of order  $\alpha \notin \mathbb{Z}$ , given by

$${}^R D_t^\alpha f(t) = \frac{{}^0 D_t^\alpha f(t) + {}_t D_T^\alpha f(t)}{2 \cos(\alpha\pi/2)}. \quad (2.95)$$

### 2.3.6.1 Fractional Laplacian

Even though we define the Riesz fractional derivative in terms of a time dependency, the Riesz derivative is mostly applied to spatial derivatives. In this case, we have to adjust the lower and upper limits of the integral. Under the assumption of a double infinite domain, e.g.  $\mathbb{R}$ , one replaces lower and upper bounds of the integral with  $-\infty$  and  $+\infty$ , respectively. This yields

$${}^R D_x^\alpha f(x) = \frac{{}_{-\infty} D_x^\alpha f(x) + {}_x D_\infty^\alpha f(x)}{2 \cos(\alpha\pi/2)}. \quad (2.96)$$

Given this definition, the Riesz fractional derivative corresponds, up to scaling, with the fractional Laplacian, that is

$$(-\Delta)^{\alpha/2} f(x) \propto {}^R D_x^\alpha f(x), \quad (2.97)$$

where the fractional Laplacian in  $n$  dimensions is given as an elliptic linear integro-differential operator, defined as

$$(-\Delta)^s = c_{n,s} \int_{\mathbb{R}^n} \frac{u(x) - u(y)}{|x - y|^{n+2s}} dy. \quad (2.98)$$

*Remark 2.10.* A more detailed analysis of the fractional Laplacian as an operator defined in (2.98) can be found in the work of Ros-Oton and Serra<sup>[19,20]</sup> or Hilfer<sup>[21]</sup>.

## 2.4 Integral transform

An integral transform  $T$  of a function  $f(t)$  is defined as

$$(Tf)(s) = \int_a^b K(t, s) f(t) dt, \quad (2.99)$$

with the integral kernel  $K(t, s)$ . The inverse transform is then defined as

$$f(t) = \int_c^d K^{-1}(s, t) (Tf(s)) ds. \quad (2.100)$$

An integral transform often allows to turn difficult problems (potentially differential equations) into simpler problems (potentially algebraic equations). The problem can then be solved in the transformed domain and the result is transformed back to the original domain via the inverse transform, which might often be easier than solving the original problem directly.

An integral transform is usually applied, to transform an integro-differential problem into an algebraic problem, which can then be solved with algebraic tools instead. The final solution is then transformed back into the “integro-differential” domain, thus avoiding to solve the integro-differential equation directly.

### 2.4.1 Fourier transform

Perhaps the most important integral transform is the Fourier transform, which is often used to map the space spatial to the frequency domain. For periodic problems, the Fourier transform simplifies to the calculation of the Fourier coefficients. Furthermore, the Fourier analysis is the basis for the Discrete Fourier Transform, which in combination with the Fast Fourier Transform, finds application in various field such as mathematics, engineering, physics, signal processing and computer science.

The most common definition of the Fourier transform is the following:

$$\mathcal{F}[f(x)](\xi) = \int_{-\infty}^{\infty} f(x) e^{-2\pi i x \xi} dx =: \hat{f}(\xi), \quad (2.101)$$

with  $\xi \in \mathbb{R}$  and  $i = \sqrt{-1}$ . The Fourier transform allows to represent a function by its frequency spectrum, possibly filtering out frequencies of higher order, thus compressing the original data. This property makes Fourier transform applicable to data compression, especially for audio data types.

Fourier transform is also used for the solution of differential equations, since it maps integral and differential operator to algebraic operators, thus simplifying the problem.

The Fourier transform of certain operators and functions are given as examples below. Note, that due to the different definitions of the Fourier transform, these transformations are only valid for the definition of  $\hat{f}(\xi)$  provided in equation (2.101). A more rigorous summary of Fourier transforms is available in several books and courses for mathematicians and engineers<sup>[22–25]</sup>. For the given examples, we assume all functions to be sufficiently integrable, i.e.  $\int_{\mathbb{R}} |f(x)| dx < \infty$  and if needed also sufficiently differentiable.

*Example 2.4.1.*  $g(x) = \frac{d}{dx} f(x)$ . By definition, we have

$$\hat{g}(\xi) = \mathcal{F}[g(x)](\xi) = \int_{-\infty}^{\infty} g(x) e^{-2\pi i x \xi} dx \quad (2.102)$$

$$= \int_{-\infty}^{\infty} \frac{d}{dx} f(x) e^{-2\pi i x \xi} dx \quad (2.103)$$

$$^{IP} = - \int_{-\infty}^{\infty} f(x) \frac{d}{dx} e^{-2\pi i x \xi} dx + f(x) e^{2\pi i x \xi} \Big|_{x=-\infty}^{\infty} \quad (2.104)$$

$$= (2\pi i \xi) \int_{-\infty}^{\infty} f(x) e^{2\pi i x \xi} dx \quad (2.105)$$

$$= (2\pi i \xi) \hat{f}(\xi). \quad (2.106)$$

Where the boundary term vanishes due to the assumption that  $f$  is integrable. This rule can be extended to higher derivatives by repeating the integration by parts multiple times, yielding  $\mathcal{F}[\frac{d^n}{dx^n} f(x)](\xi) = (2\pi i \xi)^n \hat{f}(\xi)$ .

Example 2.4.2.  $g(x) = \int_{-\infty}^x f(\tau) d\tau$ . Again, we start with the definition, yielding

$$\hat{g}(\xi) = \mathcal{F}[g(x)](\xi) = \int_{-\infty}^{\infty} g(x) e^{-2\pi i x \xi} dx \quad (2.107)$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^x f(\tau) d\tau e^{-2\pi i x \xi} dx \quad (2.108)$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^x f(\tau) e^{-2\pi i x \xi} d\tau dx \quad (2.109)$$

$$= \int_{-\infty}^{\infty} \int_{\tau}^{\infty} f(\tau) e^{-2\pi i x \xi} dx d\tau \quad (2.110)$$

$$= \int_{-\infty}^{\infty} f(\tau) \int_{\tau}^{\infty} e^{-2\pi i x \xi} dx d\tau \quad (2.111)$$

$$= \int_{-\infty}^{\infty} f(\tau) \frac{-1}{2\pi\xi} e^{-2\pi i x \xi} \Big|_{x=\tau}^{\infty} d\tau \quad (2.112)$$

$$= \frac{1}{2\pi\xi} \int_{-\infty}^{\infty} f(\tau) e^{-2\pi i \tau \xi} d\tau \quad (2.113)$$

$$= \frac{1}{2\pi\xi} \hat{f}(\xi), \quad (2.114)$$

which can be extended to higher order integrals in the same way as for derivatives, thus turning (possible multiple) integration into division.

#### 2.4.1.1 Fourier transform of the Riemann-Liouville derivative

Since the Fourier transform is mostly used to transform the spatial domain, it also seems reasonable due to the relation between the Riemann-Liouville derivative and the fractional Laplacian to consider the Fourier transform of the Riemann-Liouville derivative. As we have already derived the Fourier transform of the integral and derivative operator, the transformation of the Riemann-Liouville fractional derivative can easily be computed to be

$$\mathcal{F}_{[-\infty]}^{RL} D_x^{\alpha} f(x)](\xi) = (i\xi)^{\alpha} \hat{f}(\xi), \quad (2.115)$$

and for the symmetric Riesz fractional derivative

$$\mathcal{F}^R D_x^{\alpha} f(x)](\xi) = |\xi|^{\alpha} \hat{f}(\xi), \quad (2.116)$$

which is exactly the origin of the fractional Laplacian when performing the derivation of the fractional diffusion equation later on.

### 2.4.2 Laplace transform

Another widely used integral transform in physics and mathematics is the Laplace transform, which is particularly helpful for the solution of ordinary differential equations<sup>[26]</sup>.

There exist multiple definitions of the Laplace transform, mostly varying in the integral boundaries. Perhaps the most common definition is given by

$$\mathcal{L}[f(t)](s) = \int_0^\infty e^{-st} f(t) dt =: \tilde{f}(s), \quad (2.117)$$

with  $\sigma + i\omega = s \in \mathbb{C}$ . The Laplace transform can be interpreted as a transformation from the time-domain into the frequency-domain. As already mentioned, it simplifies problems in the sense, that differentiation and integration are replaced by multiplication and division, respectively, thus potentially transforming ordinary differential equations into algebraic problems.

Tables of Laplace transforms of the most widely used functions and operators can be found throughout the literature<sup>[26–29]</sup>. However, since we are mostly dealing with differential and integral operators, we are going to derive the corresponding Laplace transform explicitly. We again assume, that the functions are sufficiently differentiable or integrable.

*Example 2.4.3.*  $h(x) = \frac{d^n}{dx^n} f(x)$ . Let us first derive the Laplace transform of the first derivative. Therefore, we need to calculate

$$\tilde{g}(s) = \int_0^\infty \frac{d}{dx} f(x) e^{-sx} dx. \quad (2.118)$$

Integration by parts, yields

$$\tilde{g}(s) = f(x) e^{-isx} \Big|_{x=0}^\infty - \int_0^\infty f(x) \frac{d}{dx} e^{-sx} dx, \quad (2.119)$$

$$\Leftrightarrow \tilde{g}(s) = -f(0) + s \int_0^\infty f(x) e^{-sx} dx, \quad (2.120)$$

$$\Leftrightarrow \tilde{g}(s) = s \tilde{f}(s) - f(0). \quad (2.121)$$

By repeating this process for higher orders, it is easy to see that

$$\tilde{h}(s) = \int_0^\infty \frac{d^n}{dx^n} f(x) e^{-sx} dx = s^n \tilde{f}(s) - \sum_{i=0}^n s^{i-1} f^{(n-i)}(0). \quad (2.122)$$

Example 2.4.4.  $g(t) = \int_0^t f(x) dx$ . By definition we have

$$\tilde{g}(s) = \int_0^\infty \int_0^x f(\tau) d\tau e^{-sx} dx \quad (2.123)$$

$$= \int_0^\infty \int_0^x f(\tau) e^{-sx} d\tau dx. \quad (2.124)$$

If we switch the order of integration, we get

$$\tilde{g}(s) = \int_0^\infty \int_\tau^\infty f(\tau) e^{-sx} dx d\tau \quad (2.125)$$

$$= \int_0^\infty f(\tau) \int_\tau^\infty e^{-sx} dx d\tau \quad (2.126)$$

$$= \int_0^\infty f(\tau) \frac{1}{s} e^{-s\tau} d\tau \quad (2.127)$$

$$= \frac{\tilde{f}(s)}{s}. \quad (2.128)$$

Again, we turn integration into division.

#### 2.4.2.1 Laplace transform of the Caputo derivative

Given the Laplace transform of the derivative and integral operator above, we can derive the Laplace transform of the Caputo derivative  ${}_0^c D_t^\alpha f(t)$ . At first we use the fact, that for the Caputo derivative, we differentiate first and have the integration afterwards. Therefore, we can use the generalization of Example 2.4.4 in a first step and the results from Example 2.4.3 afterwards to obtain

$$\mathcal{L}[{}_0^c D_t^\alpha f(t)](s) = \int_0^\infty e^{-st} \cdot {}_0^c D_t^\alpha f(t) dt = s^{-(n-\alpha)} \mathcal{L}[f^{(n)}(t)](s) \quad (2.129)$$

$$= s^\alpha \tilde{f}(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} f^{(k)}(0+), \quad (2.130)$$

for  $n-1 < \alpha < n$ .



# 3

## Derivation of the fractional diffusion equation

### 3.1 What's so special about the albatross?

We have been able to derive the classical diffusion equation via several independent approaches, as described in the first chapter. To derive the fractional diffusion equation, it is useful to reconsider the random walk. Let  $x$  denote the position of a given particle. For the description of the random walk, we use two probability density functions. We sample from  $w(\xi)$  the step lengths, i.e. the distance  $x_i - x_{i-1}$  and from  $\psi(\tau)$  the waiting times  $t_i - t_{i-1}$ .

So far, we implicitly assumed that  $w(\xi)$  and  $\psi(\tau)$  do not allow arbitrary large jumps or waiting times, as their probability rapidly tends towards zero for large values of  $\xi$  and  $\tau$ , respectively. Therefore, the classical random walk is a local problem in space and time as the influence of particles is local due to finite jumps and finite waiting times.

However, empirical observations suggest, that this is not true for all processes that can be considered a random walk. For example, in 1996, Viswanathan et al. discovered, that the flight of an albatross can be modelled as a Lévy flight<sup>[30]</sup>, i.e. a random walk that allows large step lengths. This can be described with a heavy-tailed probability density function  $w(\xi)$ , which decays slower for large values of  $\xi$  than an exponential. For Lévy

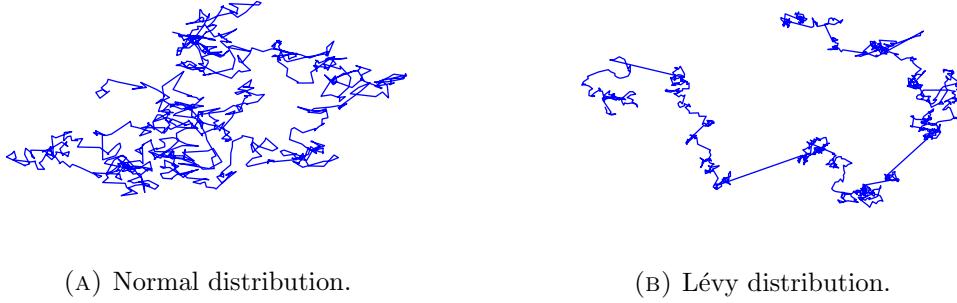


FIGURE 3.1: Random walk of a single particle with different path-length distribution.

flights, Mandelbrot<sup>[31]</sup> suggested a distribution for the step length  $U$  as

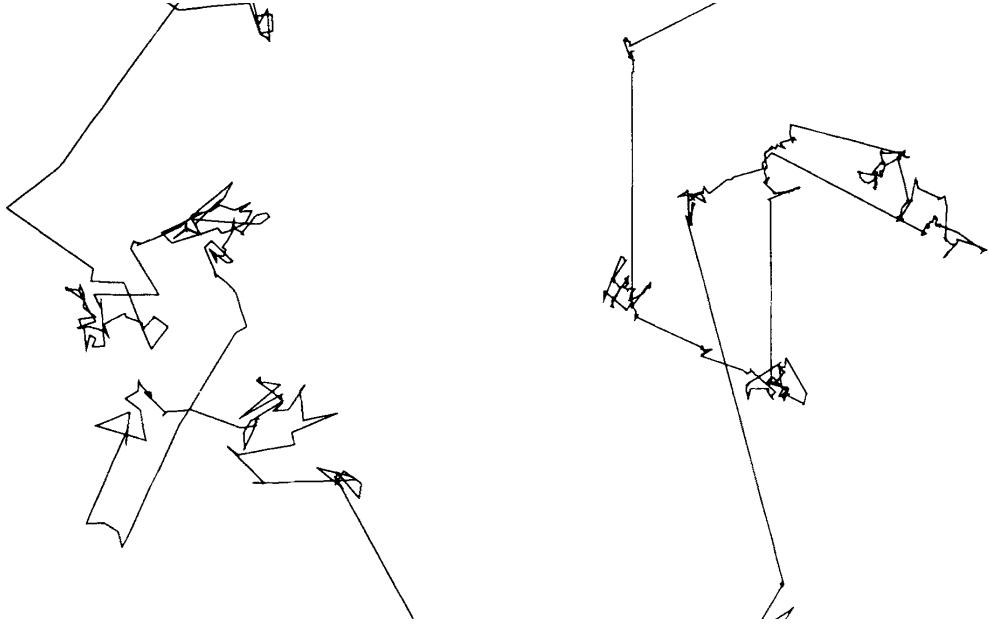
$$Pr(U > u) = \begin{cases} 1 & \text{for } u < 1, \\ u^{-D} & \text{for } u \geq 1, \end{cases} \quad (3.1)$$

where  $D \geq 1$  is related to the fractional dimension. Since the distribution is heavy-tailed, this yields an infinite variance, different from an exponentially decaying distribution. In Figure (3.1) we can see the results of an isotropic 2D random walk simulation after 1000 steps where the step-length has been sampled from a normal distribution (A) and a Cauchy distribution (B), which corresponds to the simulation of a Lévy flight. Note the large jumps in (B), which result from the heavy-tailed probability density function. For comparison, Figure (3.2) presents the observed flight patterns of an albatross. The qualitative behaviour of the Lévy process and the observation by Viswanathan et al. are similar in the case, that both movements contain steps with significantly larger length, than the more frequent smaller steps. This pattern can not be observed for the standard Brownian motion.

This observation should motivate a reconsideration of the classical random walk model. The above described phenomena has not only been observed in biology, but can also be found in photon transport in clouds, for correlated background media or fractals, within quantum physics<sup>[32]</sup>, for chemical reactions<sup>[33]</sup>, in stock market prediction<sup>[34]</sup>, in epidemic models<sup>[35]</sup> and many more.

## 3.2 The time-fractional master equation

We are now going to derive the fractional diffusion equation in time based on the approach presented by Scalas, Gorenflo, Mainardi and Raberto<sup>[36]</sup>. Assume that we consider the probability density functions  $w(\xi)$  and  $\psi(\tau)$ , such that  $\xi_i$  and  $\tau_i$  are both identically independent distributed random variables. Let  $p(x, t)$  denote the probability

FIGURE 3.2: Two observations of the flight of an albatross<sup>[30]</sup>.

of finding a particle at time  $t$  at position  $x$  and assume the initial distribution to be the delta function, i.e.  $p(x, 0) = \delta(x)$ . The master equation of the continuous time random walk (CTRW) is then given by

$$p(x, t) = \delta(x)\Psi(t) + \int_0^t \psi(t-t') \int_{-\infty}^{\infty} w(x-x')p(x', t')dx'dt', \quad (3.2)$$

with

$$\Psi(t) = \int_t^{\infty} \psi(t')dt' = 1 - \int_0^t \psi(t')dt', \quad \psi(t) = -\frac{d}{dt}\Psi(t). \quad (3.3)$$

Thus, the probability of finding a particle at  $(t, x)$  equals the probability of finding a particles at a prior time  $t'$  and position  $x'$  that moves the distance  $x - x'$  after waiting  $t - t'$ . Furthermore, we have to add the number of particles that did not jump from the initial position until time  $t$ , which is described by  $\delta(x)\Psi(t)$ . Recall the definition for the Fourier transformation in space and the Laplace transformation in time, respectively.

$$\mathcal{F}[f(x)](\kappa) = \int_{-\infty}^{\infty} e^{i\kappa x} f(x)dx =: \hat{f}(\kappa), \quad (3.4)$$

and

$$\mathcal{L}[f(t)](s) = \int_0^{\infty} e^{-st} f(t)dt =: \tilde{f}(s), \quad (3.5)$$

with  $i^2 = -1$ . If we now apply the Fourier-Laplace transform of the master equation (3.2), we obtain

$$\hat{\tilde{p}}(\kappa, s) = \tilde{\Psi}(s) \frac{1}{1 - \hat{w}(\kappa) \tilde{\psi}(s)}. \quad (3.6)$$

Mainardi et al. suggest an equivalent formulation<sup>[37]</sup>

$$\tilde{\Phi}(s)[s\hat{\tilde{p}}(\kappa, s) - 1] = [\hat{w}(\kappa) - 1]\hat{\tilde{p}}(\kappa, s), \quad (3.7)$$

where we define

$$\tilde{\Phi}(s) = \frac{\tilde{\Psi}(s)}{1 - s\tilde{\Psi}(s)}. \quad (3.8)$$

To get back to space-time domain, we apply the inverse Fourier-Laplace transformation to obtain

$$\int_0^t \Phi(t-t') \frac{\partial}{\partial t'} p(x, t') dt' = -p(x, t) + \int_{-\infty}^{\infty} w(x-x') p(x', t) dx'. \quad (3.9)$$

In this context,  $\Phi(t)$  has the role of a “memory function” and the process is no longer Markovien<sup>[37]</sup>, i.e. memoryless, unless the above function degenerates into a delta function, such that  $\psi(t) = c \cdot \phi(t)$  with a positive constant  $c$ . If we assume  $\tilde{\Phi}(s) = 1$ , we obtain  $\Phi(t) = \delta(t)$  and further  $\tilde{\psi}(s) = 1 \cdot \tilde{\Psi}(s) = \frac{1}{1+s}$  which yields by application of the inverse Laplace transformation  $\psi(t) = 1 \cdot \Phi(t) = e^{-t}$  for  $t \geq 0$ . This means, that we have memoryless exponential decay of the waiting time distribution and equation (3.9) reduces to

$$\frac{\partial}{\partial t} p(x, t) - p(x, t) + \int_{-\infty}^{\infty} w(x-x') p(x', t) dx'. \quad (3.10)$$

Therefore, with the assumptions of exponential decay, we reconstruct the classical master equation for a Markovian continuous time random walk (also called the Kolmogorov-Feller equation), which we could use to reconstruct the classical diffusion equation.

However, we can also consider different approaches for the memory function  $\Phi(t)$ . If  $\Phi(t)$  has power law decay, it corresponds to possibly arbitrary large waiting times, i.e. a heavy-tailed probability density function for the waiting time. With the choice

$$\Phi(t) = \frac{t^{-\beta}}{\Gamma(1-\beta)}, \quad t \geq 0, \quad 0 < \beta < 1, \quad (3.11)$$

we can model the power law decay. Additionally, since  $\delta(t)$  can formally be written as  $\delta(t) = t^{-1}/\Gamma(0)$ , we see that  $\Phi(t) = \delta(t)$  as  $\beta \rightarrow 1$ . If we plug  $\Phi(t)$  from equation (3.11)

into equation (3.9), we get

$$0 = \int_0^t \Phi(t-t') \frac{\partial}{\partial t'} p(x, t') dt' + p(x, t) - \int_{-\infty}^{\infty} w(x-x') p(x', t) dx' \quad (3.12)$$

$$= \frac{1}{\Gamma(1-\beta)} \int_0^t (t-t')^{-\beta} \frac{\partial}{\partial t'} p(x, t') dt' + p(x, t) - \int_{-\infty}^{\infty} w(x-x') p(x', t) dx' \quad (3.13)$$

$$= \frac{\partial^{\beta}}{\partial t^{\beta}} p(x, t) + p(x, t) - \int_{-\infty}^{\infty} w(x-x') p(x', t) dx'. \quad (3.14)$$

Where we use the definition of the Caputo derivative in the last step, namely

$$\frac{\partial^{\beta}}{\partial t^{\beta}} f(t) = \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{p'(t')}{(t-t')^{\beta}} dt'. \quad (3.15)$$

Another way to derive equation (3.14) is done via the Laplace transformation of the definition of  $\Phi(t)$  in (3.11), given by  $\tilde{\Phi}(s) = 1/s^{1-\beta}$ . If we plug this into the formulation of Mainardi et al. from equation (3.7), we obtain

$$s^{\beta} \hat{p}(\kappa, s) - s^{\beta-1} = [\hat{w}(\kappa) - 1] \hat{p}(\kappa, s), \quad (3.16)$$

for  $0 < \beta < 1$ . The Laplace transform of the fractional differential operator  $\partial^{\beta}/\partial t^{\beta}$  is defined as

$$\mathcal{L}[\partial^{\beta}/\partial t^{\beta} f(t)](s) = s^{\beta} \tilde{f}(s) - s^{\beta-1} \tilde{f}(0^+), \quad (3.17)$$

and thus we can use the inverse Fourier and Laplace transform of equation (3.16) to derive

$$\frac{\partial^{\beta}}{\partial t^{\beta}} p(x, t) + p(x, t) - \int_{-\infty}^{\infty} w(x-x') p(x', t) dx' = 0, \quad (3.18)$$

with initial condition  $p(x, 0) = \delta(x)$ .

Note, that the definition  $\Phi(t) = \frac{t^{-\beta}}{\Gamma(1-\beta)}$ ,  $t \geq 0$ ,  $0 < \beta < 1$  implies that we have

$$\tilde{\Psi}(s) = \frac{s^{\beta-1}}{1+s^{\beta}} \quad \text{and} \quad \tilde{\psi}(s) = \frac{1}{1+s^{\beta}} \quad \text{for } 0 < \beta < 1. \quad (3.19)$$

Applying the inverse Laplace transform, this yields

$$\Psi(t) = E_{\beta}(-t^{\beta}) \quad \text{and} \quad \psi(t) = -\frac{d}{dt} E_{\beta}(-t^{\beta}) \quad \text{for } 0 < \beta < 1. \quad (3.20)$$

Here  $E_{\beta}$  is again the special case  $E_{\beta,1}$ , where  $E_{\beta,\alpha}$  defines the Mittag-Leffler function. Recall, that the Mittag-Leffler function interpolates between an exponential decay for

small waiting times and a power law decay for large waiting times<sup>[36]</sup>, i.e.

$$E_\beta(-t^\beta) = \begin{cases} \exp(-t^\beta/\Gamma(1+\beta)) & \text{for } t \rightarrow 0, \\ t^{-\beta}/\Gamma(1-\beta) & \text{for } t \rightarrow \infty. \end{cases} \quad (3.21)$$

### 3.3 Diffusion limit

Performing the diffusion limit in space allows us to derive two different types of equations. Depending on the decay of the path-length distribution  $w(x)$ , we can derive the Laplace operator  $\Delta$  for the spatial derivative or a spatial derivative of fractional order. For simplicity, we assume  $w(x) = w(-x)$ , i.e. the process is isotropic. The following derivation follows the approach presented by Gorenflo and Mainardi<sup>[38]</sup>.

For  $0 < \alpha < 2$ ,  $b > 0$  and  $|x| \rightarrow \infty$  we define

$$w(x) = \frac{b}{|x|^{\alpha+1}}, \quad (3.22)$$

where we have an asymptotic representation of the Fourier transform as<sup>[39]</sup>

$$\hat{w}(\kappa) \approx 1 - \eta|\kappa|^\alpha + o(|\kappa|^\alpha), \quad (3.23)$$

as  $\kappa \rightarrow 0$ , with  $\eta = \frac{b\pi}{\Gamma(\alpha+1)\sin(\alpha\pi/2)}$  for  $0 < \alpha < 2$ <sup>[40]</sup>.

We are now going to rescale the process, to be able to perform the diffusion limit later on.

If we replace jumps of length  $X$  by scaled jumps  $hX$ , meaning we replace  $w(x)$  with  $w_h(x) = w(x/h)/h$ , this can be interpreted as performing smaller and smaller jumps as  $h$  tends to zero. Furthermore, we accelerate the spatially rescaled process by  $1/(\eta h^\alpha)$ , the re-speeding factor. These two components scale the process in space.

Using the subscript  $h$ , we can write the rescaled process of equation (3.18) as

$$\eta h^\alpha \frac{\partial^\beta}{\partial t^\beta} p_h(x, t) + p_h(x, t) - \int_{-\infty}^{\infty} w_h(x - x') p_h(x', t) dx' = 0, \quad (3.24)$$

whose Laplace-Laplace transform is

$$\eta h^\alpha [s^\beta \hat{p}_h(\kappa, s) - s^{\beta-1}] = [\hat{w}_h(\kappa) - 1] \hat{p}_h(\kappa, s), \quad (3.25)$$

$$\Leftrightarrow [s^\beta \hat{p}_h(\kappa, s) - s^{\beta-1}] = \frac{\hat{w}_h(\kappa) - 1}{\eta h^\alpha} \hat{p}_h(\kappa, s). \quad (3.26)$$

Since

$$\lim_{h \rightarrow 0} \frac{\hat{w}(h\kappa) - 1}{\eta h^\alpha} = -|\kappa|^\alpha, \quad (3.27)$$

for  $0 < \alpha \leq 2$  and  $\kappa \in \mathbb{R}$ , we can define  $\rho_h(\kappa) = \frac{\hat{w}(h\kappa) - 1}{\eta h^\alpha}$  and obtain

$$[s^\beta \hat{p}_h(\kappa, s) - s^{\beta-1}] = \rho_h(\kappa) \hat{p}_h(\kappa, s), \quad (3.28)$$

and in the limit  $h \rightarrow 0$

$$[s^\beta \hat{p}_0(\kappa, s) - s^{\beta-1}] = -|\kappa|^\alpha \hat{p}_0(\kappa, s). \quad (3.29)$$

Since  $-|\kappa|^\alpha$  is the Fourier transform of the space-fractional Riesz derivative  $\partial^\alpha / \partial |x|^\alpha$ , we use the inverse Fourier-Laplace transformation to derive the space-time fractional diffusion equation

$$\frac{\partial^\beta}{\partial t^\beta} p_0(x, t) = \frac{\partial^\alpha}{\partial |x|^\alpha} p_0(x, t), \quad (3.30)$$

$$p_0(x) = \delta(x). \quad (3.31)$$

Some further remarks should be made, concerning the scaling and the limit  $h \rightarrow 0$ . By rescaling and accelerating the complete process, we decrease the jumps, while simultaneously making the waiting times between the jumps smaller. For the limit  $h \rightarrow 0$  in equation (3.28) we use a Lemma of Gorenflo<sup>[41]</sup>, that ensures the result of equation (3.27), which holds with the explicit definition  $\eta = \frac{b\pi}{\Gamma(\alpha + 1) \sin(\alpha\pi/2)}$  if  $0 < \alpha < 2$  as mentioned before. According to Lukacs<sup>[42]</sup>, we have convergence in the distribution of  $\hat{p}_h(\kappa, s)$  towards  $\hat{p}_0(\kappa, s)$  by the continuity theorem of probability.

As derived in this section, we can see, that under certain assumptions on the probability density functions of the waiting time distribution and the step length distribution respectively, we are able to derive the fractional diffusion equation, which generalized the derivative operator from first or second order to arbitrary order in space and time. For the case, that  $\alpha = 2$  and  $\beta = 1$  the derived fractional diffusion equation coincides with the standard diffusion equation, given by

$$\frac{\partial}{\partial t} p_0(x, t) = \frac{\partial^2}{\partial x^2} p_0(x, t), \quad (3.32)$$

$$p_0(x) = \delta(x). \quad (3.33)$$

*Remark 3.1.* Even though we did not cover the situation, where  $\beta \rightarrow 2$ , it is possible to show, that the fractional differential equation converges towards the standard wave

equation, i.e.

$$\frac{\partial^2}{\partial t^2} p_0(x, t) = \frac{\partial^2}{\partial x^2} p_0(x, t), \quad (3.34)$$

$$p(x, 0) = p_0(x, t), \quad (3.35)$$

which is covered by various authors in the literature. See for example the work of Luchko<sup>[43]</sup>, El-Sayed<sup>[44]</sup>, Mainardi<sup>[45]</sup> or Metzler and Nonnemacher<sup>[46]</sup>. Even though the extension of derivatives for arbitrary order allows a transition from the diffusion process to the wave process, this work solely focusses on the diffusive case. This is due to the fact, that the diffusive process can be derived from the random walk model on the molecular level which is not the case for the wave equation. Additionally a restriction to the diffusive case is a necessary criteria for the convergence of some of the numerical methods later on. However, we will see, that for example the spectral method for the solution of the diffusion equation converges also for  $\beta \rightarrow \beta^{max} < 2$ , but breaks down for  $\beta = 2$ . For numerical methods for the solution of the fractional wave equation, the reader may refer to a variety of sources throughout the literature<sup>[47–50]</sup>.

# 4

## Numerical Methods

Due to its non local nature, fractional differential equations are often harder to solve than integer order differential equations. One of the reasons therefore is the fact, that the sparsity in the used differentiation matrices vanishes and dense matrices need to be computed and used. Therefore, applying the same algorithms that are used for standard differential equations in an adapted fashion often yields unsatisfactory results.

Methods that exploit the non local structure of the problem, might be advantageous in their application to fractional problems. This is what is done in the spectral methods presented in section 4.2 and 4.3, whereas in section 4.1 we are going to extend the most basic and well known method, namely the finite difference approach, to the fractional setting. Here we will observe the problem of dense matrices, which do not occur for the approximation of integer order derivatives.

### 4.1 Finite Differences

With finite difference schemes being one of the most obvious and easiest to use numerical methods for the approximation of standard derivatives, it seems reasonable to also consider varieties of finite difference schemes for fractional order derivatives. Especially with the Grünwald-Letnikov definition of the fractional derivative, the finite difference

approximation seems obvious. Recall, that in the Grünwald-Letnikov setting, according to definition (2.7), the fractional derivative is given by

$${}_0^{GL}D_x^\nu f(x) = \lim_{h \rightarrow 0} \frac{1}{h^n} \sum_{m=0}^{\infty} (-1)^m \binom{\nu}{m} f(x + mh). \quad (4.1)$$

A finite approximation of the above definition can easily be obtained by truncating the sum at some upper bound  $N$  and fixing a value of  $h$ .

$${}_0^{GL}\Delta_x^\nu f(x) = \frac{1}{h^n} \sum_{m=0}^N (-1)^m \binom{\nu}{m} f(x + mh). \quad (4.2)$$

The above discretization was one of the first to approximate the fractional derivative<sup>[51,52]</sup>. Since the consistency is only of order one and has frequent numerical instabilities<sup>[51]</sup> shifted and stabilized numerical variants of the discretization have been developed and analyzed<sup>[53,54]</sup>. However, in recent years most finite difference approximations of the fractional derivative have focussed more on the Riemann-Liouville definition instead of the Grünwald-Letnikov definition<sup>[51,55,56]</sup>. Therefore, we are also going to follow this approach in our analysis.

#### 4.1.1 A weighted finite difference method by Sousa & Li

As an ambassador for the class of finite difference methods for the solution of the fractional diffusion equation, we choose the algorithm presented by Sousa & Li in their 2011 paper<sup>[51]</sup>. The following theoretical analysis of convergence and consistency is a summary of the results obtained in the original paper.

In the Appendix (A) we also attach a proof for the extension of the spatial consistency to fourth order, which replaces the 3-point stencil and linear hat functions used in the paper from Sousa & Li by a 5-point stencil and Cubic Hermite Splines.

Let us consider the case, where the left-sided spatial fractional derivative of order  $1 < \alpha < 2$  is given according to the Riemann-Liouville derivative as

$$\frac{\partial^\alpha}{\partial x^\alpha} u(x, t) = \frac{1}{\Gamma(2 - \alpha)} \frac{\partial^2}{\partial x^2} \int_{-\infty}^x u(\xi, t) (x - \xi)^{1-\alpha} d\xi. \quad (4.3)$$

*Remark 4.1.* For the fractional diffusion equation, we use the symmetric variant of the Riemann-Liouville derivative. However, since the symmetric variant is a linear combination of the left-sided and right-sided Riemann-Liouville derivative the results hold

analogously. To further simplify the analysis and to be consistent with the original authors, we will only consider the case of the left-sided derivative, since the right-sided derivative can be analyzed by a similar procedure or an integral transform.

For second order convergence in space, we need two ingredients. At first, we have to approximate the derivative with second order accuracy. Secondly, we need to evaluate the integrals in the definition of the fractional derivative with sufficiently high accuracy to keep second order after differentiating them.

We consider the case where the spatial and temporal grid discretization is equidistant, i.e.  $x_j = j\Delta x$  and  $t^k = k\Delta t$ . For convenience, we define

$$\mathcal{I}_\alpha(x) = \int_{-\infty}^x u(\xi, t)(x - \xi)^{1-\alpha} d\xi, \quad 1 < \alpha < 2. \quad (4.4)$$

Using the standard stencil for the approximation of the second order derivative results in

$$\frac{\partial^2}{\partial x^2} \mathcal{I}_\alpha(x_j) \approx \frac{1}{\Delta x^2} (\mathcal{I}_\alpha(x_{j-1}) - 2\mathcal{I}_\alpha(x_j) + \mathcal{I}_\alpha(x_{j+1})). \quad (4.5)$$

For the approximation of the integral  $\mathcal{I}_\alpha$ , we use

$$\mathcal{I}_\alpha(x_j) \approx I_\alpha(x_j) = \int_{-\infty}^{x_j} s_j(\xi)(x_j - \xi)^{1-\alpha} d\xi, \quad (4.6)$$

where  $s_j$  is the spline given by

$$s_j(\xi) = \sum_{k=-\infty}^j u(x_k, t) s_{j,k}(\xi), \quad (4.7)$$

and  $s_{j,k}(\xi)$  is the standard linear hat function with compact support on  $[x_{k-1}, x_{k+1}]$ .

Under the assumption of linear splines, we can compute (4.6) analytically and obtain

$$I_\alpha(x_j) = \frac{\Delta x^{2-\alpha}}{(2-\alpha)(3-\alpha)} \sum_{k=-\infty}^j u(x_k, t) a_{j,k}, \quad (4.8)$$

where the  $a_{j,k}$  are simple algebraic expressions. Observe, that the semi infinite sum is a consequence of the one sided application of the Riemann-Liouville derivative.

Combining equation (4.8) with (4.5), we derive an expression for the approximation of the space fractional derivative:

$$\begin{aligned} \frac{\partial^2}{\partial x^2} \mathcal{I}_\alpha(x_j) \approx \\ \frac{\Delta x^{-\alpha}}{(2-\alpha)(3-\alpha)} \left( \sum_{k=-\infty}^{j-1} u(x_k, t) a_{j-1,k} - 2 \sum_{k=-\infty}^j u(x_k, t) a_{j,k} + \sum_{k=-\infty}^{j+1} u(x_k, t) a_{j+1,k} \right). \end{aligned} \quad (4.9)$$

Consequently, equation (4.3) is approximated by  $\delta_\alpha \Delta x^{-\alpha} U_j^n$  where we use

$$\delta_\alpha U_j^n = \frac{1}{\Gamma(4-\alpha)} \sum_{k=-\infty}^{j+1} q_{j,k} U_k^n, \quad (4.10)$$

and  $q_{j,k}$  collects the corresponding coefficients of the formulation in equation (4.9) and  $U_k^n := u(x_k, t^n)$ .

We now apply the derived discretization to the problem, used by Sousa & Li. Consider the one-dimensional space fractional diffusion equation

$$\frac{\partial}{\partial t} u(x, t) - d(x) \frac{\partial^\alpha}{\partial x^\alpha} u(x, t) = -p(x, t), \quad (4.11)$$

with  $x \in \mathbb{R}$ ,  $1 < \alpha < 2$  and possibly nonlinear  $d(x) > 0$ . Initial and boundary conditions are given by

$$u(x, 0) = f(x) \quad \text{for } x \in \mathbb{R}, \quad (4.12)$$

$$u(x, t) = 0 \quad \text{for } x \rightarrow \pm\infty. \quad (4.13)$$

*Remark 4.2.* Homogeneous initial conditions can be obtained by substituting  $v(x, t) = u(x, t) - u(x, 0)$  and appropriately modifying the right-hand side.

Since the time derivative is of integer order, we can use standard methods for the time discretization. Denote with  $\mu_j^\alpha = d_j \frac{\Delta t}{\Delta x^\alpha}$  the fractional Courant-Friedrich-Lowy (CFL) number at each spatial point. The implicit and explicit Euler time steps are then given as

$$U_j^{n+1} = U_j^n + \mu_j^\alpha \delta_\alpha U_j^n + \Delta t p_j^n \quad \text{and} \quad (4.14)$$

$$U_j^{n+1} = U_j^n + \mu_j^\alpha \delta_\alpha U_j^{n+1} + \Delta t p_j^{n+1}. \quad (4.15)$$

Weighting the explicit and implicit steps with  $(1 - \tau)$  and  $\tau$ , respectively, this yields

$$U_j^{n+1} = U_j^n + \mu_j^\alpha \left[ (1 - \tau) \delta_\alpha U_j^n + \tau \delta_\alpha U_j^{n+1} \right] + \tau \Delta t p_j^{n+1} + (1 - \tau) \Delta t p_j^n, \quad (4.16)$$

where we require  $\tau \in [0.5, 1]$ . For  $\tau = 0.5$ , we obtain the well known Crank-Nicolson method<sup>[57]</sup>.

If written in matrix form, we have to solve a tridiagonal system for  $\alpha \neq 2$ , due to the non local structure of the fractional derivative. If we later consider the symmetric Riesz derivative, the system will be full.

If we are able to show, that the method is consistent and convergent in space, standard results for time integration can be used to proof convergence of first order for  $\tau \in (0.5, 1]$  and second order for  $\tau = 0.5$  in time<sup>[57]</sup>.

As mentioned before, we have two sources that contribute an error to the approximation, i.e.

$$\frac{\partial^\alpha}{\partial x^\alpha} u(x_j) - \frac{\delta_\alpha}{\Delta x^\alpha} u(x_j) = \epsilon_1(x_j) + \epsilon_2(x_j). \quad (4.17)$$

The approximation error of  $\frac{\partial^2}{\partial x^2} \mathcal{I}_\alpha(x_j)$  by the standard 3-point stencil is denoted by  $\epsilon_1$ , which is known to be of second order<sup>[58]</sup>.

More interesting is the propagation of the error due to the spline interpolation. Let  $E_s(x_j)$  be given by the identity

$$\mathcal{I}_\alpha(x_{j-1}) - 2\mathcal{I}_\alpha(x_j) + \mathcal{I}_\alpha(x_{j+1}) = I_\alpha(x_{j-1}) - 2I_\alpha(x_j) + I_\alpha(x_{j+1}) + E_s(x_j). \quad (4.18)$$

Then for  $\epsilon_2 \propto \frac{1}{\Delta x^2} E_s(x_j)$  to be of second order,  $E_s(x_j)$  has to be fourth order accurate since we lose two orders by the second order stencil.

For the error due to the spline interpolation, we assume  $u$  to be sufficient smooth, i.e. in this case we want  $u \in C^4(\mathbb{R})$ . Then it can be shown<sup>[59]</sup>, that

$$u(\xi) - s_{j,k}(\xi) = - \sum_{r=2}^3 \frac{1}{r!} u^{(r)}(\xi) l_{k,r}(\xi) + \frac{1}{4!} u^{(4)}(\eta_k) l_{k,r}(\xi), \quad (4.19)$$

with  $\xi$  and  $\eta_k \in [x_{k-1}, x_k]$  and  $|l_{k,r}(\xi)| \leq \Delta x^r$ . That is, a linear spline interpolates the original curve with second order accuracy.

However, it remains to show that  $E_s(x_j)$  is of fourth order accuracy, for which we refer to the literature<sup>[51]</sup> or the derivation of even higher accuracy in the appendix A. The underlying idea is, to insert the spline approximation into the integral representation and afterwards apply the finite difference stencil to the error. In the appendix A, this prove is rigorously derived for every higher order accuracy under the assumption of a larger stencil and cubic splines. The proof of second order is given by the original authors.

Finally, we are left with a second order method in space.

A convergence analysis with the von Neumann method is performed by Sousa & Li as well and shows, that the scheme is unconditionally stable for  $\tau \in [0.5, 1]$ .

#### 4.1.2 Numerical results for the finite difference method

We will now reproduce some of the results produced by Zayernouri and Karniadakis. In the original paper, examples are provided which do have analytical solutions. Given the case, where

$$u(x, 0) = x^\lambda \quad x \in [0, 1], \quad (4.20)$$

$$u(0, t) = u(1, t) = e^{-t}, \quad (4.21)$$

$$d(x) = \frac{\Gamma(\lambda + 1 - \alpha)}{\Gamma(\Lambda + 1)} x^{\alpha+1}, \quad (4.22)$$

$$p(x, t) = -(1 + x)e^{-t} x^\lambda, \quad (4.23)$$

then the problem in equation (4.11) is well defined with solution

$$u(x, t) = e^{-t} x^\lambda. \quad (4.24)$$

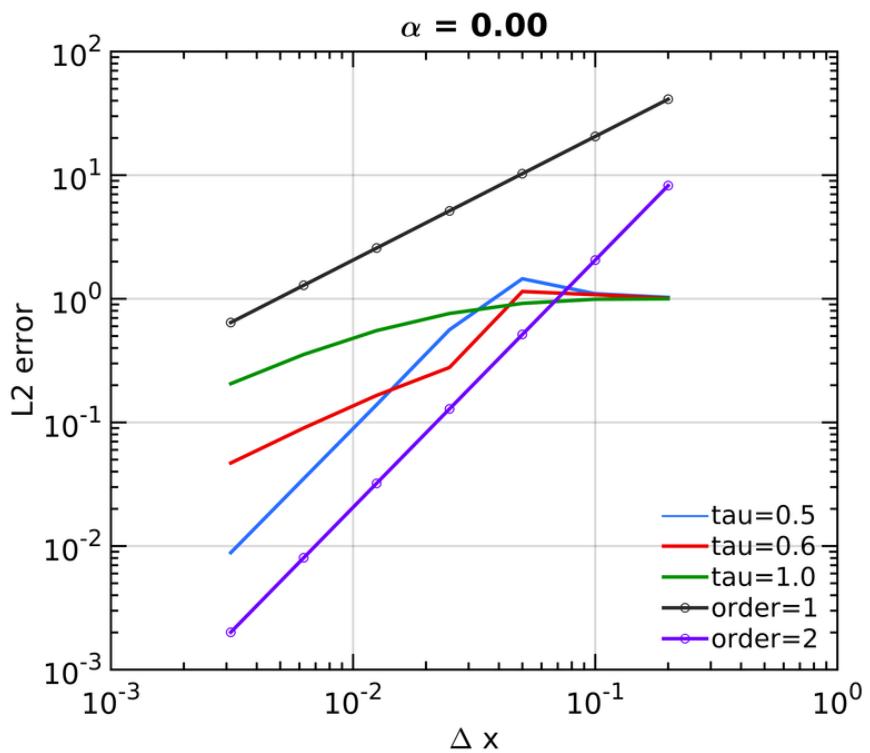
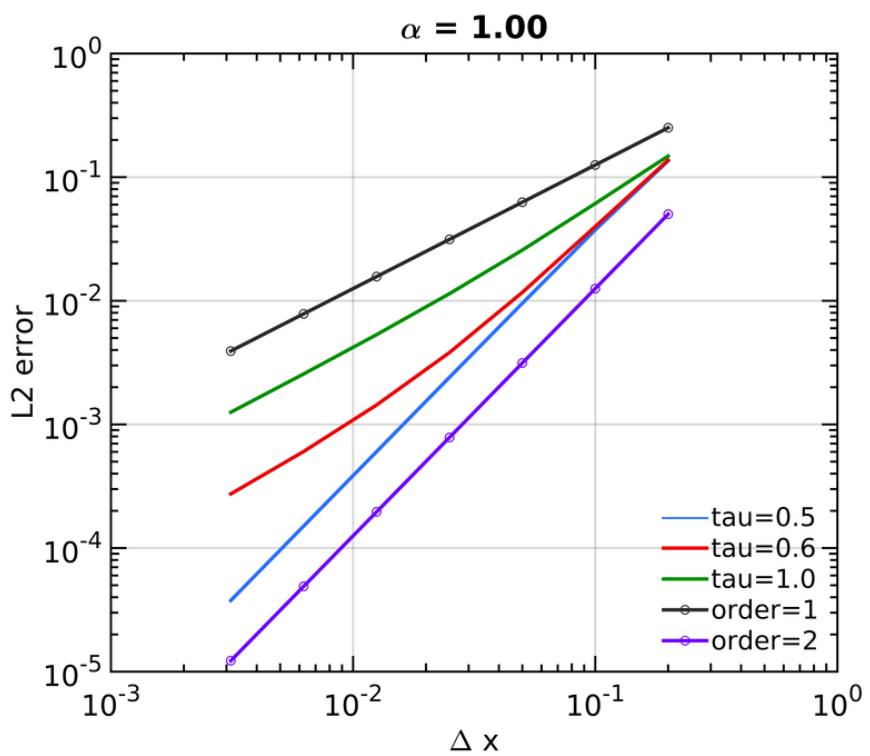
In Figures 4.1 to 4.4 we see the convergence results for different values of  $\alpha$  and  $\Delta t = \Delta x$ . Here,  $\alpha = 0$  corresponds to the identity operator,  $\alpha = 1$  to the solution of the advection equation and  $\alpha = 2$  to the solution of the standard heat equation, respectively. For  $\alpha = 1.5$ , we see the convergence results for the solution of the fractional diffusion equation. Each plot shows the convergence behaviour for different values of  $\tau$ , i.e. the weighting of the implicit and explicit time steps. The values are given by  $\tau = 0.5$ ,  $\tau = 0.6$  and  $\tau = 1$ . As predicted by the theoretical analysis, for  $\tau = 0.5$  we expect second order convergence, due to the fact that the error is of order  $\mathcal{O}(\Delta x^2, \Delta t^2)$  for  $\tau = 0.5$  and  $\mathcal{O}(\Delta x^2, \Delta t)$  for  $\tau \in (0.5, 1]$ . Since the plots are scaled logarithmic in x-direction and y-direction, the slope in the plot corresponds to the order of convergence in space for the corresponding method, which are inserted into the plot for comparison in black (first order) and in purple (second order). For  $\alpha \in (0, 2]$  we see, that the method is always of first order, if  $\tau \neq 0.5$  and of second order, once  $\tau = 0.5$ . Additionally, one can observe, that for  $\tau$  close to 0.5 the error is smaller than for the case where  $\tau = 1$ , even though both methods are still of first order accuracy. In Figure 4.1, we notice that the error increases at first when reducing the step size, but then turns into second and first order convergence. However, since this is for the case  $\alpha = 0$  and our analytic derivation assumed  $\alpha \in [1, 2]$ , which is the only case where we have the fractional derivative defined as equation (4.3), one can not impose convergence conditions on the method for  $\alpha < 1$ . The fact, that the method still converges for  $\alpha = 0$  suggests, that for the given setting, the choice of  $n$ , such that

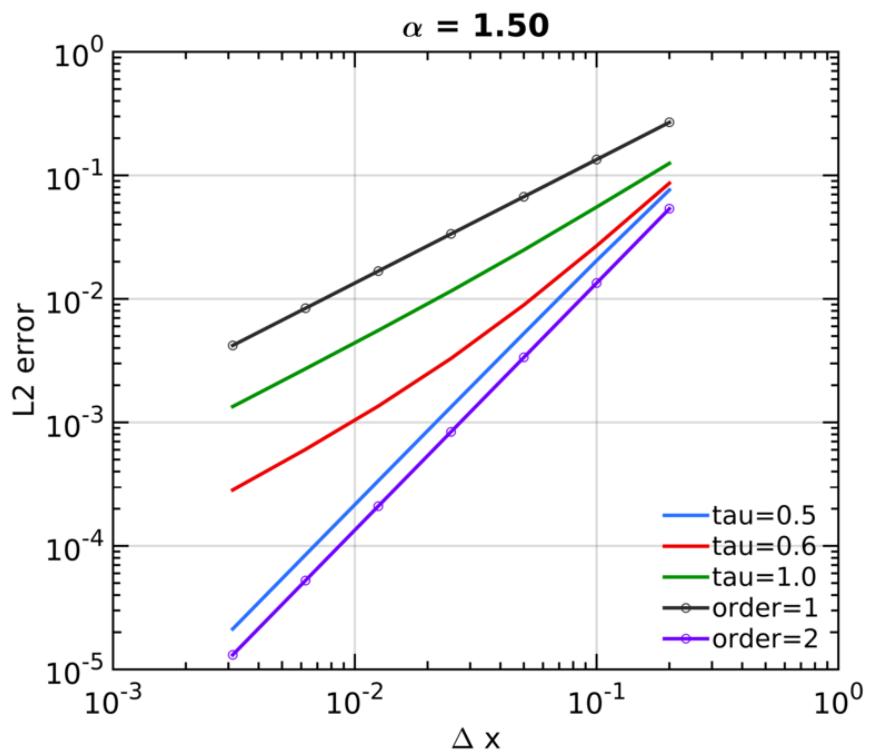
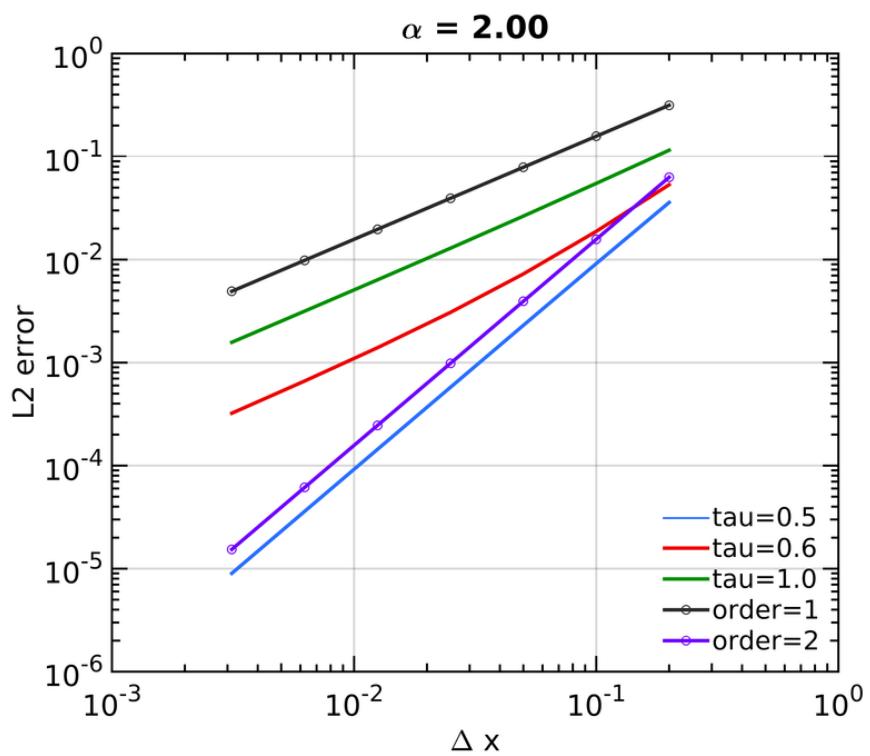
$n - 1 < \alpha < n$  is not relevant and  $n$  can be chosen rather flexible. A theoretical analysis of this phenomena would require further investigation, which we will not perform, since we are mainly interested in fractional diffusion equations for which the case of  $\alpha = 0$  is not relevant. In Figure 4.5, we see the dependency between the convergence and the value of  $\alpha$  for different values of  $\tau$ . For  $\tau \neq 0.5$  we notice, that the error is almost independent of the value of  $\alpha \in (1, 2)$ . That we observe better convergence for  $\alpha$  close to 2 in the case of  $\tau = 0.5$  suggests, that in this case, the main contribution to the error is due to the temporal discretization. However, with second order convergence for  $\tau = 0.5$  the error due to the time discretization becomes smaller, than the error due to the spatial discretization. For this case, we see a different error for different values of  $\alpha$ , which can also be observed in the theoretical derivation of the spatial error.

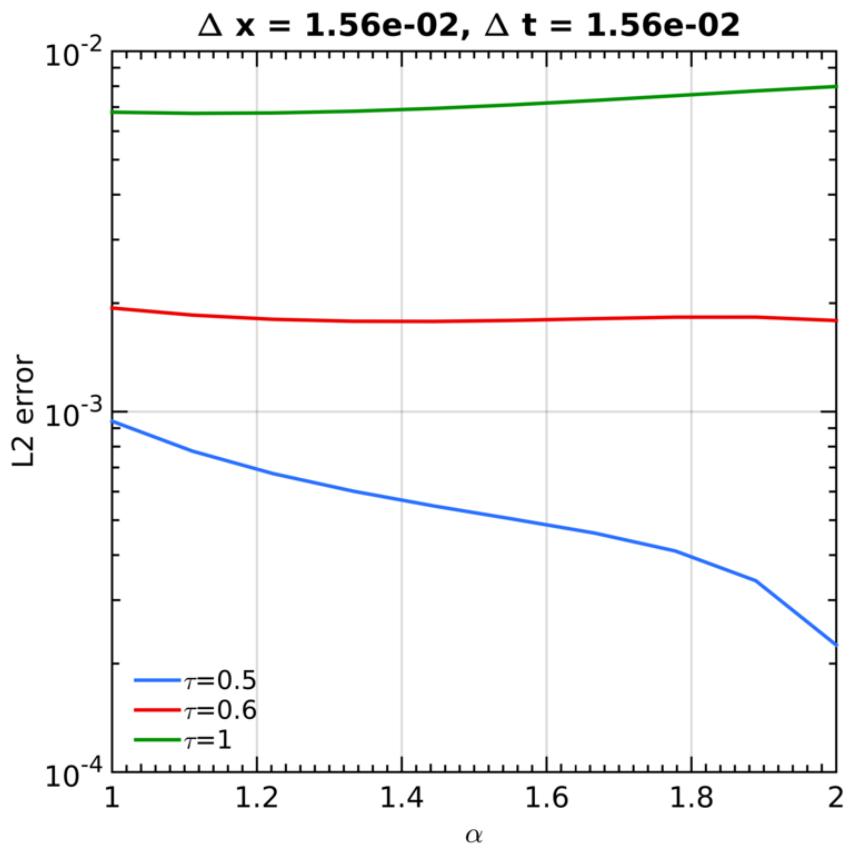
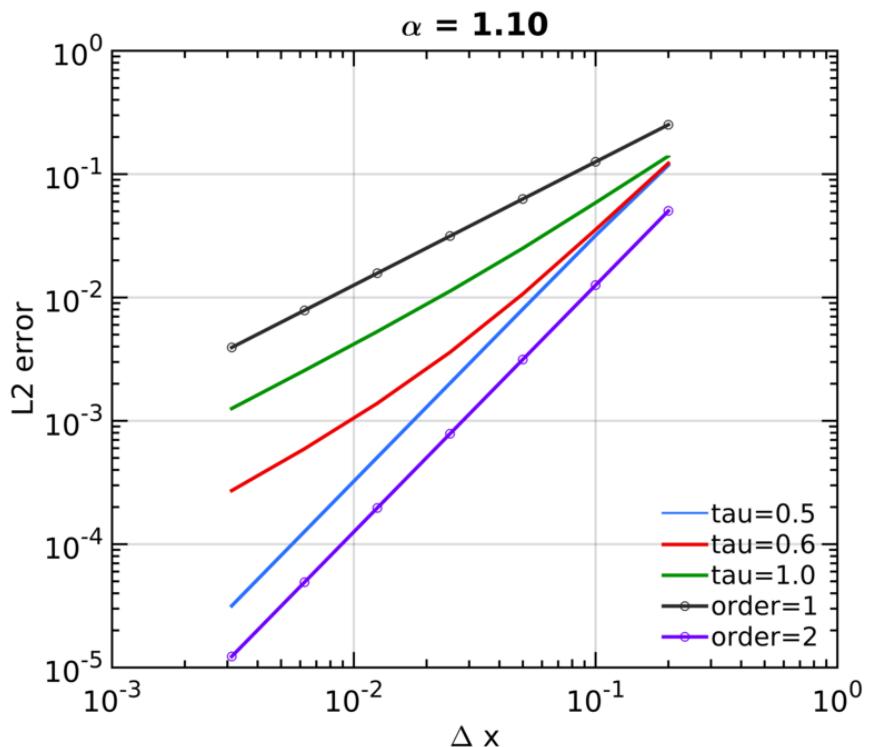
If we apply the method of Zayernouri and Karniadakis to different settings, we observe the same convergence behaviour as for the first example. If we consider the symmetric Riesz fractional derivative, then under the assumption of constant diffusion coefficient  $d$ , homogeneous boundary conditions and no source term, the convergence behaviour for  $\alpha = 1.1$  and the initial conditions

$$u(x, 0) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-1)^2}{2\sigma}\right), \quad (4.25)$$

and  $\sigma = 0.01$  are presented in Figure 4.6. Again, we observe first order convergence for  $\alpha \neq 0.5$  and second order convergence for  $\alpha = 0.5$ . However, for the computation we now have to solve a dense matrix system instead.

FIGURE 4.1: Spatial derivative of order  $\alpha = 0$ .FIGURE 4.2: Spatial derivative of order  $\alpha = 1$ .

FIGURE 4.3: Spatial derivative of order  $\alpha = 1.5$ .FIGURE 4.4: Spatial derivative of order  $\alpha = 2$ .

FIGURE 4.5: Convergence depending on  $\alpha$ .FIGURE 4.6: Spatial derivative of order  $\alpha = 1.1$  for Gaussian-like initial function.

## 4.2 Pseudo spectral collocation methods

We have shown, that the fractional differential operators are global operators in the corresponding space. Therefore, it seems reasonable to consider global methods for the solution of the fractional differential equations. The underlying idea of global methods is to express the quantity of interest in an appropriate, global basis. We then require the projection of the differential equation onto the expansion basis to vanish. Fully spectral methods require, that this projection vanishes almost everywhere, i.e. the integral of the differential equation against the basis has to vanish. In contrast, when we require that the projection vanishes only when summed over certain points, we call this a collocation method. The finite set of points which is used to approximate the integral by finite summation is called collocation points and has to be chosen carefully with respect to the concrete problem. Let us now write down this procedure in detail.

Consider the differential equation

$$\frac{\partial}{\partial t} u(t, x) = \mathcal{L}u(t, x), \quad (4.26)$$

where  $\mathcal{L}$  is some (fractional) differential operator in space. For example, in the case of the  $n$  dimensional fractional Laplacian we could have  $\mathcal{L} = \sum_{i=1}^n \partial_{|x_i|}^\alpha$  or  $\mathcal{L} = \partial_{xx} + \partial_{yy}$  for the two dimensional standard Laplacian.

Let now  $T^s = \text{span}\{\phi_0, \dots, \phi_\infty\}$  be the spatial trial space and  $T^t = \text{span}\{\psi_0, \dots, \psi_\infty\}$  the temporal trial space, where the  $\phi_i$  and  $\psi_i$  are an orthonormal basis, i.e.  $\langle \phi_i, \phi_j \rangle = \delta_{ij}$  and  $\langle \psi_i, \psi_j \rangle = \delta_{ij}$ . Since the basis is orthonormal, we are able to express  $u(t, x)$  in this basis as

$$u(t, x) = \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} a_{k,l} \psi_l(t) \phi_k(x), \quad (4.27)$$

with expansion coefficients  $a_{k,l}$ . An approximation of  $u(t, x)$  is then given by

$$u(t, x) \approx u^{M,N}(t, x) = \sum_{k=0}^M \sum_{l=0}^N a_{k,l} \psi_l(t) \phi_k(x). \quad (4.28)$$

The residual of the differential equation applied to the approximation of  $u(t, x)$  is then defined as

$$R(t, x) = \frac{\partial}{\partial t} u^{M,N}(t, x) - \mathcal{L}u^{M,N}(t, x) \quad (4.29)$$

$$= \sum_{l=0}^M \sum_{k=0}^N a_{k,l} \frac{\partial}{\partial t} \psi_l(t) \phi_k(x) - \sum_{l=0}^M \sum_{k=0}^N a_{l,k} \psi_l(t) \mathcal{L} \phi_k(x). \quad (4.30)$$

For the collocation method, we now need two sets of collocation points for time and space, respectively. Let the spatial set of collocation points be given by  $\{x_0, \dots, x_N\}$  and the temporal set of collocation points as  $\{t_0, \dots, t_M\}$ . The projection of  $R(t, x)$  onto  $\psi_i$  and  $\phi_j$  is done by the discrete analogon of the scalar product, i.e.

$$\langle R, \psi_i, \phi_j \rangle = \langle \langle R, \psi_i \rangle, \phi_j \rangle \quad (4.31)$$

$$\begin{aligned} &= \sum_{l=0}^M \sum_{k=0}^N a_{k,l} \sum_{m=0}^M \frac{\partial}{\partial t} \psi_l(t_m) \psi_i(t_m) \sum_{n=0}^N \phi_k(x_n) \phi_j(x_n) \\ &\quad - \sum_{l=0}^M \sum_{k=0}^N a_{l,k} \sum_{m=0}^M \psi_l(t_m) \psi_i(t_m) \sum_{n=0}^N \mathcal{L} \phi_k(x_n) \phi_j(x_n), \end{aligned} \quad (4.32)$$

which we can simplify under the assumption of orthonormality to get

$$\langle R, \psi_i, \phi_j \rangle = \sum_{l=0}^M \sum_{k=0}^N a_{l,k} \sum_{m=0}^M \frac{\partial}{\partial t} \psi_l(t_m) \psi_i(t_m) \delta_{k,j} \quad (4.33)$$

$$\begin{aligned} &\quad - \sum_{l=0}^M \sum_{k=0}^N a_{l,k} \delta_{l,i} \sum_{n=0}^N \mathcal{L} \phi_k(x_n) \phi_j(x_n) \\ &= \sum_{l=0}^M a_{l,j} \sum_{m=0}^M \frac{\partial}{\partial t} \psi_l(t_m) \psi_i(t_m) \\ &\quad - \sum_{k=0}^N a_{i,k} \sum_{n=0}^N \mathcal{L} \phi_k(x_n) \phi_j(x_n). \end{aligned} \quad (4.34)$$

If we now require the residual to vanish when projecting it onto the basis functions, we obtain

$$\langle R, \psi_i, \phi_j \rangle = 0 \quad \forall i = 0, \dots, M, \forall j = 0, \dots, N. \quad (4.35)$$

Solving the resulting linear system for  $a_{j,k}$  gives exactly the expansion coefficient for the approximation of  $u(t, x)$  via  $u^N(t, x)$ .

When using the collocation method for the solution of partial differential equations, it is especially important to choose the “correct” set of trial functions and the “correct” set of collocation points. In this context, “correct” means, that we want high order convergence while keeping the computational costs at an acceptable level. Since the choice of the basis functions and the collocation points is highly dependent on the problem, we will now consider concrete problems in the context of fractional diffusion.

### 4.2.1 A fractional spectral collocation method by Zayernouri & Karniadakis

In the following section, we will refer to the paper of Zayernouri & Karniadakis from 2014<sup>[60]</sup>. For the detailed theoretical analysis we refer to the original paper. The method is summarized and applied to examples below. Our implementation is used to derive numerical results.

Let us consider a general differential equation, that might be fractional in time and space.

$${}_0D_t^\tau u(x, t) = \mathcal{L}^\nu u(x, t), \quad x \in [-1, 1], t \in [0, T], \quad (4.36)$$

$$u(x, 0) = g(x), \quad (4.37)$$

$$u(-1, t) = 0, \quad \text{if } \nu \in (0, 1), \quad (4.38)$$

$$u(-1, t) = u(1, t) = 0, \quad \text{if } \nu \in (1, 2). \quad (4.39)$$

Here we either have to fix one or two boundary conditions, since the order of the differential operator is at first not specified.

The main idea for the choice of the basis function is now to consider the fractional Sturm-Liouville equation. To reduce computational costs, it is desirable to choose a basis that consists of eigenfunctions of the corresponding Sturm-Liouville problem. It can be shown<sup>[61]</sup>, that for the fractional Sturm-Liouville problem given by

$$\mathcal{L}^\mu \phi_\lambda(x) + \lambda(1-x)^\mu(1+x)^{-\mu} \phi_\lambda(x) = 0, \quad (4.40)$$

the corresponding eigenfunctions are given by

$$\phi_n(x) = (1+x)^\mu P_{n-1}^{-\nu, \nu}(x) =: \mathcal{P}_n^\mu(x). \quad (4.41)$$

In this context,  $P_{n-1}^{-\nu, \nu}(x)$  are the standard Jacobi polynomials and the  $\mathcal{P}_n^\mu(x)$  are referred to as the Jacobi polyfractionals.

Consequently, we consider the basis  $V_N^n = \text{span}\{\mathcal{P}_n^\mu(x), n = 1, \dots, N\}$  such that

$$u_N(x) = \sum_{j=1}^N \hat{u}_j \mathcal{P}_j^\mu(x), \quad (4.42)$$

for  $u_N(x) \in V_N^n$ . Comparing the order of the polynomials and polyfractionals involved, we can see, that we can also interpolate  $u_N(x)$  by making use of the fractional Lagrange

interpolants, i.e.

$$u_N(x) = \sum_{j=1}^N u_N(x_j) h_j^\mu(x), \quad (4.43)$$

with

$$h_j^\mu(x) \left( \frac{x - x_1}{x_j - x_1} \right)^\mu \prod_{k=1, k \neq j}^N \left( \frac{x - x_k}{x_j - x_k} \right), \quad j = 2, \dots, N, \quad (4.44)$$

and  $\{x_j\}_{j=1}^N$  being the set of interpolation points that satisfy  $-1 = x_1 < \dots < x_N = 1$ . Note, that  $h_j^\mu(x_k) = \delta_{j,k}$ .

Let us now be more specific regarding the differential operators applied to  $u_N(x)$ . At first we consider the simple one sided Riemann-Liouville derivative. Since we will later deal with homogeneous boundary and initial conditions, this is identically with the Caputo derivative. We also make use of the homogeneous boundary conditions by denoting, that  $u_N(x_1) = 0$ . We then plug in equation (4.44) into our expression for  $u_N(x)$ . Consider at first the case where  $\mu \in (0, 1)$ .

$${}_{-1}D_x^\mu u_N(x) = \sum_{j=2}^N u_N(x_j) {}_{-1}D_x^\mu h_j^\mu(x) \quad (4.45)$$

$$= \sum_{j=2}^N u_N(x_j) {}_{-1}D_x^\mu [(1+x)^\mu \mathcal{G}_j] \frac{1}{(x_j - x_1)^\mu}, \quad (4.46)$$

where  $\mathcal{G}_j = \prod_{k=1, k \neq j}^N \left( \frac{x - x_k}{x_j - x_k} \right)$ . Furthermore, we define  $a_j = \frac{1}{(x_j - x_1)^\mu}$ . Since the Jacobi polynomials are an orthogonal basis, it is also possible to rewrite  $\mathcal{G}_j$  in terms of the Jacobi polynomials as

$$\mathcal{G}_j = \sum_{n=1}^N \beta_n^j P_{n-1}^{-\mu, \mu}(x), \quad (4.47)$$

with some expansion coefficients  $\beta_n^j$  that can be computed analytically. Plugging the expression (4.47) into (4.46) and making use of the fact that we obtain the eigenfunctions

of the differential operator, we further compute

$${}_{-1}D_x^\mu u_N(x) = \sum_{j=2}^N u_N(x_j) {}_{-1}D_x^\mu [(1+x)^\mu \mathcal{G}_j] a_j \quad (4.48)$$

$$= \sum_{j=2}^N u_N(x_j) {}_{-1}D_x^\mu \left[ (1+x)^\mu \sum_{n=1}^N \beta_n^j P_{n-1}^{-\mu, \mu}(x) \right] a_j \quad (4.49)$$

$$= \sum_{j=2}^N u_N(x_j) {}_{-1}D_x^\mu \left[ (1+x)^\mu \sum_{n=1}^N \beta_n^j P_{n-1}^{-\mu, \mu}(x) \right] a_j \quad (4.50)$$

$$= \sum_{j=2}^N u_N(x_j) a_j \sum_{n=1}^N \beta_n^j {}_{-1}D_x^\mu [(1+x)^\mu P_{n-1}^{-\mu, \mu}(x)] \quad (4.51)$$

$$= \sum_{j=2}^N u_N(x_j) a_j \sum_{n=1}^N \beta_n^j {}_{-1}D_x^\mu [\mathcal{P}_n^{-\mu, \mu}(x)] \quad (4.52)$$

$$= \sum_{j=2}^N u_N(x_j) a_j \sum_{n=1}^N \beta_n^j \lambda_n P_{n-1}(x). \quad (4.53)$$

If we now evaluate the above expression at the collocation points, we obtain

$${}_{-1}D_x^\mu u_N(x)|_{x_i} = \sum_{j=2}^N u_N(x_j) a_j \sum_{n=1}^N \beta_n^j \lambda_n P_{n-1}(x_i) \quad (4.54)$$

$$= \sum_{j=2}^N D_{ij}^\mu u_N(x_j) \quad \forall i = 2, \dots, N, \quad (4.55)$$

where  $D_{ij}^\mu$  can be used as entries of a discrete differentiation matrix  $D^\mu \in \mathbb{R}^{(N-1) \times (N-1)}$ .

A similar computation can be performed to obtain  ${}_{-1}D_x^{1+\mu}$ . Simply note, that  ${}_{-1}D_x^{1+\mu} = \frac{d}{dx} {}_{-1}D_x^\mu$  and use  $\frac{d}{dx} P_{n-1}(x) = \frac{n}{2} P_{n-2}^{1,1}(x)$ . The computation is performed in detail in the original paper and results in a differentiation matrix  $D_x^{1+\mu}$ , similar to  $D_x^\mu$ . Furthermore, we note, that the differentiation matrix for the time derivative, i.e.  ${}_0D_t^\nu$  can be obtained by using the collocation points  $\{t_i\}_{i=1}^N$  with the transformation  $t_i = (x_i + 1)T/2$ .

For the implementation, Zayernouri and Karniadakis provide different choices of collocation points. It is noted, that the choice of the collocation points does not influence the order of convergence (which will always be spectral), but the condition number of the resulting matrices and therefore the numerical computation. Since the choice of collocation points is discussed in detail in the original paper, we would like to name only two of them. One are the equidistant points in time and space, i.e.  $t_i = i\Delta t$  and  $x_k = -1 + k\Delta x$ . The second type are the the extrema of the Chebyshev polynomial, which are Gauss-Lobatto type points that include the boundary points automatically.

Let us now consider concrete applications. Since we are able to express differentiation matrices for first order in time and space, as well as for second order in space, we are able to solve time-dependent advection-diffusion problems that are fractional in time and space with different orders of the three involved fractional indices. In general, this means that our problems can be of the type

$${}_0D_t^\tau u(x, t) + c_{-1}D_x^{\nu_2}u(x, t) - K_{-1}D_x^{1+\nu_1}u(x, t) = f(x, t), \quad (4.56)$$

$$u(1, t) = u(-1, t) = 0, \quad (4.57)$$

$$u(x, 0) = 0, \quad (4.58)$$

with  $\tau, \nu_1, \nu_2 \in (0, 1)$ . Using the prior defined differentiation matrices and defining  $U$  as the approximation of  $u$ , i.e.  $U_{j,m} = u^{M,N}(x_j, x_m)$  and  $F$  by  $F_{j,m} = f(x_j, t_m)$ , we obtain the system

$$UD^{\tau T} + [cD^{\nu_1} - KD^{\nu_2}]U + F, \quad (4.59)$$

which is equivalent to the solution of the Lyapunov equation

$$AU + UB = F, \quad (4.60)$$

where  $A = cD^{\nu_1} - KD^{\nu_2}$  and  $B = D^{\tau T}$ , with the superscript  $T$  for the transpose operator. An advantage of the collocation method, is the treatment of nonlinear problems. Since we only need to solve the original problem at certain grid points. This means, that we do not have to consider singularities in the computation of the scalar product. In a further example, Zayernouri and Karniadakis apply the method also to the Burgers equation which we will not consider in this work.

#### 4.2.2 Numerical results for the collocation method

We will now provide several examples, where we apply the collocation method to solve the time-dependent advection diffusion equation with varying order of the fractional derivative in time, the first order differentiation corresponding to the advection term and the second order differentiation corresponding to the diffusion term, respectively. Let  $\tau$  denote the order of the fractional derivative in time  $\nu_1$  the order of differentiation related to the diffusion term and  $\nu_2$  the order corresponding to the advection term, respectively. In contrast to the finite difference method, the restrictions for  $\tau, \nu_1$  and  $\nu_2$  to be in the domain  $(0, 1)$  are strict. This means, that the presented method will break down when trying to recover integer order derivatives in time and space. However, we are able to choose all three orders arbitrarily close to 0 or 1. One way to resolve this issue, could be

by implementing a switching method, that chooses standard differentiation methods for integer order derivatives. To be comparable with the original work by Zayernouri and Karniadakis, we will not consider this and assume, that  $\tau, \nu_1, \nu_2 \in (0, 1)$ . In contrast to the original work, we will replace the one-sided spatial derivative corresponding to the diffusion term by the symmetrized variant  $D_{|x|}^\nu = -_1D_x^\nu + xD_1^\nu$ . In addition to the order of the derivative, we can also adjust the contribution of the advection term and the diffusion term by providing two parameters  $c$  and  $K$  in agreement with the usage in equation (4.56). Even though Zayernouri and Karniadakis perform their analysis with different types of collocation points, they notice, that this does not influence the order of convergence, but only the condition number of the corresponding matrices. We therefore always choose equidistant points in time and space, respectively.

We will consider the scenario, where the right-hand side  $f(x, t)$  is a composition of a Gaussian in space and linear in time. Since we want the boundary conditions to be homogeneous, we multiply the Gaussian in space with  $x(1 - x)$  to enforce homogeneous boundary conditions on  $[0, 1]$ . We then obtain  $f(x, t) = \exp(-(x - 1)^2) \cdot x(1 - x) \cdot t$ , which is consistent with the homogeneous initial conditions, that were assumed during the derivation

To model a standard diffusion equation, we first assume  $\tau = 0.99, \nu_1 = 0.99$  and then ignore the differentiation matrix corresponding to the advection term by setting  $c = 0$  and  $K = 1$ . This means, that we solve

$$_0D_t^{0.99}u(x, t) - D_{|x|}^{1+99}u(x, t) = \exp(-(x - 1)^2) \cdot x(1 - x) \cdot t, \quad (4.61)$$

$$u(1, t) = u(-1, t) = 0, \quad (4.62)$$

$$u(x, 0) = 0. \quad (4.63)$$

As a reference solution, we take the results produced by the spectral collocation method with spatial and temporal expansion order equally high, i.e.  $N_{space} = N_{time} = 64$ . The convergence is measured in the  $L_2$ -norm. In the discrete setting, we define  $\|u\|_2^2 = \sum_{i=0}^{M_{space}} \sum_{j=0}^{M_{time}} u(x_i, t_j)^2$ . where  $M_{space}$  and  $M_{time}$  denote the number of grid points on which we reconstruct the solution. The value is fixed to  $M_{space} = M_{time} = 100$  throughout all computations.

In Figure 4.7 we then see the results for the first test case. We observe spectral convergence in the order of the spatial expansion  $N$ , independent of the order of the temporal expansion  $M$ . Even for low numbers of  $M$  we observe spectral convergence rate as  $N$  grows.

In a first step, we now replace the almost integer order derivative in space by a fractional derivative. For  $\nu_1 = 0.5$ , we obtain a fractional Laplacian  $\Delta^{1.5/2}$ . Keeping all other

parameters as before, we again observe spectral convergence in Figure 4.8. The fact, that the convergence behavior is also quantitative similar to the results obtained in Figure 4.7 suggest, that when modelling the diffusion equation, the order of the fractional derivative in space does not influence the convergence. This is in agreement with the theoretical analysis, where we choose our polynomial basis to consist of eigenfunctions of the spatial differential operator. Therefore, different orders of spatial derivatives only scale the corresponding eigenvalues differently and do not influence the computation at any other location.

That the methodology is not restricted to diffusion problems only, can be seen in Figure 4.9. Here we let the advection term influence the solution by setting  $\nu_2 = 0.4$  and  $c = 1.0$ . We also change the contribution of diffusive effects by setting  $K = 5$ , which means that we model an advection-diffusion equation with dominant diffusive terms. Additionally, we changed the order of the spatial derivative to be  $\tau = 0.9$  and use the Laplacian  $\Delta^{1.9/2}$ . This means, that we solve the fractional advection-diffusion equation that is fractional in time and space. We observe spectral order convergence in this case, too. The fact, that the expansion order in time has almost no influence on the solution can be explained by the fact, that due to the high diffusion, the steady state solution is reached earlier and therefore, the error introduced due to the temporal approximation is smaller.

When we now move on to the case, where advection and diffusion contribute equally to the equation, we can see the convergence results in Figure 4.10. Since the process that is modelled by the equation is less diffusive, the temporal order of expansion now again influences the solution. At first we observe, that the spectral convergence is still present for all values of  $M$ . However, except for the value of  $N = 8$  the convergence is similar for all values of  $M$ . The difference in convergence for different values of  $M$  when  $N = 8$  can not directly be explained by considering the theoretical analysis. From a quantitative viewpoint, a direct comparison with the diffusion dominant case shows, that for the scenario where advection and diffusion contribute equally, the overall convergence is slower, though it is still spectral. It again seems reasonable to assume, that problems with higher diffusion are numerically easier to solve, since an almost steady state solution is reached faster and the advection processes take place on a smaller scale and therefore have smaller influence on the accuracy of the solution. As a last example, we consider the case where  $\tau = 0.1$ ,  $\nu_1 = 0.1$  and  $\nu_2 = 0.9$  in Figure 4.11. This setting shall mimic an almost time-independent process, since for  $\tau$  close to zero, we recover the identity operator. That the process is not completely time-independent can be seen in the results. In the case of  $M$  being small ( $M = 8$ ) the convergence is slightly worse for sufficient high values of  $M$  ( $M = 12$  or  $M = 16$ ). Advection and diffusion contribute equally to the problem, however, by setting  $\nu_1 = 0.1$  and  $\nu_2 = 0.9$  both spatial derivatives approach

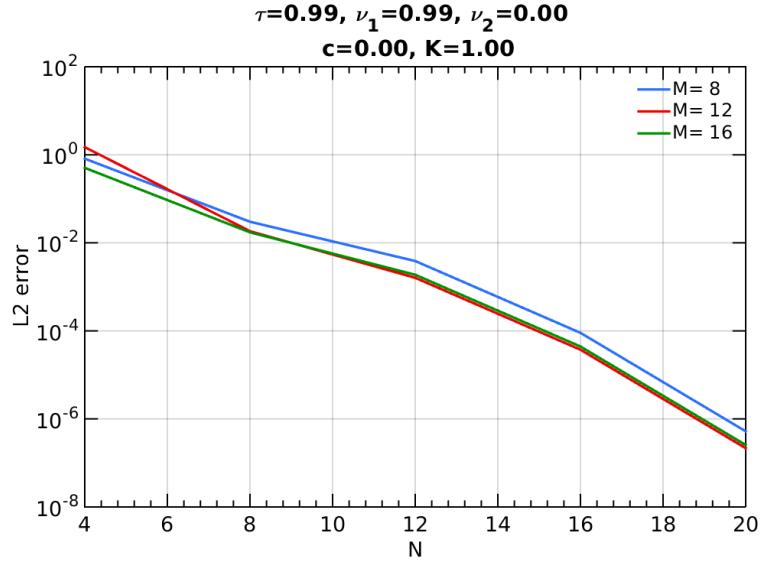


FIGURE 4.7: Approximating the standard heat equation.

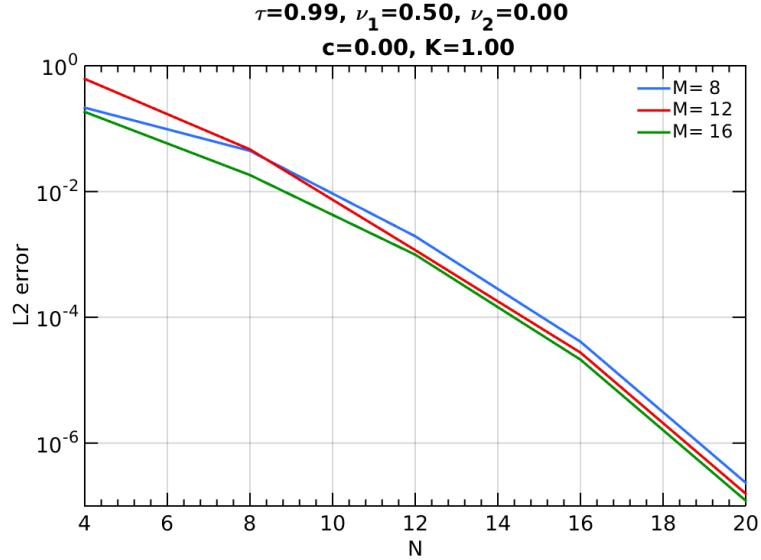


FIGURE 4.8: Approximating the space fractional heat equation.

the first order integer derivative in space. Even though,  $c = K = 1$  we can not argue, that for this case the spatial derivative vanishes, since for the differentiation matrix corresponding to the diffusion process, we symmetrize the differentiation, whereas this is not the case for the advection part.

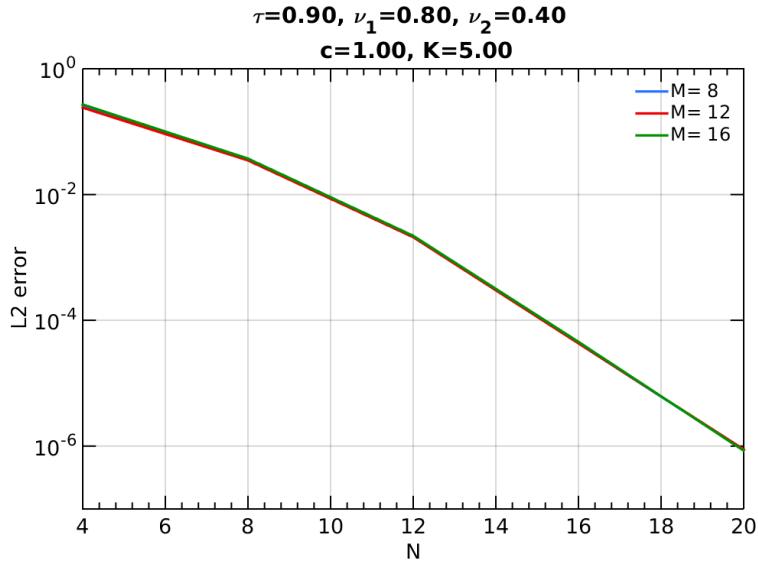


FIGURE 4.9: Advection-diffusion equation with dominant diffusion.

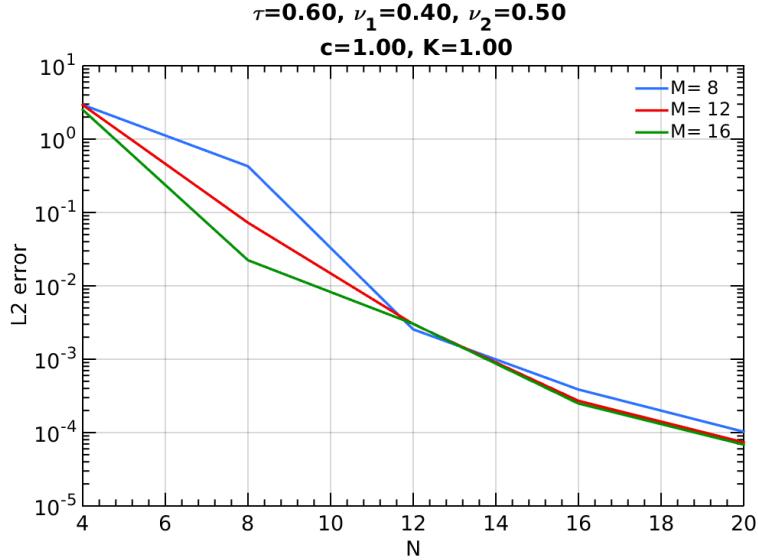


FIGURE 4.10: Advection and diffusion contribute equally to the equation.

### 4.3 Spectral Galerkin methods

One of the standard methods for solving partial differential equations is the Galerkin method. As before, we plug in an ansatz for our solution into the original equation and require the residual of the projection onto the space spanned by the test functions to vanish.

Consider the one dimensional diffusion equation

$$\partial_t u(x, t) - \partial_{xx} u(t, x) = f(x, t), \quad (4.64)$$

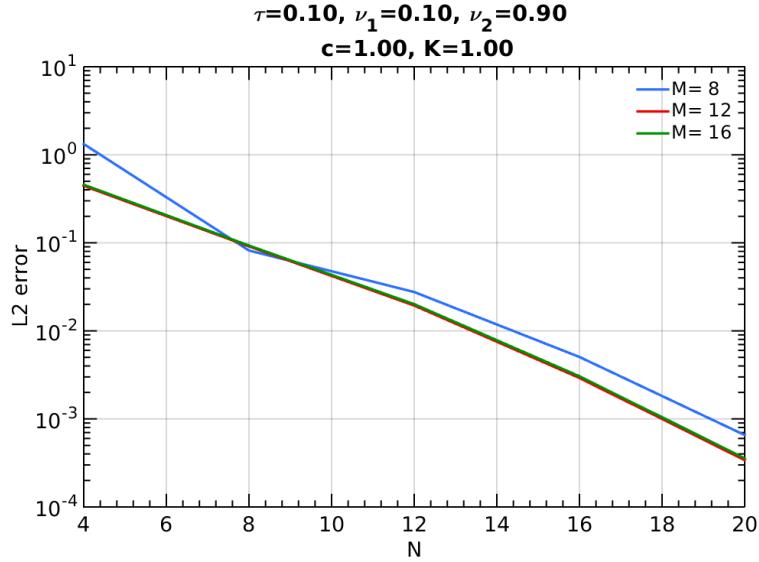


FIGURE 4.11: Almost no temporal derivative.

with homogeneous initial and boundary conditions. If we further consider some space  $V$ , we obtain the weak formulation of (4.94) by finding  $u \in V$  such that

$$\mathcal{A}(u, v) = \mathcal{F}(v) \quad \forall v \in V, \quad (4.65)$$

with the bilinear form

$$\mathcal{A}(u, v) = \langle \partial_t u, v \rangle_V + \langle \partial_x u, \partial_x v \rangle_V, \quad (4.66)$$

and

$$\mathcal{F}(v) = \langle f, v \rangle_V. \quad (4.67)$$

We then seek solutions  $u_N \in V_N$  where  $V_N \subset V$ . The weak problem in the subspace is then to find  $u_N \in V_N$  such that

$$\mathcal{A}(u_N, v_N) = \mathcal{F}(v_N) \quad \forall v_N \in V_N. \quad (4.68)$$

If the bilinear form is continuous and coercive and  $\mathcal{F}$  is bounded, then it is well known, that by Cea's lemma the error of the approximation can be bounded by

$$\|u - u_N\| \leq \inf_{v_N \in V_N} \|u - v_N\|. \quad (4.69)$$

This means, that we have the best approximation property and the error bound only depends on the approximation of the space. By choosing an appropriate basis we are then able to achieve spectral convergence simply as a result of the choice of basis functions.

### 4.3.1 A space-time spectral method for time fractional diffusion equations by Li & Xi

We will now review one of the main contributions to fully spectral numerical methods in the context of fractional differential equations. In their paper from 2009, Li & Xi present a space-time spectral method for the solution of the time fractional heat equation. Let us consider from now on the one dimensional time fractional diffusion equation

$${}_0\partial_t^\alpha u(x, t) - \partial_{xx}u(t, x) = f(x, t), \quad (4.70)$$

with  $(x, t) \in \Omega := \Lambda \times I = (-1, 1) \times (0, T)$  with homogeneous initial and boundary conditions

$$u(x, 0) = 0, \quad (4.71)$$

$$u(-1, t) = u(1, t) = 0. \quad (4.72)$$

Since we have the homogeneous initial and boundary conditions, the Riemann-Liouville and Caputo derivative coincide. The authors therefore choose the definition according the Riemann-Liouville throughout their paper.

For the spectral expansion in space and time, Li & Xi provide suitable basis polynomials. Let  $P_M(\Lambda)$  and  $P_N(I)$  define the set of polynomials of degree  $M$  in space and  $N$  in time, respectively. Since we assume  $u(\partial\Lambda, t) \equiv 0$  as well as  $u(x, 0) \equiv 0$ , we choose polynomials in space from

$$P_M^0(\Lambda) = P_M(\Lambda) \cap H_0^1(\Lambda), \quad (4.73)$$

as well as for time

$$P_N^E(I) = \{v \in P_N(I) | v(0) \equiv 0\}. \quad (4.74)$$

For sake of convenience, define the multiindex  $L = (M, N)$  and

$$S_L := P_M^0(\Lambda) \otimes P_N^E(I). \quad (4.75)$$

Then the Galerkin problem is given by finding  $u_L \in S_L$  such that

$$\mathcal{A}(u_L, v_L) = \mathcal{F}(v_L) \quad \forall v_L \in S_L. \quad (4.76)$$

However, it remains to specify the bilinear form in the context of fractional derivatives. For  $\mathcal{A}$  to be symmetric, we need some way to symmetrize the scalar product  $\langle {}_0D_t^\alpha u, v \rangle$ .

We therefore cite the following two lemmas from the original paper.

*Lemma 4.3.* For  $0 < \alpha < 1$  and  $u \in H^\alpha(I)$ ,  $v \in C_0^\infty(I)$  we have

$$\langle {}_0D_t^\alpha u, v \rangle_I = \langle u, {}_tD_T^\alpha v \rangle_I. \quad (4.77)$$

*Proof.* Applying integration by parts to the definition of the scalar product yields

$$\langle {}_0D_t^\alpha u, v \rangle_I = \int_0^T \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t \frac{u(\tau)}{(t-\tau)^\alpha} d\tau v(t) dt \quad (4.78)$$

$$= \underbrace{\left[ \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u(\tau)}{(t-\tau)^\alpha} v(t) \right]_0^T}_{=0, \text{ since } v \in C_0^\infty} - \int_0^T \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u(\tau)}{(t-\tau)^\alpha} d\tau v'(t) dt \quad (4.79)$$

$$= - \int_0^T \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u(\tau)}{(t-\tau)^\alpha} d\tau v'(t) dt. \quad (4.80)$$

By changing the order of integration and by employing the fact, that for  $v \in C_0^\infty$  the Riemann-Liouville definition and the Caputo definition coincide, we further obtain

$$\langle {}_0D_t^\alpha u, v \rangle_I = - \int_0^T \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u(\tau)}{(t-\tau)^\alpha} d\tau v'(t) dt \quad (4.81)$$

$$= - \int_0^T \frac{1}{\Gamma(1-\alpha)} \int_t^T \frac{v'(\tau)}{(t-\tau)^\alpha} dt u(\tau) d\tau \quad (4.82)$$

$$= - \int_0^T \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t \frac{v(\tau)}{(t-\tau)^\alpha} dt u(\tau) d\tau \quad (4.83)$$

$$= \langle u, {}_tD_T^\alpha v \rangle_I. \quad (4.84)$$

□

*Lemma 4.4.* For all  $0 < \alpha < 1$  and  $u \in {}_0H^1(I)$ ,  $v \in {}_0H^{\alpha/2}(I)$  we have

$$\langle {}_0D_t^\alpha u, v \rangle_I = \langle {}_0D_t^{\alpha/2} u, {}_tD_t^{\alpha/2} v \rangle_I. \quad (4.85)$$

*Proof.* The idea is, to use the fact, that  ${}_0D_t^\alpha u = {}_0D_t^{\alpha/2} {}_0D_t^{\alpha/2} u$  and Lemma 4.3. □

This yields the Galerkin problem that is considered in the following. Try to find  $u_L \in S_L$  such that

$$\mathcal{A}(u_L, v_L) = \mathcal{F}(v_L) \quad \forall v_L \in S_L, \quad (4.86)$$

where the bilinear form is given by

$$\mathcal{A}(u, v) = \langle {}_0\partial_t^{\alpha/2} u, {}_t\partial_T^{\alpha/2} v \rangle_\Omega + \langle \partial_x u, \partial_x v \rangle_\Omega. \quad (4.87)$$

It can then be shown, that in the given context, the requirements for the Lax-Milgram theorem are satisfied and convergence and uniqueness, as well as spectral convergence rate by Cae's lemma are ensured.

Let us now specify the basis for both, time and space. In space, we choose the standard Lagrangian polynomials as a basis, i.e.  $P_M^0(\Lambda) = \text{span}\{h_i, i = 1, \dots, M - 1\}$  where  $h_i$  are the Lagrangian polynomials associated with the Gauss-Lobatto-Legendre quadrature points. To achieve good convergence for the time approximation, the authors introduce a linear combination of Jacobi polynomials, which differ for the space of test functions and trial functions. Define

$$\phi_j(t) = J_j^{-\alpha/2,0}\left(\frac{2t}{T} - 1\right) + J_{j-1}^{-\alpha/2,0}\left(\frac{2t}{T} - 1\right), \quad (4.88)$$

$$\psi_n(t) = \frac{n}{n - \alpha/2} J_n^{-\alpha/2,0}\left(\frac{2t}{T} - 1\right) + J_{n-1}^{-\alpha/2,0}\left(\frac{2t}{T} - 1\right), \quad (4.89)$$

where both  $i$  and  $j$  run from 1 to  $N$  and  $J_k^{\alpha,\beta}$  are the standard Jacobi polynomials. Even though this choice might seem arbitrary, it can be verified, that these polynomials form a suitable basis that allows easy evaluation of the involved integrals in combination with the fractional differential operators. We note, that both, the set of  $\psi_n(t)$  and  $\phi_j(t)$  form a basis of  $P_N^E(I)$ . Our polynomial expansion of  $u(t, x)$  is then given by

$$u(x, t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} u_{ij} h_i(x) \phi_j(t) \approx \sum_{i=1}^{M-1} \sum_{j=1}^N u_{ij} h_i(x) \phi_j(t) =: u_L(x, t). \quad (4.90)$$

In contrast to the standard Galerkin approach, where test and trial functions are chosen from the same space, we choose the test functions to be the space of Lagrangian polynomials times the space spanned by the  $\psi_n$ , which yields the linear system

$$Au = f, \quad (4.91)$$

with  $u, f \in \mathbb{R}^{(M-1)N}$  and  $A \in \mathbb{R}^{(M-1)N \times (M-1)N}$  where

$$a_{mn,ij} = \langle h_{i0} \partial_t^{\alpha/2} \phi_j, h_{mt} \partial_T^{\alpha/2} \psi_n \rangle_L + \langle \partial_x h_i \phi_j, \partial_x h_m \psi_n \rangle_L, \quad (4.92)$$

$$f_{mn} = \langle f, h_m \psi_n \rangle_L. \quad (4.93)$$

*Remark 4.5.* Computing these integrals naively by high order quadrature methods implies high computational costs, since the global nature of the fractional differential operator implies dense matrices. Li & Xi therefore provide suitable quadrature methods and a comprehensive appendix with transformations of the original integral to ensure faster computation of the entries of  $A$ . While this allows faster computation of the stiffness

matrix, it is restricted to the specific choice of basis functions which we will change later and will therefore not be considered here.

#### 4.3.1.1 Extension to time and space fractional diffusion equations

Since our original interest was in the field of fractional diffusion equations, it is desirable to extend the method provided by Li & Xi to include the fractional Laplacian, which was not considered in the original paper. Furthermore, we would like to consider fractional diffusion problems which have non homogeneous, but symmetric initial conditions. Also the restriction to homogeneous boundary conditions might be a problem when choosing suitable polynomials for the expansion in space. We therefore replace homogeneous boundary conditions by periodic boundary conditions. Summarizing this, we consider problems of the type

$${}_0\partial_t^\alpha u(x, t) - \partial_{|x|}^{2\beta} u(t, x) = f(x, t), \quad (4.94)$$

with  $(x, t) \in \Omega := \Lambda \times I = (0, 2\pi) \times (0, T)$  and

$$u(x, 0) = u_0(x), \quad (4.95)$$

$$u(0, t) = u(2\pi, t). \quad (4.96)$$

With  $\alpha, \beta \in (0, 1)$  and consistency in the initial and boundary conditions. The space fractional derivative  $\partial_{|x|}^{2\beta}$  is defined by  $2\partial_{|x|}^{2\beta} u(t, x) = \partial_x^{2\beta} u(t, x) + {}_x\partial^{2\beta} u(t, x)$ , i.e. the symmetric combination of the left- and right-sided fractional derivative. We can transform this problem into a problem with homogeneous initial conditions by defining  $v(x, t) := u(x, t) - u(x, 0)$  and substituting  $u(x, t) = v(x, t) + u(x, 0)$  in the original equation to obtain

$${}_0\partial_t^\alpha v(x, t) - \partial_{|x|}^{2\beta} v(t, x) = f(x, t) + \partial_{|x|}^{2\beta} u(x, 0) =: \tilde{f}(x, t), \quad (4.97)$$

$$v(x, 0) = 0, \quad (4.98)$$

$$v(0, t) = v(2\pi, t). \quad (4.99)$$

Under the assumption, that the problem is periodic, our initial conditions are symmetric and by denoting that the fractional differential operator in space is also symmetric, we can apply Lemma 4.3 to obtain the bilinear form

$$\mathcal{A}(u, v) = \langle {}_0\partial_t^{\alpha/2} u, {}_T\partial_T^{\alpha/2} v \rangle_\Omega + \langle \partial_{|x|}^\beta u, \partial_{|x|}^\beta v \rangle_\Omega. \quad (4.100)$$

Since we apply a fractional differential operator in space, we have to consider a change of the basis functions from the proposed Lagrangian polynomials by Li & Xi. As shown by Zhan & Liu<sup>[62]</sup>, in the case of the Riesz fractional differential operator, which is up to scaling by a constant identically to  $\partial_{|x|}^{2\beta}$ , the complex Fourier expansion polynomials provide a suitable basis of eigenfunctions. Let us therefore consider the space

$$P_M(\Lambda) = \text{span}\{e^{imx}/\sqrt{2\pi}, m \in (-M, M)\}. \quad (4.101)$$

This choice of basis polynomials is orthonormal with respect to the standard scalar product on  $\Lambda$ , i.e.  $\langle e^{imx}/\sqrt{2\pi}, e^{inx}/\sqrt{2\pi} \rangle_\Lambda = \delta_{mn}$ . Zhan & Liu have shown, that the terms  $e^{imx}$  are eigenfunctions of the considered differential operator with eigenvalues  $(im)^{2\beta}$  and therefore,  $\langle \partial_{|x|}^\beta e^{imx}/\sqrt{2\pi}, \partial_{|x|}^\beta e^{inx}/\sqrt{2\pi} \rangle_\Lambda = \delta_{mn} m^{2\beta}$ . This property is obviously desirable, since we are able to avoid the calculation of the scalar products by numerical quadrature rules and we are able to explore sparsity. The ansatz for approximating  $u(x, t)$  is then given by

$$u(x, t) = \sum_{i=1}^{\infty} \sum_{j=-\infty}^{\infty} u_{ij} f_i(x) \phi_j(t) \approx \sum_{m=-M}^M \sum_{j=1}^N u_{ij} f_m(x) \phi_j(t) =: u_L(x, t), \quad (4.102)$$

with  $f_m(x) = e^{imx}/\sqrt{(2\pi)}$  and  $\phi_j(t)$  defined as before.

*Remark 4.6.* For the convergence to be spectral we need  $u(x, t)$  to be sufficiently smooth. Since we consider a periodic domain with initial conditions  $u(x, 0) \not\equiv 0$ , we will see that it is necessary to require additional smoothness conditions on  $u(x, 0)$ , i.e. we want  $u^{(n)}(x, 0) = u^{(n)}(x, 2\pi)$  for as many orders of the derivative  $n$  as possible. This is not only necessary for spectral convergence of the method, but also for the approximation by the Fourier series in space, since we would otherwise encounter the Gibbs phenomenon.

### 4.3.2 Numerical results for the Galerkin method

We will now apply the derived method to several problems and show convergence results as well as the phenomenological influence of the fractional order of the derivatives in time and space, respectively. All examples will be based on the general formulation in equation (4.94)

At first, we will consider a standard scenario in diffusive processes. Let us omit the source term  $f$  at first. For  $u(x, 0)$  we assume a standard normal distribution as the

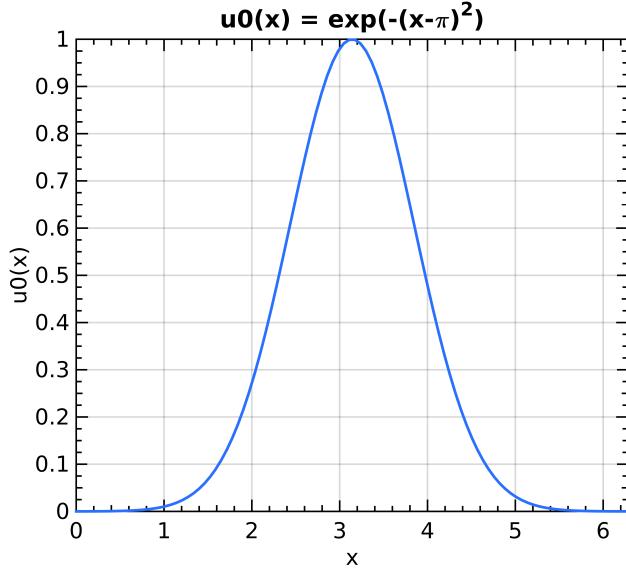


FIGURE 4.12: Initial conditions for the results shown in Figure 4.13.

initial conditions, i.e.  $u(x, 0) = \exp(-(x - \pi)^2)$ . We then solve

$${}_0\partial_t^\alpha v(x, t) - \partial_{|x|}^{2\beta} v(t, x) = \partial_{|x|}^{2\beta} \exp(-(x - \pi)^2), \quad (4.103)$$

$$v(x, 0) = 0, \quad (4.104)$$

$$v(0, t) = v(2\pi, t). \quad (4.105)$$

The qualitative influence of the order of the fractional derivative can be seen in Figure 4.13, where all combinations of equation (4.94) with  $\alpha \in \{0, 0.5, 1\}$  and  $2\beta \in \{0, 1.5, 2\}$  are presented. For  $\alpha = 0$  we only have diffusion in space and the solution is time invariant, which corresponds to the first row of plots. It can be seen, that the higher the value for  $\beta$ , the more spread out the value of  $v(x)$  is over the spatial domain. For  $\alpha = 0$  and  $2\beta = 2$  we then recover the equation  $(I + \Delta^2)v = \Delta^2 u_0(x)$ .

If we now increase  $\alpha$ , we obtain a time-dependent problem. Similar to the case, where we increase  $\beta$ , an increase in  $\alpha$  causes higher diffusivity in time. For  $\alpha = 0.5$  and  $2\beta = 1.5$  we recover the fully time and space fractional diffusion equation. Setting  $\alpha = 1$  yields the classical time derivative and together with  $2\beta = 2$  we are left with the classical heat equation.

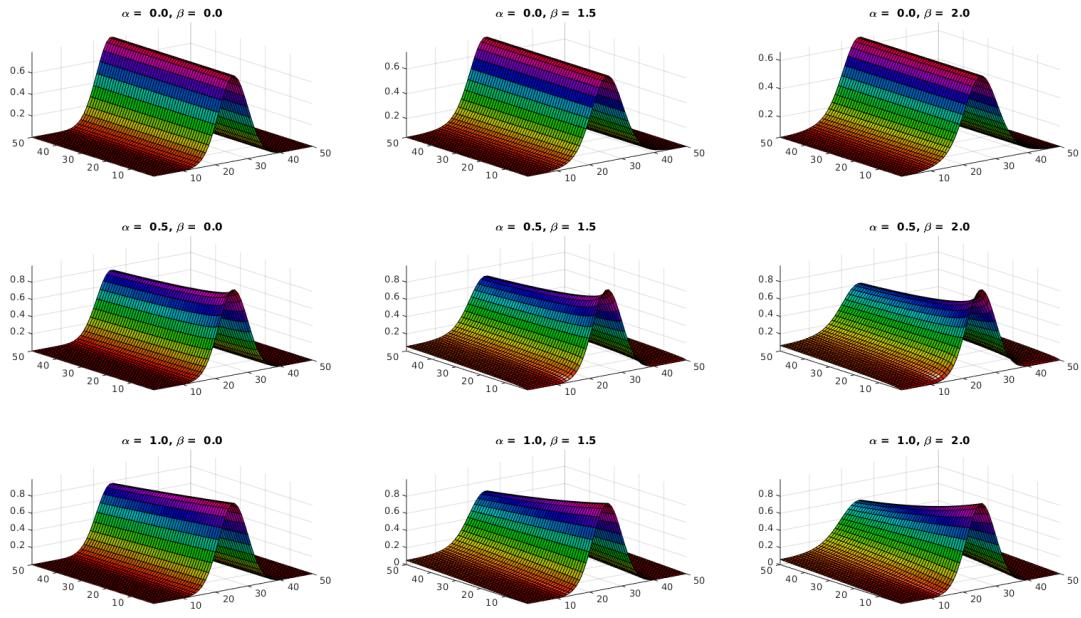
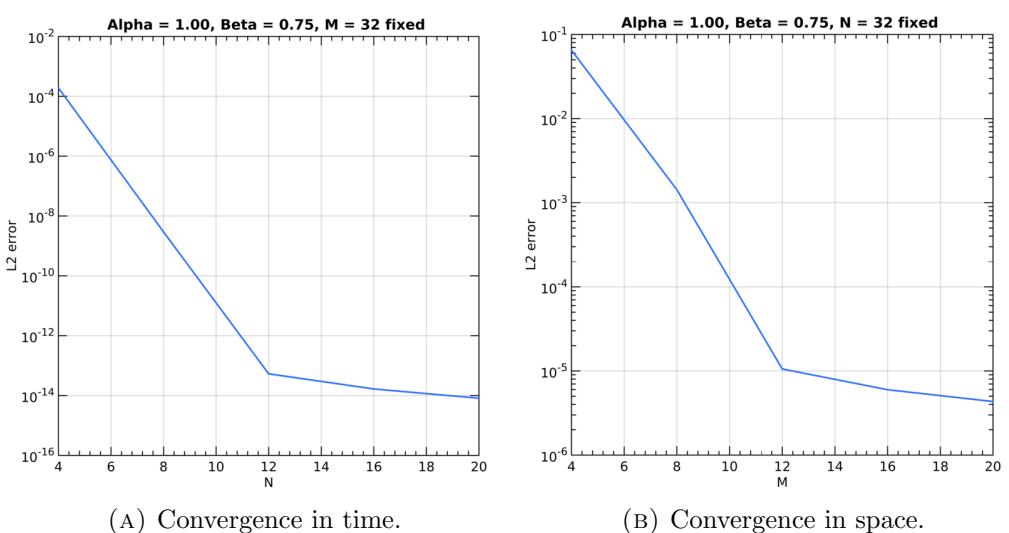
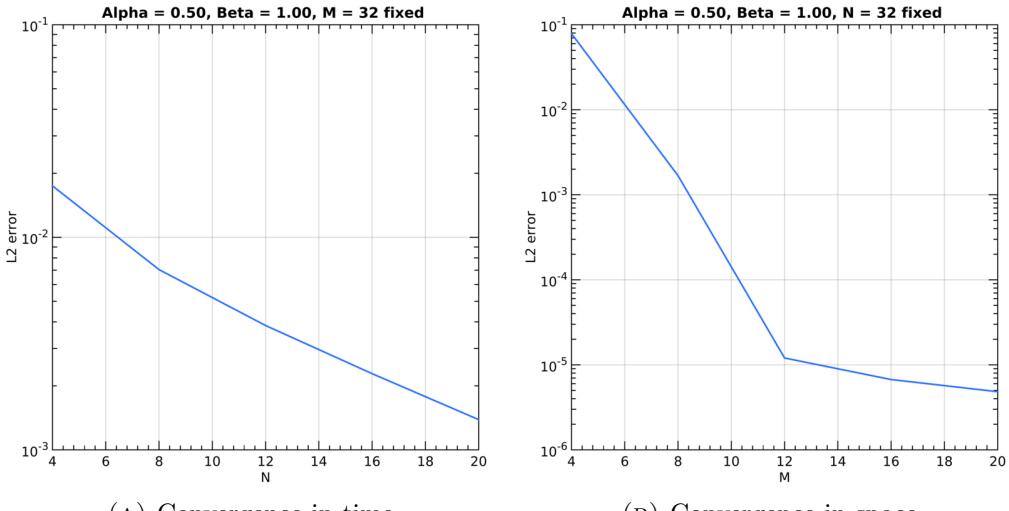


FIGURE 4.13: Solution  $u(x, t)$  of the diffusion equation for different values of  $\alpha$  and  $2\beta$ .

Since our method is spectral in space and time, respectively, we also expect spectral convergence of the solution in both cases. However, we know that the convergence rate of the spectral Galerkin approach depends on the smoothness of the analytic solution to the problem. Since the initial conditions have discontinuities in the derivative at the periodic boundary, this might be a limiting factor in the convergence rate. From Figure 4.14a up to 4.16b we then see the convergence results in dependency of the temporal expansion order  $N$ , presented in the left column, and the spatial expansion order  $M$  in the right column. The presented cases are a sample of all of the performed simulations from Figure 4.13. We only show the results, for the cases where either one or two derivatives are of fractional order. In Figures 4.14a and 4.14b we set the temporal derivative  $\alpha = 0.5$  and leave the spatial derivative of integer order. In Figures 4.15a and 4.15b, the temporal derivative is the first derivative and we have a fractional derivative in space with  $2\beta = 1.5$ . The last row presents the results for the time and space fractional diffusion equation in Figures 4.16a and 4.16b. We are able to derive several conclusions from the given convergence plots. From the results in Figures 4.14a and 4.16a, the convergence rate in time for the fractional derivative is significantly slower, than for the integer order case in 4.15a where we converge to machine precision for even low values of  $N$ . The results suggest, that for non homogeneous initial conditions, the convergence rate in time is reduced, given  $\alpha \notin \mathbb{N}$ . This behaviour is in agreement with the theoretical analysis if we recall, that for fractional order derivatives, the decay is algebraic and not

exponential. Therefore, any error in the initial conditions is damped slower in the case where  $\alpha = 0.5$ . This is also in agreement with the observations made for the case, where we will later use homogeneous initial conditions, but a right-hand side that is also non zero as for this simulation, shown in Figures 4.22a to 4.24b.

If we now also consider the convergence in space, we observe that the methods converges fast at first, but then flattens out for  $M$  greater 12. This observation can be justified with recalling, that our analytic solution is not smooth enough, due to discontinuities in the derivatives at the periodic boundary. On the other hand we note, that the convergence rate is almost independent of the order of the derivative in space, which means, that our method is able to recover solutions for fractional spatial order derivatives in the same quality as for the integer order case.



To support our claim, that the spatial convergence rate is reduced due to discontinuities in the solution, we consider initial conditions that allow a smoother solution in the next case. If we multiply the original initial conditions with  $x^k(2\pi - x)^k$  we obtain smooth derivatives at the boundary up to order  $k$ . This smoothed initial conditions can be seen

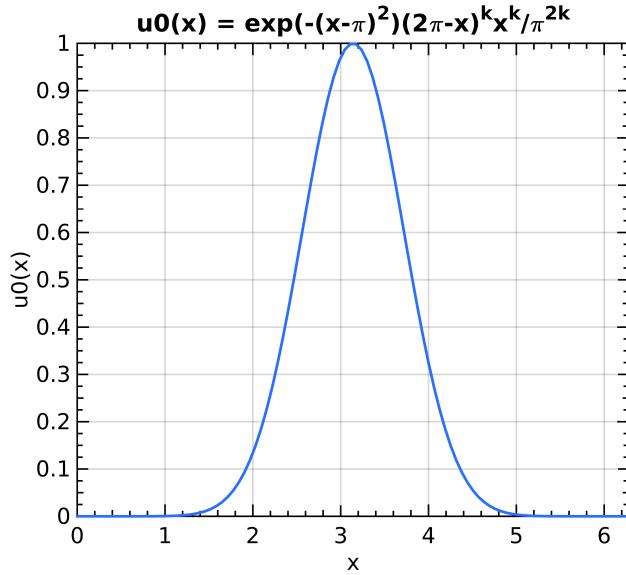
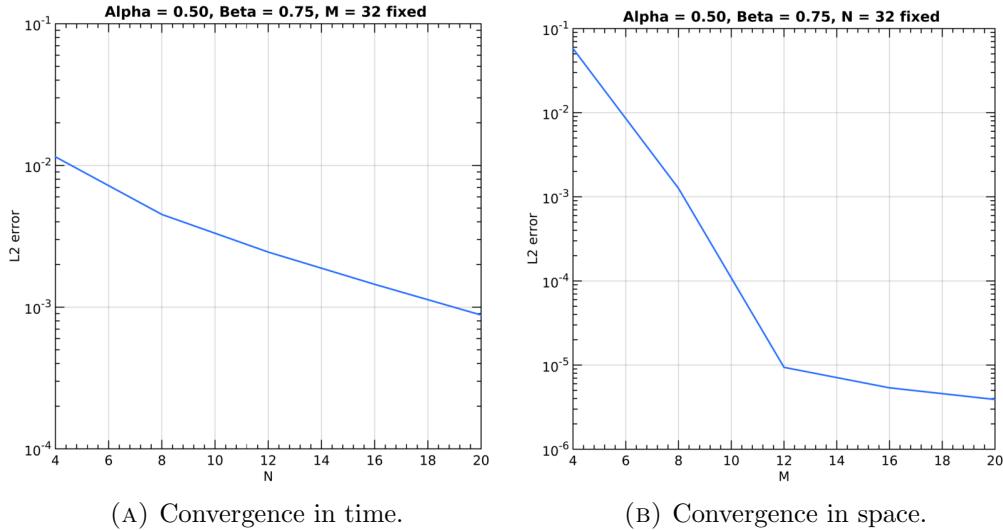
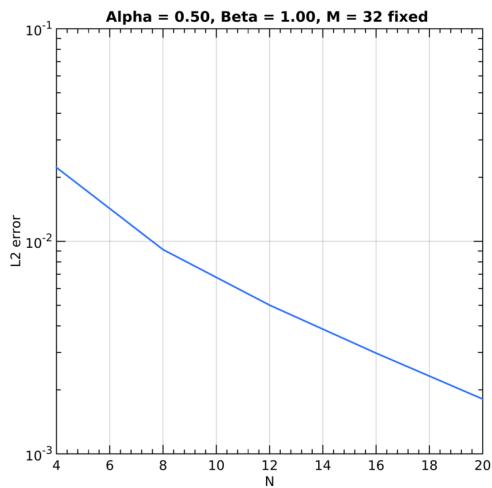


FIGURE 4.17: Initial conditions with continuous derivatives at the periodic boundary for  $k = 5$ .

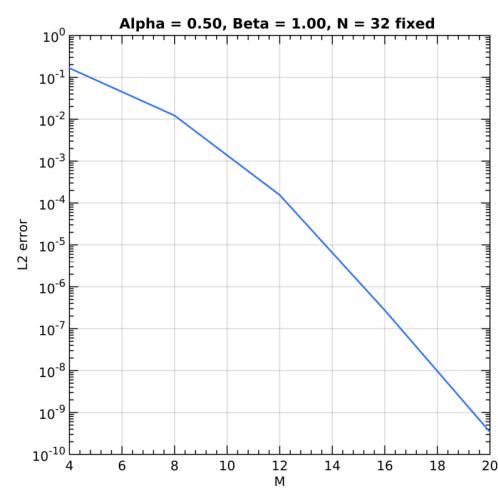
in Figure 4.17, where we also scale the initial conditions with  $(2\pi)^{-k}$  to keep the order of magnitude of the solution.

The results for this modified problem are then presented in Figures 4.18a up to 4.20b. Since we do not introduce a new time-dependent quantity, the convergence in time remains unchanged in comparison with the original problem. However, for the convergence in space, we no observe spectral convergence throughout all expansion orders  $M$ . Again, the convergence in space is independent of the value for  $\beta$ .

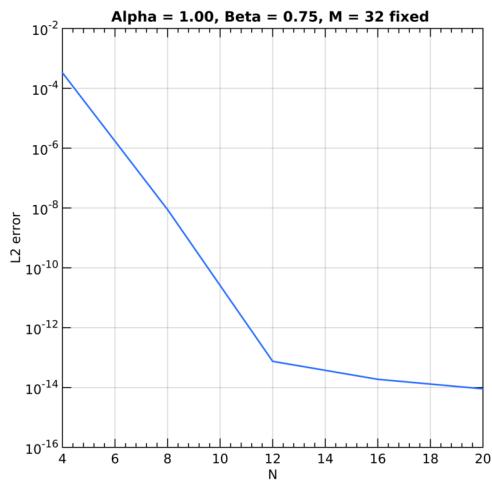
To obtain faster spectral convergence in time, we now consider a case with solution  $u(x, t)$  that fulfils  $u(x, 0) \equiv 0$ . This can be achieved, by introducing homogeneous initial conditions with a right-hand side  $f(x, t)$  that also satisfies  $f(x, 0) \equiv 0$ . In this example, we consider the case where we use a right-hand side  $f(x, t)$  that combines the smoothed



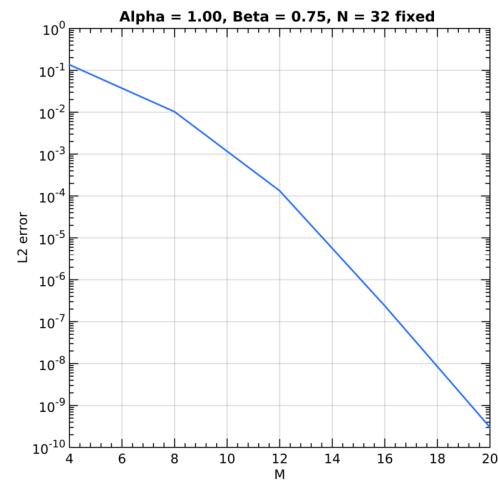
(A) Convergence in time.



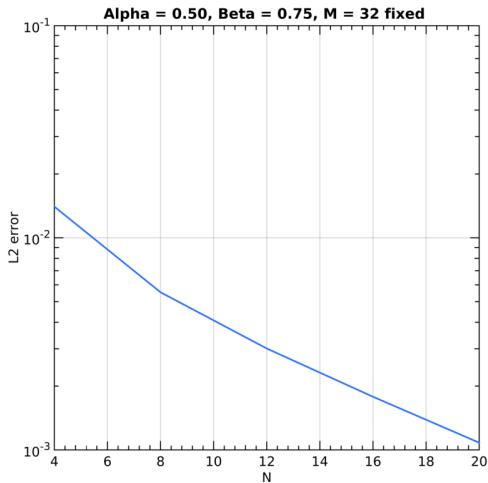
(B) Convergence in space.



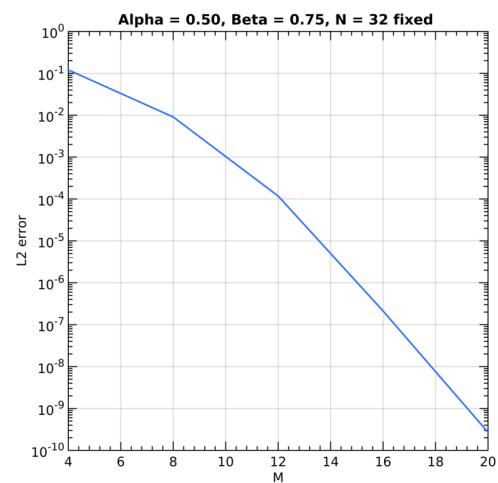
(A) Convergence in time.



(B) Convergence in space.



(A) Convergence in time.



(B) Convergence in space.

initial conditions with forcing term to set  $f(x, 0) \equiv 0$ . One possible  $f(x, t)$  that satisfies these requirements is given by

$$f(x, t) = t^k(T - t)^k \cdot x^k(2\pi - x)^k \exp(-(x - \pi)^2), \quad (4.106)$$

and is visualized in Figure 4.21. The convergence results for this computation are given in Figures 4.22a up to 4.24b. We note, that the convergence in space stays almost unchanged. However, for the convergence in time we now observe much faster spectral convergence, due to the fact that our solution vanishes for  $t = 0$ . Comparing Figures 4.22a and 4.24a to 4.23a, we still observe faster convergence for the integer order derivative case. A possible, heuristic explanation for this might be given, by considering fundamental property of fractional derivatives. Since integer order derivatives are local operators and fractional derivatives operate globally, this also influences the way that errors are propagated throughout the domain.

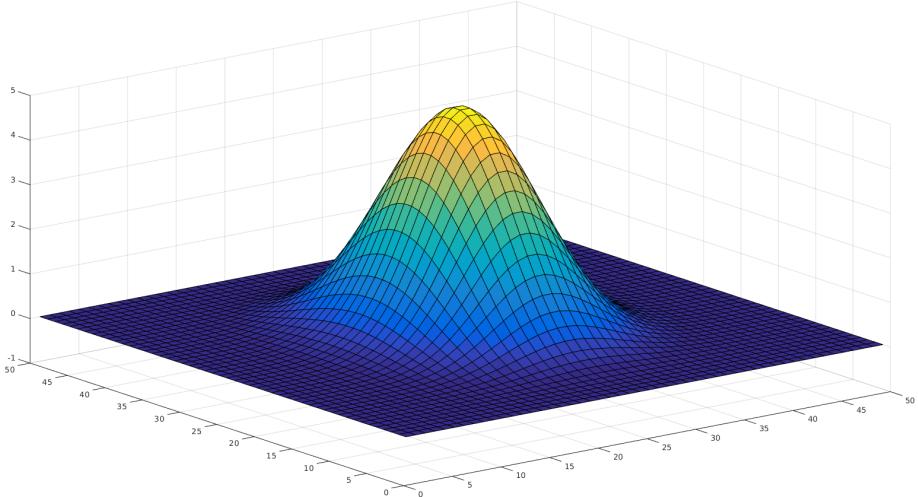
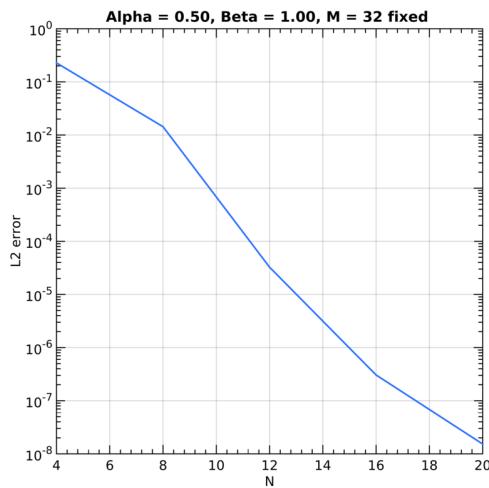
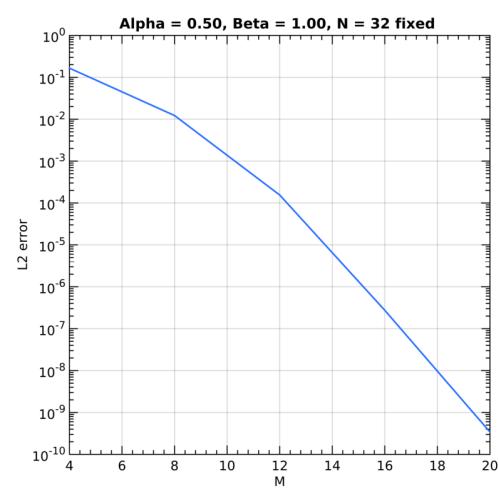


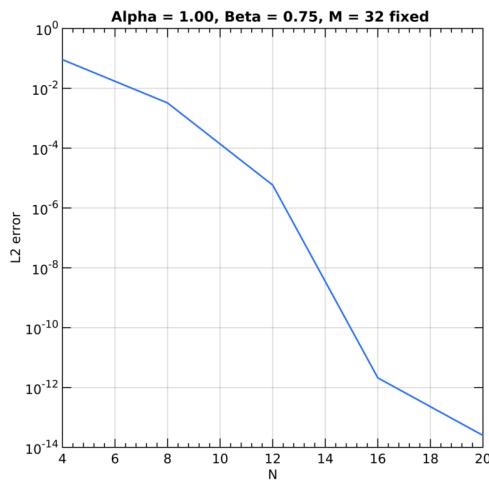
FIGURE 4.21: Smooth right hand side with zero values on spatial and temporal boundaries.



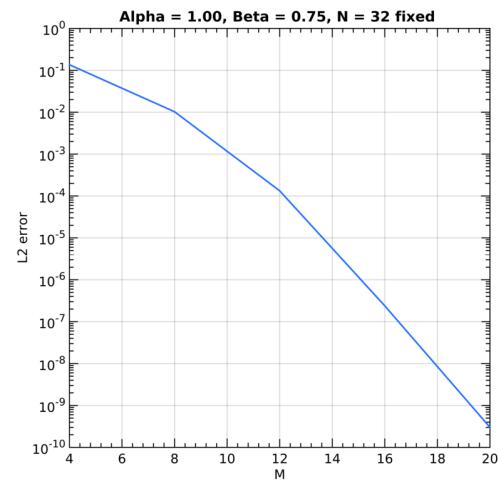
(A) Convergence in time.



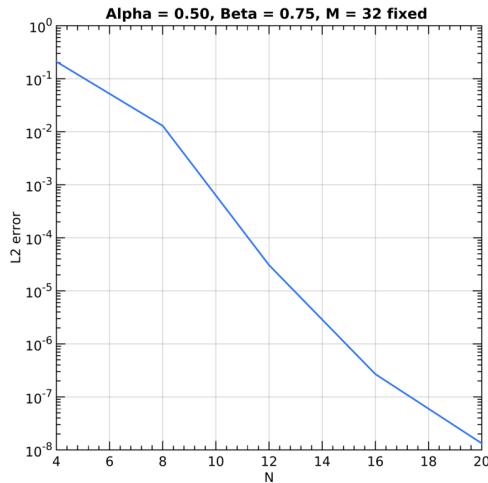
(B) Convergence in space.



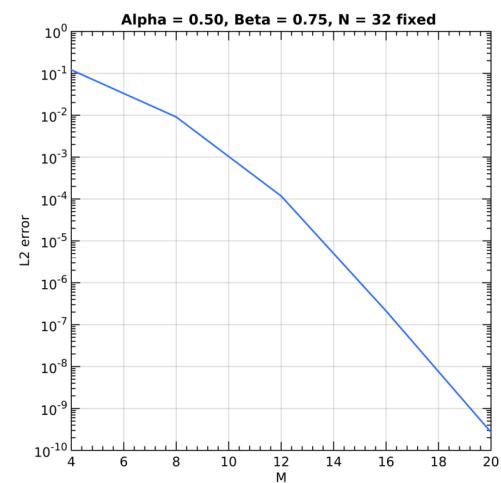
(A) Convergence in time.



(B) Convergence in space.



(A) Convergence in time.



(B) Convergence in space.

*Remark 4.7.* Since the theoretical analysis of the spectral fractional Galerkin methods assumes, that  $\alpha/2 \in (0, 1)$  and not  $\alpha \in (0, 1)$ , we can approach values of  $\alpha = 2$  arbitrary close. However, for  $\alpha = 2$  the method breaks down, since the Jacobi polynomials are not defined for this case. Setting  $\alpha = 1.999$  and  $2\beta = 2$ , we approach the classical wave equation  $\partial_{tt}u(x, t) - \partial_{xx}u(x, t) = f(x, t)$ . For the case of zero source term and sinusoidal initial conditions, the solution of the system is given in Figure 4.25 and for a higher frequency of the initial conditions and a longer domain in time in Figure 4.26.

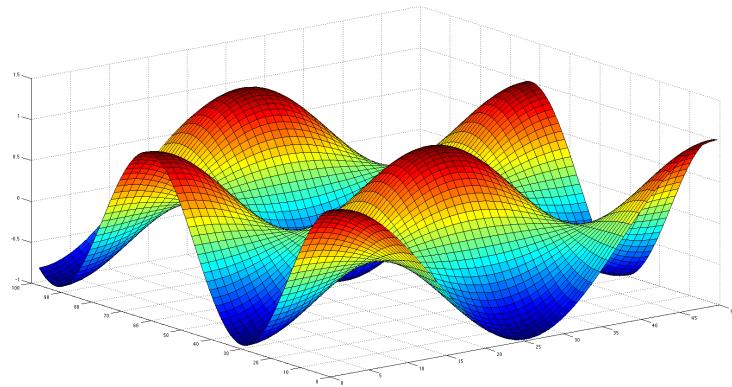


FIGURE 4.25: Approaching the solution of the wave equation.

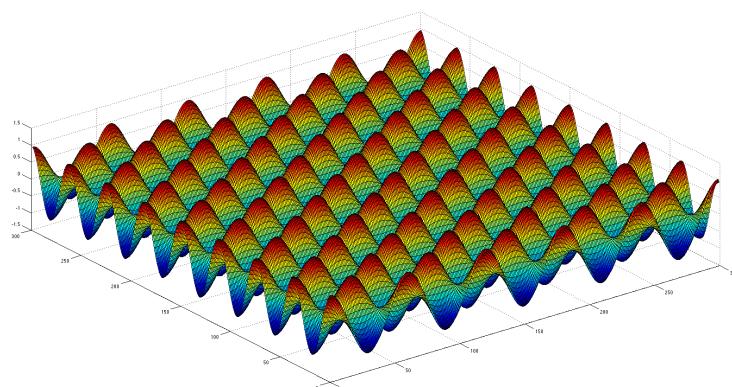


FIGURE 4.26: Approaching the solution of the wave equation.

# 5

## Summary and Outlook

With this work, an introduction into the theoretical and numerical concepts of fractional partial differential equations, especially fractional diffusion equations was given. By first considering the derivation of classical diffusion by random walks, we were able to point out the underlying assumptions, that differ, when deriving the concept of fractional diffusion. By switching from exponential decay in the waiting time and path length distributions to algebraic decay in the asymptotic expansion, we could formulate the Fourier-Laplace transform of the underlying differential equations, whose inversion yields the fractional derivatives in time and space, respectively. The relevant existing definitions of fractional derivatives according to Riemann-Liouville and Caputo are presented, analyzed and compared. In this context, we also provide a profound background in the area of fractional calculus with the relevant non classical function definitions and rules for computing when dealing with fractional derivatives or integrals. The theoretical background is then used to analyze and implement three different numerical algorithms for the solution of fractional diffusion equations in different settings. The extension of the finite difference method by Souse & Li applies the standard second order finite difference approximation to the fractional integrals to derive the differentiation matrix of fractional order. Since fractional operators are global operators the resulting linear systems are dense systems. We were able to show, that the algorithm is of second order

accuracy in space as well as first or second order in time, depending of the weights associated with the explicit and implicit time steps.

Due to the global nature of the differential operators, we considered a global method next. The pseudo spectral collocation method by Zayernouri & Karniadakis was analyzed and implemented. By choosing the appropriate basis for the polynomial expansion in time and space and with the right choice of collocation points, the solution of the resulting system showed spectral convergence in the number of expansion polynomials. By choosing polynomials that are eigenfunctions with respect to the fractional operators, the relevant differentiation matrices for the temporal derivatives, as well as for the derivatives corresponding to the advection and diffusion terms were derived. The explicit calculation of the scalar products for the projection was bypassed by the approximation via collocation points and weights.

Finally, we were able to extend the fully spectral algorithm of Li & Xu for the solution of the time fractional diffusion equations to obtain a spectral algorithm that is able to solve time and space fractional diffusion equations. This has been realized by introducing the complex Fourier basis polynomials for the expansion in space. Due to their property of being eigenfunctions to the differential operator, the Galerkin approach could be implemented without having to compute the required scalar products for the projection of the residual. Spectral convergence was achieved in both, space and time expansion of the solution. We have seen, that the convergence rate depends on the smoothness of the analytic solution, which is in agreement with theoretical predictions.

For future work, we plan to further investigate the underlying physical causes that contribute to the algebraic decaying distributions, used for the derivation of the fractional differential equations. Extending the implemented numerical algorithms to work with a greater class of problem settings, as well as with a more flexible choice of basis functions is also highly desirable. Furthermore, it is of interest to apply the derived numerical methods to the solution of real world problems, which will require a more performance oriented implementation of the presented algorithms.

# A

## Appendix

### A.1 Extension to higher order convergence in space

In the following, we are going to extend the convergence results from Sousa & Li<sup>[51]</sup> from 2nd order convergence in space to 4th order. The presented lemmata, theorems and proofs are derived by applying higher order stencils and splines to the procedure, that Sousa & Li followed to prove their results.

According to Riemann-Liouville, we have the fractional derivative as

$$\frac{\partial^\alpha}{\partial x^\alpha} u(x, t) = \frac{1}{\Gamma(2 - \alpha)} \frac{\partial^2}{\partial x^2} \int_{-\infty}^x u(\xi, t) (x - \xi)^{1-\xi} d\xi, \quad 1 < \alpha < 2, \quad (\text{A.1})$$

and define

$$\mathcal{I}_\alpha(x) = \int_{-\infty}^x u(\xi, t) (x - \xi)^{1-\xi} d\xi, \quad 1 < \alpha < 2. \quad (\text{A.2})$$

Thus we want to approximate the 2nd derivative of  $\mathcal{I}_\alpha(x)$  to get the fractional derivative of  $u(x, t)$ .

*Lemma A.1.* To approximate the second derivative of  $\mathcal{I}_\alpha$  at  $x_j$  with error of order  $\mathcal{O}(\Delta x^4)$  we can use the following 5-point stencil.

$$\frac{\partial^2}{\partial x^2} \mathcal{I}_\alpha(x_j) \approx \frac{1}{12\Delta x^2} (-\mathcal{I}_\alpha(x_{j-2}) + 16\mathcal{I}_\alpha(x_{j-1}) - 30\mathcal{I}_\alpha(x_j) + 16\mathcal{I}_\alpha(x_{j+1}) - \mathcal{I}_\alpha(x_{j+2})). \quad (\text{A.3})$$

*Proof.* Use Taylor expansion or provided proofs throughout the literature<sup>[63,64]</sup>.

*Lemma A.2.* A cubic hermite spline  $s$  approximates a function  $u \in C^4$  with order  $\mathcal{O}(\Delta x^4)$ , i.e.

$$\|u - s\|_\infty \leq \frac{1}{16} \Delta x^4 \|u^{(4)}\|. \quad (\text{A.4})$$

*Proof.* A proof is given by Arnold<sup>[65]</sup>.

*Definition A.3.* A cubic Hermite spline is a composition of four Hermite basis functions of the form

$$\mathbf{p}(x) = h_{00}(t)\mathbf{p}_k + h_{10}(t)(x_{k+1} - x_k)\mathbf{m}_k + h_{01}(t)\mathbf{p}_{k+1} + h_{11}(t)(x_{k+1} - x_k)\mathbf{m}_{k+1}. \quad (\text{A.5})$$

where  $h_{ij}$  are the Hermite basis functions and  $p_k, p_{k+1}, m_k, m_{k+1}$  the interpolation points and derivatives<sup>1</sup>.

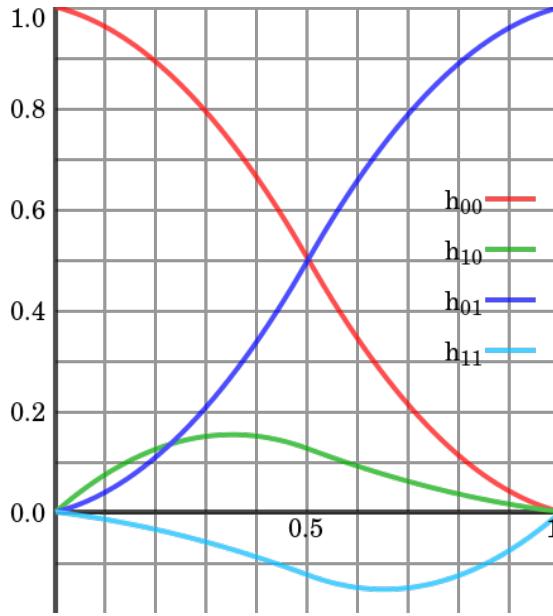


FIGURE A.1: Hermite basis functions.

<sup>1</sup>Image taken from [http://en.wikipedia.org/wiki/Cubic\\_Hermite\\_spline](http://en.wikipedia.org/wiki/Cubic_Hermite_spline)

When we replace the  $m_k$  and  $m_{k+1}$  by a finite difference approximation, we obtain the following basis functions

$$g_{k,m}(x) = \begin{cases} -h_{10}(t)/2 & m = -1, \\ h_{00}(t) - h_{11}(t)/2 & m = 0, \\ h_{10}(t) + h_{01}(t) & m = 1, \\ h_{11}(t)/2 & m = 2. \end{cases} \quad (\text{A.6})$$

with  $t = (x - x_k)/(x_{k+1} - x_k)$ .

The cubic hermite spline  $s_j(\xi)$  that interpolates the points  $\{x_k, t\}$ ,  $k \leq j$  is then defined as

$$s_j(\xi) = \sum_{k=-\infty}^j t_{j,k}(\xi) \quad \text{with} \quad (\text{A.7})$$

$$t_{j,k}(\xi) = \sum_{m=-1}^2 g_{k,m}(\xi) u(x_{k+m-1}) \cdot \mathbb{I}_{[x_k, x_{k+1}]}(x), \quad (\text{A.8})$$

where  $\mathbb{I}$  is the indicator function for the specific interval.

*Lemma A.4.* For  $u \in C^{(6)}$  and for  $\xi \in [x_{k-1}, x_k]$  and  $\eta_k \in [x_{k-1}, x_k]$  we can use Taylor expansion to derive

$$u(\xi) - t_{j,k}(\xi) = - \sum_{r=4}^5 \frac{1}{r!} u^{(r)}(\xi) l_{k,r}(\xi) - \frac{1}{6!} u^{(6)}(\eta_k) l_{k,6}(\xi). \quad (\text{A.9})$$

with  $|l_{k,r}| \leq \Delta x^r$ .

*Definition A.5.*  $I_\alpha(x_j)$  approximates  $\mathcal{I}_\alpha(x_j)$  by the use of the cubic spline  $s_j(\xi)$  via

$$I_\alpha(x_j) = \int_{-\infty}^{x_j} s_j(\xi) (x_j - \xi)^{1-\alpha} d\xi \quad (\text{A.10})$$

$$= \int_{-\infty}^{x_j} \sum_{k=-\infty}^j t_{j,k}(\xi) (x_j - \xi)^{1-\alpha} d\xi \quad (\text{A.11})$$

$$= \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} t_{j,k}(\xi) (x_j - \xi)^{1-\alpha} d\xi, \quad (\text{A.12})$$

since the  $t_{j,k}$  are only non zero in  $[x_{k-1}, x_k]$ .

*Theorem A.6.* (Order of the approximation of for the fractional derivative)

Let  $1 < \alpha \leq 2$  and let  $u \in C^{(6)}(\mathbb{R})$  such that  $u^{(6)}(x) = 0$  for  $x \leq a$  with a real constant  $a$ , then

$$\frac{\partial^\alpha}{\partial x^\alpha} \mathcal{I}_\alpha(x_j) - \frac{\delta^\alpha u}{\Delta x^\alpha} = \epsilon_1(x_j) + \epsilon_2(x_j), \quad (\text{A.13})$$

with

$$\frac{\delta^\alpha u}{\Delta x^\alpha} = \frac{1}{12\Delta x^2} (-I_\alpha(x_{j-2}) + 16I_\alpha(x_{j-1}) - 30I_\alpha(x_j) + 16I_\alpha(x_{j+1}) - I_\alpha(x_{j+2})), \quad (\text{A.14})$$

and

$$|\epsilon_1(x_j)| \leq C_1 \Delta x^4, \quad (\text{A.15})$$

$$|\epsilon_2(x_j)| \leq C_2 \Delta x^4. \quad (\text{A.16})$$

*Proof.* For notation define  $S(f)(x_j)$  as the 5-point stencil above, i.e.

$$S(f)(x_j) = \frac{1}{12} (-f(x_{j-2}) + 16f(x_{j-1}) - 30f(x_j) + 16f(x_{j+1}) - f(x_{j+2})). \quad (\text{A.17})$$

For  $1 < \alpha \leq 2$  we have

$$\frac{\partial^\alpha}{\partial x^\alpha} \mathcal{I}_\alpha(x_j) = \frac{1}{\Gamma(2-\alpha)} \mathcal{I}_\alpha(x_j) = \frac{1}{\Gamma(2-\alpha)} \frac{1}{\Delta x^2} S(\mathcal{I}_\alpha)(x_j) + \epsilon_1(x_j), \quad (\text{A.18})$$

with  $\epsilon_1(x_j) \in \mathcal{O}(\Delta x^4)$  according to Lemma(A.1).

Now define  $E_s(x_j)$  to be the error due to the spline approximation, i.e.

$$S(\mathcal{I}_\alpha)(x_j) = S(I_\alpha)(x_j) + E_s(x_j). \quad (\text{A.19})$$

Inserting equation (A.19) into equation (A.20), we obtain

$$\frac{\partial^\alpha}{\partial x^\alpha} \mathcal{I}_\alpha(x_j) = \frac{1}{\Gamma(2-\alpha)} \frac{1}{\Delta x^2} S(I_\alpha)(x_j) + \frac{1}{\Gamma(2-\alpha)} \frac{1}{\Delta x^2} E_s(x_j) + \epsilon_1(x_j). \quad (\text{A.20})$$

and define  $\epsilon_2(x_j) = \frac{1}{\Gamma(2-\alpha)} \frac{1}{\Delta x^2} E_s(x_j)$ . To complete the proof, we now have to show that  $E_s(x_j) \in \mathcal{O}(\Delta x^6)$ . By definition,  $E_s(x_j) = S(\mathcal{I}_\alpha)(x_j) - S(I_\alpha)(x_j) = S(\mathcal{I}_\alpha(x_j) - I_\alpha(x_j))$  since  $S$  is a linear operator. We will start with the computation of  $\mathcal{I}_\alpha(x_j) - I_\alpha(x_j)$ .

Omitting the time dependency, we have

$$\mathcal{I}_\alpha(x_j) - I_\alpha(x_j) = \int_{-\infty}^{x_j} u(\xi)(x_j - \xi)^{1-\alpha} d\xi - \int_{-\infty}^{x_j} s_j(\xi)(x_j - \xi)^{1-\alpha} d\xi \quad (\text{A.21})$$

$$= \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} u(\xi)(x_j - \xi)^{1-\alpha} d\xi - \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} t_{j,k}(\xi)(x_j - \xi)^{1-\alpha} d\xi \quad (\text{A.22})$$

$$= \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} (u(\xi) - t_{j,k}(\xi)) (x_j - \xi)^{1-\alpha} d\xi. \quad (\text{A.23})$$

Applying lemma (A.4), we get

$$\mathcal{I}_\alpha(x_j) - I_\alpha(x_j) = - \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} \left[ \sum_{r=4}^5 \frac{1}{r!} u^{(r)}(\xi) l_{k,r}(\xi) - \frac{1}{6!} u^{(6)}(\eta_k) l_{k,6}(\xi) \right] (x_j - \xi)^{1-\alpha} d\xi \quad (\text{A.24})$$

$$=: -E_4(x_j) - E_5(x_j) - E_6(x_j), \quad (\text{A.25})$$

with

$$E_i(x_j) = \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} \frac{1}{i!} u^{(i)}(\xi) l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} d\xi, \quad (\text{A.26})$$

for  $i = 4, 5$  and for  $i = 6$

$$E_6(x_j) = \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} \frac{1}{6!} u^{(6)}(\eta_k) l_{k,6}(\xi) (x_j - \xi)^{1-\alpha} d\xi. \quad (\text{A.27})$$

Thus our error  $E_s(x_j)$  is given by

$$E_s(x_j) = S(-E_4(x_j) - E_5(x_j) - E_6(x_j)) \quad (\text{A.28})$$

$$= -S(E_4(x_j)) - S(E_5(x_j)) - S(E_6(x_j)) \quad (\text{A.29})$$

$$=: -E_4^s(x_j) - E_5^s(x_j) - E_6^s(x_j). \quad (\text{A.30})$$

We will now compute the  $E_i^s$  and show, that they are of required order.

For  $i = 4, 5$  we have

$$-i! S(E_i(x_j)) = S \left( \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} u^{(i)}(\xi) l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} d\xi \right) \quad (\text{A.31})$$

$$= -\frac{1}{12} \sum_{k=-\infty}^{j-2} \int_{x_{k-1}}^{x_k} u^{(i)}(\xi) l_{k,i}(\xi) (x_{j-2} - \xi)^{1-\alpha} d\xi \quad (\text{A.32})$$

$$\begin{aligned} &+ \frac{4}{3} \sum_{k=-\infty}^{j-1} \int_{x_{k-1}}^{x_k} u^{(i)}(\xi) l_{k,i}(\xi) (x_{j-1} - \xi)^{1-\alpha} d\xi \\ &- \frac{5}{2} \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} u^{(i)}(\xi) l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} d\xi \\ &+ \frac{4}{3} \sum_{k=-\infty}^{j+1} \int_{x_{k-1}}^{x_k} u^{(i)}(\xi) l_{k,i}(\xi) (x_{j+1} - \xi)^{1-\alpha} d\xi \\ &- \frac{1}{12} \sum_{k=-\infty}^{j+2} \int_{x_{k-1}}^{x_k} u^{(i)}(\xi) l_{k,i}(\xi) (x_{j+2} - \xi)^{1-\alpha} d\xi. \end{aligned}$$

A change of variable in  $\xi$  yields

$$-i! S(E_i(x_j)) = -\frac{1}{12} \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} u^{(i)}(\xi - 2\Delta x) l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} d\xi \quad (\text{A.33})$$

$$\begin{aligned} &+ \frac{4}{3} \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} u^{(i)}(\xi - \Delta x) l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} d\xi \\ &- \frac{5}{2} \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} u^{(i)}(\xi) l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} d\xi \\ &+ \frac{4}{3} \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} u^{(i)}(\xi + \Delta x) l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} d\xi \\ &- \frac{1}{12} \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} u^{(i)}(\xi + 2\Delta x) l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} d\xi \\ &= \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} \left[ -\frac{1}{12} u^{(i)}(\xi - 2\Delta x) \right. \\ &\quad \left. + \frac{4}{3} u^{(i)}(\xi - \Delta x) - \frac{5}{2} u^{(i)}(\xi) \right. \\ &\quad \left. - \frac{1}{12} u^{(i)}(\xi + \Delta x) + \frac{4}{3} u^{(i)}(\xi + 2\Delta x) \right] d\xi \quad (\text{A.34}) \end{aligned}$$

$$= \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} \left[ \Delta x^2 u^{(i+2)}(\xi) + \mathcal{O}(\Delta x^6) \right] d\xi \quad (\text{A.35})$$

$$= \Delta x^2 \sum_{k=N_a+1}^j u^{(i+2)}(\xi_k) c_{j,k,i} + \mathcal{O}(\Delta x^6), \quad (\text{A.36})$$

where we assume, that  $u^{(i+2)}(x) \equiv 0, \forall x \leq x_a$  and  $c_{j,k,i} = \int_{x_{k-1}}^{x_k} l_{k,i}(\xi) (x_j - \xi)^{1-\alpha} d\xi$ . By lemma (A.4) we can bound

$$|c_{j,k,i}| \leq \Delta x^i \int_{x_{k-1}}^{x_k} (x_j - \xi)^{1-\alpha} d\xi \quad (\text{A.37})$$

$$\leq \Delta x^i \frac{1}{2-\alpha} (x_j - x_a)^{2-\alpha}, \quad (\text{A.38})$$

yielding for  $i = 4, 5$

$$|E_i(x_j)| \leq C \Delta x^6 \|u^{(i+2)}\|_\infty (x_j - x_a)^{2-\alpha}. \quad (\text{A.39})$$

For the case  $i = 6$ , we bound the different terms in  $E_6^s(x_j)$ , i.e. for  $\kappa = -2, \dots, 2$

$$|E_6(x_{j+\kappa})| = \left| \sum_{k=-\infty}^{j+\kappa} \int_{x_{k-1}}^{x_k} \frac{1}{6!} u^{(6)}(\eta_k) l_{k,6}(\xi) (x_{j+\kappa} - \xi)^{1-\alpha} d\xi \right| \quad (\text{A.40})$$

$$\leq \frac{1}{\Delta x^6} \frac{1}{6!} \|u^{(6)}\|_\infty \sum_{k=N_a+1}^{j+\kappa} \int_{x_{k-1}}^{x_k} |(x_{j-\kappa} - \xi)^{1-\alpha}| d\xi \quad (\text{A.41})$$

$$\leq \frac{1}{\Delta x^6} \frac{1}{6!} \|u^{(6)}\|_\infty \frac{1}{2-\alpha} (x_{j+\max(\kappa)} - x_a)^{2-\alpha}, \quad (\text{A.42})$$

which is of order  $\mathcal{O}(\Delta x^6)$  for every possible  $\kappa$ .

Thus  $E_s(x_j) \in \mathcal{O}(\Delta x^6)$ , implying  $\epsilon_2(x_j) \in \mathcal{O}(\Delta x^4)$ , which proves theorem (A.6).  $\square$



## Bibliography

- [1] Helmut Mehrer and Nicolaas A Stolwijk. Heroes and highlights in the history of diffusion. 2009.
- [2] Jean Philibert. One and a half century of diffusion: Fick, einstein, before and beyond. *Diffusion Fundamentals*, 4(6.1-6.19):146, 2006.
- [3] Jurica Hižak and Robert Logožar. A derivation of the mean absolute distance in one-dimensional random walk. *Tehnički glasnik*, 5(1):10–16, 2011.
- [4] Albert Einstein. On the movement of small particles suspended in a stationary liquid demanded by the molecular-kinetic theory of heat. *Annalen der physik*, 17: 549–560, 1905.
- [5] Langlands Henry and Straka. An introduction to fractional diffusion. 2010.
- [6] Bertram Ross. A brief history and exposition of the fundamental theory of fractional calculus. In *Fractional calculus and its applications*, pages 1–36. Springer, 1975.
- [7] R Vilela Mendes. Introduction to fractional calculus (based on lectures by r. gorenflo, f. mainardi and i. podlubny). 2008.
- [8] Bextram Ross Kenneth S. Miller. *An introduction to the fractional calculus and fractional differential equations*. Higb Wukey and Sons, Inc., 1993. ISBN 0-471-58884-9.
- [9] Mehdi Delkhosh. Introduction of Derivatives and Integrals of Fractional Order and Its Applications. *Applied Mathematics and Physics*, 1(4):103–119, January 2013. doi: 10.12691/amp-1-4-3. URL <http://pubs.sciepub.com/amp/1/4/3/index.html>.
- [10] H. J. Haubold, A. M. Mathai, and R. K. Saxena. Mittag-Leffler Functions and Their Applications. *ArXiv e-prints*, September 2009.
- [11] H.J. Seybold and R. Hilfer. Numerical results for the generalized mittag-leffler function. *Fractional Calculus and Applied Analysis*, 8(2):127–139, 2005.

- [12] Rudolf Gorenflo, Yuri Luchko, and Francesco Mainardi. Analytical properties and applications of the wright function. *arXiv preprint math-ph/0701069*, 2007.
- [13] R. Gorenflo and F. Mainardi. Fractional Calculus: Integral and Differential Equations of Fractional Order. *ArXiv e-prints*, May 2008.
- [14] Changpin Li, Deliang Qian, and YangQuan Chen. On riemann-liouville and caputo derivatives. *Discrete Dynamics in Nature and Society*, 2011:15, 2011. URL <http://dx.doi.org/10.1155/2011/562494>.
- [15] Changpin Li and Weihua Deng. Remarks on fractional derivatives. *Applied Mathematics and Computation*, 187(2):777–784, 2007. doi: 10.1016/j.amc.2006.08.163. URL <http://dx.doi.org/10.1016/j.amc.2006.08.163>.
- [16] Manuel Duarte Ortigueira and Fernando Coito. From differences to derivatives. *Fractional Calculus and Applied Analysis*, 7(4):459, 2004.
- [17] J.B. Diaz and T.J. Osler. Differences of fractional order. *Mathematics of Computation*, 28(125):185–202, 1974.
- [18] Marie Christine Neel and Maminirina Joelson. Generalizing grünwald-letnikov’s formulas for fractional derivatives. 2011.
- [19] X. Ros-Oton and J. Serra. The extremal solution for the fractional Laplacian. *ArXiv e-prints*, May 2013.
- [20] X. Ros-Oton and J. Serra. The Dirichlet problem for the fractional Laplacian: regularity up to the boundary. *ArXiv e-prints*, July 2012.
- [21] Rudolf Hilfer et al. Threefold introduction to fractional derivatives. *Anomalous transport: Foundations and applications*, pages 17–73, 2008.
- [22] Dr. Lee G. Mundy. Fourier transform properites and pairs. University of Maryland, 2010. URL [http://www.astro.umd.edu/~lgm/ASTR410/ft\\_ref2.pdf](http://www.astro.umd.edu/~lgm/ASTR410/ft_ref2.pdf).
- [23] Dr. Lee G. Mundy. And more fourier transform properites. University of Maryland, 2010. URL [http://www.astro.umd.edu/~lgm/ASTR410/ft\\_ref3.pdf](http://www.astro.umd.edu/~lgm/ASTR410/ft_ref3.pdf).
- [24] R.N. Bracewell. *The Fourier Transform and Its Applications*. Electrical engineering series. McGraw Hill, 2000. ISBN 9780073039381. URL <http://books.google.com.tr/books?id=ZNQQAQAAIAAJ>.
- [25] H. Meikle. *A New Twist to Fourier Transforms*. Wiley, 2004. ISBN 9783527404414. URL <http://books.google.com.tr/books?id=I3I2N5BY50kC>.

- [26] Eric W. Weisstein. Laplace transform. From MathWorld—A Wolfram Web Resource. URL <http://mathworld.wolfram.com/LaplaceTransform.html>. Last visited on 2014/8/19.
- [27] Brian Davies and Brian Martin. Numerical inversion of the laplace transform: a survey and comparison of methods. *Journal of Computational Physics*, 33(1):1 – 32, 1979. ISSN 0021-9991. doi: [http://dx.doi.org/10.1016/0021-9991\(79\)90025-1](http://dx.doi.org/10.1016/0021-9991(79)90025-1). URL <http://www.sciencedirect.com/science/article/pii/0021999179900251>.
- [28] J.L. Schiff. *The Laplace Transform: Theory and Applications*. Springer Undergraduate Texts in Mathematics and Technology. Springer, 1999. ISBN 9780387986982. URL <http://books.google.de/books?id=RU-5jSP1KMcc>.
- [29] P.P.G. Dyke. *An Introduction to Laplace Transforms and Fourier Series: With 51 Figures*. Springer Undergraduate Mathematics Series. Springer London, 1999. ISBN 9781852330156. URL <http://books.google.de/books?id=vx2G2BHPMLUc>.
- [30] G. M. Viswanathan, V. Afanasyev, S. V. Buldyrev, E. J. Murphy, P. A. Prince, and H. E. Stanley. Levy flight search patterns of wandering albatrosses. *Nature*, 381(6581):413–415, May 1996. doi: 10.1038/381413a0. URL <http://dx.doi.org/10.1038/381413a0>.
- [31] B. B. Mandelbrot. *The Fractal Geometry of Nature*. Freeman, 1968.
- [32] Ido Almog Nir Davidson Yoav Sagi, Miri Brook. Observation of anomalous diffusion and fractional self-similarity in one dimension. *Phys. Lett.*, Phys. Rev. Lett. 108, 093002 (2012), 2012.
- [33] E. V. Albano and H. O. Martin. Temperature-programmed reactions with anomalous diffusion. *The Journal of Physical Chemistry*, 92(12):3594–3597, 1988. doi: 10.1021/j100323a054. URL <http://pubs.acs.org/doi/abs/10.1021/j100323a054>.
- [34] M. Raberto, G. Cuniberti, M. Riani, E. Scales, F. Mainardi, and G. Servizi. Learning short-option valuation in the presence of rare events. *International Journal of Theoretical and Applied Finance*, 03(03):563–564, 2000. doi: 10.1142/S0219024900000590. URL <http://www.worldscientific.com/doi/abs/10.1142/S0219024900000590>.
- [35] Eva Schumacher Emmanuel Hanert and Eric Deleersnijder. Front dynamics in fractional-order epidemic models. *Journal of Theoretical Biology*, 2010. doi: doi: 10.1016/j.jtbi.2011.03.012.
- [36] E. Scales, R. Gorenflo, F. Mainardi, and M. Raberto. Revisiting the derivation of the fractional diffusion equation. *Fractals*, 11(sup01):281–289, 2003.

- doi: 10.1142/S0218348X0300194X. URL <http://www.worldscientific.com/doi/abs/10.1142/S0218348X0300194X>.
- [37] F. Mainardi, M. Raberto, R. Gorenflo, and E. Scalas. Fractional calculus and continuous-time finance II: the waiting-time distribution. *Physica A Statistical Mechanics and its Applications*, 287:468–481, December 2000. doi: 10.1016/S0378-4371(00)00386-1.
- [38] R. Gorenflo and F. Mainardi. Continuous time random walk, Mittag-Leffler waiting time and fractional diffusion: mathematical aspects. *ArXiv e-prints*, May 2007.
- [39] Rudolf Gorenflo and Francesco Mainardi. Random walk models for space-fractional diffusion processes, 1998.
- [40] Helen Wittenberg. Limiting distributions of random sums of independent random variables. *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete*, 3(1): 7–18, 1964. ISSN 0044-3719. doi: 10.1007/BF00531680. URL <http://dx.doi.org/10.1007/BF00531680>.
- [41] J. Elschner, I. Gohberg, and B. Silbermann. *Problems and Methods in Mathematical Physics: The Siegfried Prössdorf Memorial Volume : Proceedings of the 11th TMP, Chemnitz (Germany), March 25-28, 1999*. Operator theory. Springer, 2001. ISBN 9783764364779. URL <http://books.google.de/books?id=0QhNiAMxVKUC>.
- [42] E. Lukacs. *Characteristic functions*. Griffin's statistical monographs & courses. Hafner Pub. Co., 1960. URL <http://books.google.de/books?id=3xZzdUs9JtcC>.
- [43] Y. Luchko. Fractional wave equation and damped waves. *Journal of Mathematical Physics*, 54(3):031505, March 2013. doi: 10.1063/1.4794076.
- [44] AhmedM.A. El-Sayed. Fractional-order diffusion-wave equation. *International Journal of Theoretical Physics*, 35(2):311–322, 1996. ISSN 0020-7748. doi: 10.1007/BF02083817. URL <http://dx.doi.org/10.1007/BF02083817>.
- [45] F. Mainardi. The fundamental solutions for the fractional diffusion-wave equation. *Applied Mathematics Letters*, 9(6):23 – 28, 1996. ISSN 0893-9659. doi: [http://dx.doi.org/10.1016/0893-9659\(96\)00089-4](http://dx.doi.org/10.1016/0893-9659(96)00089-4). URL <http://www.sciencedirect.com/science/article/pii/0893965996000894>.
- [46] Ralf Metzler and Theo F. Nonnenmacher. Space-and time-fractional diffusion and wave equations, fractional fokker–planck equations, and physical motivation. *Chemical Physics*, 284(1):67–90, 2002.

- [47] Fawang Liu, Mark M Meerschaert, Robert J McGough, Pinghui Zhuang, and Qingxia Liu. Numerical methods for solving the multi-term time-fractional wave-diffusion equation. *Fractional Calculus and Applied Analysis*, 16(1):9–25, 2013.
- [48] Yuan-Ming Wang and Tao Wang. A compact locally one-dimensional method for fractional diffusion-wave equations. *Journal of Applied Mathematics and Computing*, pages 1–27, 2014. ISSN 1598-5865. doi: 10.1007/s12190-014-0823-0. URL <http://dx.doi.org/10.1007/s12190-014-0823-0>.
- [49] Ya-nan Zhang, Zhi-zhong Sun, and Xuan Zhao. Compact alternating direction implicit scheme for the two-dimensional fractional diffusion-wave equation. *SIAM Journal on Numerical Analysis*, 50(3):1535–1555, 2012.
- [50] Jianfei Huang, Yifa Tang, Luis Vázquez, and Jiye Yang. Two finite difference schemes for time fractional diffusion-wave equation. *Numerical Algorithms*, 64(4):707–720, 2013.
- [51] E. Sousa and C. Li. A weighted finite difference method for the fractional diffusion equation based on the Riemann-Liouville derivative. *ArXiv e-prints*, September 2011.
- [52] Igor Podlubny. *Fractional Differential Equations. An Introduction to Fractional Derivatives, Fractional Differential Equations, Some Methods of Their Solution and Some of Their Applications*. Academic Press, San Diego - New York - London, 1999.
- [53] Yumin Lin and Chuanju Xu. Finite difference/spectral approximations for the time-fractional diffusion equation. *Journal of Computational Physics*, 225(2):1533–1552, 2007.
- [54] Mark M Meerschaert and Charles Tadjeran. Finite difference approximations for two-sided space-fractional partial differential equations. *Applied Numerical Mathematics*, 56(1):80–90, 2006.
- [55] H. Zhou, W. Tian, and W. Deng. Compact Finite Difference Approximations for Space Fractional Diffusion Equations. *ArXiv e-prints*, April 2012.
- [56] Diego A. Murio. Implicit finite difference approximation for time fractional diffusion equations. *Computers & Mathematics with Applications*, 56(4):1138 – 1145, 2008. ISSN 0898-1221. doi: <http://dx.doi.org/10.1016/j.camwa.2008.02.015>. URL <http://www.sciencedirect.com/science/article/pii/S0898122108001156>.
- [57] J. Crank and P. Nicolson. A practical method for numerical evaluation of solutions of partial differential equations of the heat-conduction type. *Advances in*

- Computational Mathematics*, 6(1):207–226, 1996. ISSN 1019-7168. doi: 10.1007/BF02127704. URL <http://dx.doi.org/10.1007/BF02127704>.
- [58] Isaac Newton. *The principia: mathematical principles of natural philosophy*. Univ of California Press, 1999.
- [59] Yu.N. Subbotin (originator). Spline interpolation. *Encyclopedia of Mathematics*, 2011. URL [http://www.encyclopediaofmath.org/index.php?title=Spline\\_interpolation&oldid=11892](http://www.encyclopediaofmath.org/index.php?title=Spline_interpolation&oldid=11892).
- [60] Mohsen Zayernouri and George Em Karniadakis. Fractional spectral collocation method. *SIAM Journal on Scientific Computing*, 36(1):A40–A62, 2014.
- [61] Mohsen Zayernouri and George Em Karniadakis. Fractional sturm–liouville eigenproblems: theory and numerical approximation. *Journal of Computational Physics*, 252:495–517, 2013.
- [62] Hongmei Zhang and Fawang Liu. The fundamental solutions of the space, space–time riesz fractional partial differential equations with periodic conditions.
- [63] Bengt Fornberg. Calculation of weights in finite difference formulas. *SIAM Rev*, 40:685–691, 1998.
- [64] Bengt Fornberg. Generation of finite difference formulas on arbitrarily spaced grids. *Mathematics of computation*, 51(184):699–706, 1988.
- [65] Douglas N Arnold. A concise introduction to numerical analysis. 2001.