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The Grünwald–Letnikov method for fractional differential equations

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ABSTRACT

This paper is devoted to the numerical treatment of fractional differential equations. Based on the Grünwald–Letnikov definition of fractional derivatives, finite difference schemes for the approximation of the solution are discussed. The main properties of these explicit and implicit methods concerning the stability, the convergence and the error behavior are studied related to linear test equations. The asymptotic stability and the absolute stability of these methods are proved. Error representations and estimates for the truncation, propagation and global error are derived. Numerical experiments are given.

1. Introduction

The subject of fractional calculus has gained considerable popularity and importance during the past three decades mainly due to its attractive applications in numerous, seemingly diverse and wide spread fields of science and engineering. Fractional differential equations (FDEs) have been used for mathematical modeling in potential fields, hydraulics of dams, diffusion problems, waves in liquids and gases, in heat equations, especially modeling oil strata, and in Maxwell's equation. Modeling of diffusion in a specific type of porous medium is one of the most significant applications of fractional derivatives. The fractional calculus provides an excellent instrument for the description of memory and hereditary properties of various materials and processes. Valuable monographs have been published on fractional calculus and applications (e.g., [1–7]). Further theoretical results, applications and modeling for ordinary and partial FDEs were discussed (e.g., [8–10]).

Numerical methods must conserve these properties of FDEs, and various schemes were proposed (e.g., [11–22]). This paper addresses the Grünwald–Letnikov approximation and follows the statement in the monography of Podlubny [6]. In a sense the resulting scheme for FDEs of fractional order α is an extension of the Euler scheme for ordinary differential equations and the given results reduce to that case if $\alpha = 1$. Consider the initial value problem

$$y'(t) = f(y(t)), \qquad y(t_0) = y_0,$$

then the explicit or implicit Euler method scheme reads

$$y_{n+1} = y_n + hf(y_n) \quad \text{or} \quad + hf(y_{n+1}).$$

Consider the initial value problem of an FDE

$$D^\alpha y(t) = f(y(t)), \qquad y(t_0) = y_0,$$

where always the existence and uniqueness of a solution is assumed. $D^\alpha y(t)$ means the derivative of order α of the function $y(t)$. The exact definition of the Riemann–Liouville and Caputo derivative is given later. There is a small difference between

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the Riemann–Liouville and the Caputo derivative. But the Caputo definition has advantages for initial value problems. M. Caputo was the first to give application of fractional calculus to mechanics, especially to linear models of viscoelasticity [23,24]. This paper mainly deals with FDEs using the Caputo operator of fractional order α with $0 < \alpha < 1$. And the Caputo derivative is approximated by the Grünwald–Letnikov approach using finite differences of fractional order. In the case of FDEs with inhomogeneous initial values, a correction term $r_{n+1}^{\alpha} y_0$ has to be added. Then the Grünwald–Letnikov scheme reads in the explicit and implicit cases as

$$y_{n+1} = c_1^{\alpha} y_n + c_2^{\alpha} y_{n-1} + \cdots + c_{n+1}^{\alpha} y_0 + r_{n+1}^{\alpha} y_0 + h^{\alpha} f(y_n) \quad \text{or} \quad + h^{\alpha} f(y_{n+1}).$$

The Grünwald–Letnikov method is proceeding iteratively but the sum in the scheme becomes longer and longer, which reflects the memory effect. The coefficients c_{ν}^{α} are recursively defined and show very smooth properties, e.g., they are positive and show strong damping effect. Therefore, they imply smooth properties for the scheme, but the correction term causes some perturbation. A discrete version of the Gronwall lemma applied in proofs is very useful. The properties of the Grünwald–Letnikov approximation as a numerical scheme concerning the stability and error estimates related to linear test equations are studied. Because of the long sum there arise discrepancies compared with the Euler method. One has to distinguish between the individual schemes for computing y_k and their behavior when $h \to 0$ and k is fixed, and the scheme for computing y_{n+1} at the point $t = (n+1)h$ and its behavior when $h \to 0$ and $n \to \infty$. The truncation error at the point $t = (n+1)h$ satisfies $O(h^{1+\alpha})$. But the truncation error of the scheme in the first step tends to a constant when $h \to 0$ in the case of an inhomogeneous initial value and satisfies $O(h^{\alpha})$ in the case of a homogeneous initial value. The global error is estimated by the sum of the truncation errors over all previous steps provided with damping coefficients. We can expect the order of convergence to be one. The maximum value of the global error over the whole grid is dominated by the truncation error in the first step.

Interesting examples of FDEs using the Caputo definition, denoted by D_*^{α}, are the Bagley–Torvik equation [25,26], [6, pp. 224–231]

$$ay''(t) + bD_*^{3/2} y(t) + cy(t) = f(t), \qquad y(0) = y'(0) = 0,$$

a prototype of fractional differential equations, which can be reduced to a system of FDEs of order $\alpha = 1/2$ with four equations, and further, the test equation

$$D_*^{\alpha} y(t) = \lambda y(t), \qquad y(0) = y_0,$$

and the fractional extension of the heat equation as a model for oil strata [27,8,28]

$$D_*^{\alpha} u = c^2 \frac{\partial^2 u}{\partial z^2}, \quad 0 < r, z, t < \infty, \ 0 < \alpha \le 1,$$

subject to nonstandard boundary conditions.

In Section 2, we present the definition of fractional derivatives in the sense of Riemann–Liouville and Caputo and mention the Mittag-Leffler function. The definition of fractional derivatives due to Grünwald–Letnikov is also given. The fractional order binomial coefficients and coefficients relevant for error representations are studied and monotony properties are derived in Section 3. The behavior and properties of these coefficients are investigated and explained in tables. In Section 4, the Grünwald–Letnikov scheme based on finite differences is discussed. In some sense it is an extension of the classical explicit and implicit Euler methods. The paper mainly deals with FDEs using the Caputo operator of order α. In the case of FDEs with inhomogeneous initial values, a correction term has to be added. The stability of the Grünwald–Letnikov scheme is investigated in Section 5. The asymptotic stability and absolute stability are proved. If $\alpha \to 1$ the results reduce to those of the classical Euler methods. Section 6 deals with the application of the Grünwald–Letnikov scheme to a test equation and a detailed error analysis. The error coefficients are studied when the steps are increasing. The representation of the propagation error emphasizes the stability of the Grünwald–Letnikov method caused by the strong damping factors in the fractional binomial evaluation. The global error is estimated by the sum of the truncation error of the current step and all previous steps, where again the damping effect of the fractional binomial coefficients is given. Numerical experiments are given to illustrate the properties of the schemes in the last section.

2. Fractional derivatives

There exist different approaches to fractional derivatives [6]. For simplification we consider the interval $[0, t]$ instead of $[a, t]$ and omit $a = 0$ as an index in the differential operator. Suppose that the function $y(\tau)$ satisfies some smoothness conditions in every finite interval $(0, t)$ with $t \le T$. The *Riemann–Liouville* definition ($\approx$1850) [6, p. 68] reads

$$D_R^{\alpha} y(t) = \begin{cases} \dfrac{1}{\Gamma(m-\alpha)} \dfrac{\mathrm{d}^m}{\mathrm{d}t^m} \displaystyle\int_0^t \frac{y(\tau)}{(t-\tau)^{\alpha+1-m}} \mathrm{d}\tau & m-1 \le \alpha < m \\ \dfrac{\mathrm{d}^m y(t)}{\mathrm{d}t^m} & \alpha = m, \end{cases} \tag{2.1}$$

and the *Caputo* definition (1967) [23,6, p. 79]

$$D_*^\alpha y(t) = \begin{cases} \dfrac{1}{\Gamma(m-\alpha)} \displaystyle\int_0^t \frac{y^{(m)}(\tau)}{(t-\tau)^{\alpha+1-m}} \mathrm{d}\tau & m-1 \le \alpha < m \\ \dfrac{\mathrm{d}^m y(t)}{\mathrm{d}t^m} & \alpha = m. \end{cases} \tag{2.2}$$

Later, the *Grünwald–Letnikov* definition (1867) based on finite differences is given which is equivalent to the Riemann–Liouville definition. These approaches provide an interpolation between the derivatives of integer order $m-1$ and m. The two definitions (2.1) and (2.2) are not equivalent to each other, and their difference is expressed by

$$D_*^\alpha y(t) = D_R^\alpha y(t) - \sum_{\nu=0}^{m-1} r_\nu^\alpha(t) y^{(\nu)}(0), \quad r_\nu^\alpha(t) = \frac{t^{\nu-\alpha}}{\Gamma(\nu+1-\alpha)}. \tag{2.3}$$

The Caputo operator D_*^α has advantages for differential equations with initial values. In the case of Riemann–Liouville and Caputo derivatives, respectively, the initial values are usually given as

$$D_R^{\alpha-\nu} y(0) = b_\nu \quad \text{and} \quad y^{(\nu-1)}(0) = b_\nu \quad \text{for } \nu = 1, 2, \dots, m, \tag{2.4}$$

respectively, i.e., things become easier if the initial values are homogeneous. In this paper we prefer the Caputo operator and concentrate on the case $m = 1$, i.e., $0 < \alpha < 1$. Then the correction term reads

$$D_*^\alpha y(t) = D_R^\alpha y(t) - r_0^\alpha(t) y_0, \quad r_0^\alpha(t) = \frac{t^{-\alpha}}{\Gamma(1-\alpha)}. \tag{2.5}$$

We mention the derivatives of the constant function $y_0(\tau) = 1$, where

$$D_*^\alpha y_0(t) = 0 \quad \text{and} \quad D_R^\alpha y_0(t) = \frac{t^{-\alpha}}{\Gamma(1-\alpha)}, \tag{2.6}$$

and the derivatives of monomials $y(\tau) = \tau^p$ $(p > 0)$

$$D_*^\alpha t^p = D_R^\alpha t^p = \frac{\Gamma(p+1)}{\Gamma(p-\alpha+1)} t^{p-\alpha}, \tag{2.7}$$

and give the following examples (with rounded numbers)

$$D_*^\alpha t^2 = \frac{2}{\Gamma(3-\alpha)} t^{2-\alpha}, \qquad D_*^{1/3} t^2 = 1.3 t^{5/3}, \qquad D_*^{1/2} t^2 = 1.5 t^{3/2}, \qquad D_*^{3/4} t^2 = 1.8 t^{5/4}.$$

For the representation of solutions of fractional differential equations the two-parametric *Mittag-Leffler function* is very useful [6, p. 17]:

$$E_{\alpha,\beta}(z) = \sum_{\nu=0}^\infty \frac{z^\nu}{\Gamma(\alpha\nu+\beta)}, \quad \alpha, \beta > 0, \ z \in \mathbb{C}, \qquad E_{\alpha,1}(z) = E_\alpha(z), \qquad E_1(z) = \exp(z).$$

A direct definition of the fractional derivative $D^\alpha y(t)$ is based on finite differences of an equidistant grid in $[0, t]$. Assume that the function $y(\tau)$ satisfies some smoothness conditions in every finite interval $(0, t)$, $t \le T$. Choosing the grid

$$0 = \tau_0 < \tau_1 < \dots < \tau_{n+1} = t = (n+1)h \quad \text{with } \tau_{k+1} - \tau_k = h \tag{2.8}$$

and using the notation of finite differences

$$\frac{1}{h^\alpha} \Delta_h^\alpha y(t) = \frac{1}{h^\alpha} \left(y(\tau_{n+1}) - \sum_{\nu=1}^{n+1} c_\nu^\alpha y(\tau_{n+1-\nu}) \right), \tag{2.9}$$

where

$$c_\nu^\alpha = (-1)^{\nu-1} \binom{\alpha}{\nu}, \tag{2.10}$$

the Grünwald–Letnikov definition reads [6, p. 48]

$$D_R^\alpha y(t) = \lim_{h\to 0} \frac{1}{h^\alpha} \Delta_h^\alpha y(t). \tag{2.11}$$

Lemma 2.1 (*Order of Approximation [6, pp. 204–208]*). *Let the function $y(\tau)$ be smooth in $[0, T]$. Then the Grünwald–Letnikov approximation satisfies for each $0 < t < T$ and a series of step sizes h with $\frac{t}{h} \in \mathbb{N}$ and $t = (n+1)h$*

$$D_R^\alpha y(t) = \frac{1}{h^\alpha} \Delta_h^\alpha y(t) + O(h) \quad (h \to 0). \tag{2.12}$$

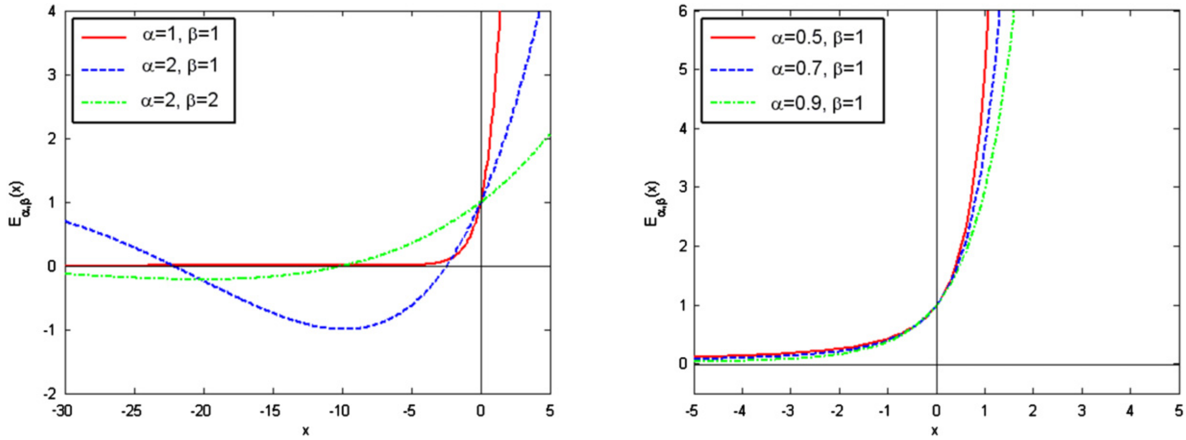

Fig. 2.1. Mittag-Leffler function $E_{\alpha,\beta}(z)$.

In the case of α a positive integer, the well known finite backward differences are given. If $\alpha = 1$, then the first order finite difference $\frac{1}{h}(y(\tau_{n+1}) - y(\tau_n))$ follows, if $\alpha = 2$, then the second order finite difference $\frac{1}{h^2}(y(\tau_{n+1}) - 2y(\tau_n) + y(\tau_{n-1}))$, and so on. It is emphasized that this definition is equivalent to the Riemann–Liouville definition (2.1) but in the case of the Caputo operator the correction term from (2.3) has to be added. The Grünwald–Letnikov approach can be used without correction term if the differential equations of the Caputo type have homogeneous initial values.

3. Fractional order binomial series

The binomial evaluation reads [29]

$$(1 - z)^\alpha = 1 - \sum_{\nu=1}^{\infty} c_\nu^\alpha z^\nu, \tag{3.1}$$

where α is any positive real number, $z \in [0, 1]$ and c_ν^α are the binomial coefficients defined in (2.10) and recursively connected by

$$c_\nu^\alpha = \left(1 - \frac{\alpha + 1}{\nu}\right) c_{\nu-1}^\alpha. \tag{3.2}$$

In the classical case α is an integer and the sum is finite. The binomial coefficients, used in the Grünwald–Letnikov definition, show interesting behavior. The first coefficient is $c_1^\alpha = \alpha$. For proving the results on stability and error estimates (in Sections 5 and 6) we introduce the following coefficients for $n \geq 0$ and $\mu \in \mathbb{N}_0$:

$$\gamma_{\mu,k}^\alpha = \frac{\Gamma(\mu\alpha + 1)}{\Gamma(k\alpha + 1)}, \quad \mu, k \in \mathbb{N}_0 \cup \{-1\}, \tag{3.3}$$

$$r_{n+1}^\alpha = \gamma_{0,-1}^\alpha (n + 1)^{-\alpha}, \tag{3.4}$$

$$S_{\mu,n+1}^\alpha = \sum_{\nu=1}^{n+1} c_\nu^\alpha (n + 1 - \nu)^{\mu\alpha}, \tag{3.5}$$

$$L_{\mu,n+1}^\alpha = S_{\mu,n+1}^\alpha + \gamma_{\mu,\mu-1}^\alpha n^{(\mu-1)\alpha}, \tag{3.6}$$

$$\hat{L}_{0,n+1}^\alpha = S_{0,n+1}^\alpha + \gamma_{0,-1}^\alpha (n + 1)^{-\alpha}, \tag{3.7}$$

$$\hat{L}_{\mu,n+1}^\alpha = \sum_{k=1}^{\mu} \gamma_{\mu,k}^\alpha S_{k,n+1}^\alpha + \gamma_{\mu,0}^\alpha \hat{L}_{0,n+1}^\alpha, \tag{3.8}$$

$$V_{\mu,n+1}^\alpha = (n + 1)^{\mu\alpha} - S_{\mu,n+1}^\alpha - \gamma_{\mu,\mu-1}^\alpha (n + 1)^{(\mu-1)\alpha} \tag{3.9}$$

$$K_{\mu,n+1}^\alpha = (n + 1)^{\mu\alpha} - S_{\mu,n+1}^\alpha - \gamma_{\mu,\mu-1}^\alpha n^{(\mu-1)\alpha}, \tag{3.10}$$

$$\hat{K}_{\mu,n+1}^\alpha = (n + 1)^{\mu\alpha} - \sum_{k=1}^{\mu} \gamma_{\mu,k}^\alpha S_{k,n+1}^\alpha - \gamma_{\mu,0}^\alpha \hat{L}_{0,n+1}^\alpha. \tag{3.11}$$

We are interested in the main case $0 < \alpha < 1$, but for larger values of α similar results can be deduced. The constants $\gamma_{0,k}^{\alpha}$ are important for error representations (6.4), (6.5). Using Stirling's formula

$$\gamma_{0,\mu}^{\alpha} \sim \frac{1}{\sqrt{2\pi}} \frac{\exp(\mu\alpha + 1)}{(\mu\alpha + 1)^{\mu\alpha + 0.5}} \quad \text{for } \mu\alpha \to \infty, \tag{3.12}$$

we notice that the coefficients $\gamma_{0,\mu}^{\alpha}$ rapidly tend to zero when $\mu \to \infty$ (see also Table 3.3).

Lemma 3.1. *The coefficients $V_{\mu,n+1}^{\alpha}$ given in (3.9) satisfy for $\mu \in \mathbb{N}_0$*

$$V_{\mu,n+1}^{\alpha} = O(h^{1-(\mu-1)\alpha}) \quad \textit{for } h \to 0 \ (n \to \infty). \tag{3.13}$$

Lemma 3.2. *Assume that $0 < \alpha < 1$, then all the coefficients c_{ν}^{α} defined in (2.10) are positive and show the behavior*

$$c_{\nu}^{\alpha} = O\left(\frac{1}{\nu^{1+\alpha}}\right) \quad (\nu \to \infty). \tag{3.14}$$

Further, the coefficients from (2.10), (3.4) and (3.5) satisfy for $n \geq 1$ the properties

$$0 < c_{n+1}^{\alpha} < c_{n}^{\alpha} < \cdots < c_{1}^{\alpha} = \alpha, \tag{3.15}$$

$$\alpha = S_{0,1}^{\alpha} < \cdots < S_{0,n}^{\alpha} < S_{0,n+1}^{\alpha} < 1, \tag{3.16}$$

$$0 < r_{n+1}^{\alpha} < r_{n}^{\alpha} < \cdots < r_{1}^{\alpha} = \frac{1}{\Gamma(1-\alpha)}. \tag{3.17}$$

Lemma 3.3. *Assume that $0 < \alpha < 1$, then the coefficients given in (3.10) and (3.11) satisfy for $h \to 0$ $(n \to \infty)$ the asymptotic properties*

$$K_{\mu,n+1}^{\alpha} = O(h^{1-(\mu-1)\alpha}) \quad \textit{for } \mu \in \mathbb{N}, \tag{3.18}$$

$$\hat{K}_{\mu,n+1}^{\alpha} = O(h^{1-(\mu-1)\alpha}) \quad \textit{for } \mu \in \mathbb{N}_0. \tag{3.19}$$

Proof. Lemma 3.1: Consider the functions $y(\tau) = 1$ and $y(\tau) = \tau^{\mu\alpha}$ and insert them into (2.12) using (2.6), (2.7) and $t = (n+1)h$, then it follows for $\mu \in \mathbb{N}_0$ and for $h \to 0$ $(n \to \infty)$

$$\gamma_{\mu,\mu-1}^{\alpha}(n+1)^{(\mu-1)\alpha}h^{(\mu-1)\alpha} = h^{(\mu-1)\alpha}\left((n+1)^{\mu\alpha} - S_{\mu,n+1}^{\alpha}h^{\mu\alpha}\right) + O(h), \tag{3.20}$$

and therefore with (3.9) the result is deduced.

Lemma 3.2: The c_{ν}^{α} from (2.10) are positive, because the binomial product $\binom{\alpha}{\nu} = \frac{1}{\nu!}\alpha(\alpha-1)\cdots(\alpha-\nu+1)$ consists of one positive term and $\nu - 1$ negative terms, compensated by $(-1)^{\nu-1}$. The recurrence relation (3.2) implies (3.15). Using

$$c_{\nu}^{\alpha} = \frac{(-1)}{\Gamma(-\alpha)} \frac{\Gamma(\nu-\alpha)}{\Gamma(\nu+1)} \tag{3.21}$$

and [5, p. 20]

$$\lim_{\nu\to\infty}\left(\nu^{1+\alpha}\frac{\Gamma(\nu-\alpha)}{\Gamma(\nu+1)}\right) = 1, \tag{3.22}$$

the result (3.14) is deduced. The Cauchy ratio test shows that setting $z = 1$ in (3.1) is allowed, which leads to $1 = \sum_{\nu=1}^{\infty} c_{\nu}^{\alpha}$. This implies $\alpha \leq S_{0,n+1}^{\alpha} \leq 1$ for each $n \geq 0$, and with $c_{\nu}^{\alpha} > 0$ the monotony (3.16). Property (3.17) is clear from definition (3.5).

Lemma 3.3: First, regarding (3.9) and (3.10) we derive the representation

$$K_{\mu,n+1}^{\alpha} = V_{\mu,n+1}^{\alpha} + \gamma_{\mu,\mu-1}^{\alpha}\left((n+1)^{(\mu-1)\alpha} - n^{(\mu-1)\alpha}\right), \tag{3.23}$$

where the first and the second part in the last line satisfy $O(h^{1-(\mu-1)\alpha})$. The first part is given by Lemma 3.1. If $\mu = 1$, the second part disappears. For $\mu \geq 2$ the sequence

$$\left((n+1)^{(\mu-1)\alpha} - n^{(\mu-1)\alpha}\right)(n+1)^{1-(\mu-1)\alpha} \tag{3.24}$$

for $n \geq 0$ is bounded. Using the abbreviation $x = (\mu - 1)\alpha$, we have for $n \to \infty$

Table 3.1
Values of c_ν^α for $\alpha = 0.8$ and $\alpha = 0.5$.

ν	1	2	3	4	5	6	7	8	9	10	11	12	14	16	18	20
$\alpha = 0.8$	0.80	0.08	0.031	0.018	0.011	0.0079	0.0059	0.0045	0.0036	0.0030	0.0026	0.0021	0.0016	0.0012	0.0010	0.0008
$\alpha = 0.5$	0.50	0.13	0.063	0.039	0.027	0.021	0.016	0.013	0.011	0.009	0.008	0.007	0.006	0.005	0.004	0.003

Table 3.2
Values of $S_{0,n+1}^\alpha$ for $\alpha = 0.8$ and $\alpha = 0.5$.

n	0	1	2	3	4	5	6	7	8	9	14
$\alpha = 0.8$	0.80	0.88	0.91	0.93	0.94	0.95	0.95	0.96	0.96	0.97	0.98
$\alpha = 0.5$	0.50	0.63	0.69	0.73	0.75	0.77	0.79	0.80	0.81	0.82	0.86

Table 3.3
Values of $\gamma_{0,k}^\alpha$ for $\alpha = 0.8$ and $\alpha = 0.5$.

k	1	2	3	4	5	6	7	8
$\alpha = 0.8$	1.07	0.70	0.34	0.13	0.04	0.01	0.0007	0.00003
$\alpha = 0.5$	1.13	1.00	0.75	0.50	0.30	0.17	0.04	0.008

Table 3.4
Values of $(-1)\hat{K}_{0,n+1}^\alpha$ for $\alpha = 0.8$ and $\alpha = 0.5$.

n	0	1	2	3	4	5	6	7	8
$\alpha = 0.8$	0.0178	0.0051	0.0025	0.0015	0.0010	0.0007	0.0005	0.0004	0.0003
$\alpha = 0.5$	0.0642	0.0239	0.0132	0.0087	0.0062	0.0047	0.0038	0.0031	0.0026

$$\frac{(n+1)^x - n^x}{(n+1)^{x-1}} = \frac{n^x\left(\left(1+\frac{1}{n}\right)^x - 1\right)}{(n+1)^{x-1}} = \frac{n^x\left(1+\frac{x}{n}+\frac{x(x-1)}{2n^2}+O\left(\frac{1}{n^3}\right)-1\right)}{(n+1)^{x-1}} \tag{3.25}$$

$$= \frac{xn^{x-1}+\frac{1}{2}x(x-1)n^{x-2}+O(n^{x-3})}{(n+1)^{x-1}} \le x. \tag{3.26}$$

Second, (3.9) and (3.11) are regarded. If $\mu = 0$, then $\hat{K}_{0,n+1}^\alpha = V_{0,n+1}^\alpha$ and $V_{0,n+1}^\alpha$ satisfies $O(h^{1+\alpha})$. If $\mu > 0$, after each term of the sum in (3.11) we complement

$$\gamma_{\mu+1-k,\mu-k}^\alpha\left(-(n+1)^{(\mu-k)\alpha} + (n+1)^{(\mu-k)\alpha}\right) \tag{3.27}$$

to get the terms $V_{\mu+1-k,n+1}^\alpha$. Therefore, the representation follows

$$\hat{K}_{\mu,n+1}^\alpha = \sum_{k=1}^{\mu} \gamma_{\mu,\mu+1-k}^\alpha V_{\mu+1-k,n+1}^\alpha + \gamma_{\mu,0}^\alpha \hat{K}_{0,n+1}^\alpha, \tag{3.28}$$

and from Lemma 3.1 the second result of Lemma 3.3 is given. □

In the limit case $\alpha \to 1$, the first coefficients in (3.10) and (3.11) become zero, i.e.,

$$\hat{K}_{0,n+1}^1 = \hat{K}_{1,n+1}^1 = K_{1,n+1}^1 = 0. \tag{3.29}$$

In Tables 3.1–3.4, used in Sections 5 and 6, some values of the coefficients c_ν^α, $\gamma_{0,k}^\alpha$, $S_{0,n+1}^\alpha$ and $\hat{K}_{0,n+1}^\alpha$ are presented, where the coefficients $\hat{K}_{0,n+1}^\alpha$ are negative:

4. The Grünwald–Letnikov approximation

We are interested in fractional differential equations using the Caputo operator D_*^α. The Caputo definition is equivalent to the Riemann–Liouville and in the case of a homogeneous initial value also to the Grünwald–Letnikov definition. But in the case of an inhomogeneous initial value the correction term (2.5) is needed. Consider the fractional differential equation using the Caputo operator

$$D_*^\alpha y(t) = f(y(t)), \qquad y(\tau_0) = y_0 \quad (0 < \alpha < 1) \tag{4.1}$$

and assume that there exists a unique solution $y = y(\tau)$ in the interval $[0, T]$. Both cases, the homogeneous and inhomogeneous initial values, are considered. For the discretization an equidistant grid is chosen

$$0 = \tau_0 < \tau_1 < \cdots < \tau_{N+1} = T \quad \text{with } \tau_{k+1} - \tau_k = h \tag{4.2}$$

and let y_k denote the approximation of the true solution $y(\tau_k)$. The Grünwald–Letnikov approximation (2.9) is applied to the left-hand side of (4.1) with respect to $\tau_{n+1} = (n+1)h$ including the correction term (2.5) and the right-hand side is approximated by $f(y_n)$ or $f(y_{n+1})$. Then the explicit or implicit Grünwald–Letnikov method reads

$$y_{n+1} - \sum_{\nu=1}^{n+1} c_\nu^\alpha y_{n+1-\nu} - r_{n+1}^\alpha y_0 = h^\alpha f(y_n) \quad \text{or} \quad = h^\alpha f(y_{n+1}), \tag{4.3}$$

where

$$r_{n+1}^\alpha = h^\alpha r_0^\alpha(\tau_{n+1}) = \gamma_{0,-1}^\alpha (n+1)^{-\alpha}. \tag{4.4}$$

The correction term $r_{n+1}^\alpha y_0$ tends to zero when $n \to \infty$, and it is zero if Eq. (4.1) with homogeneous initial value $y_0 = 0$ is considered. In a sense it is an extension of the Euler method to fractional differential equations. If $\alpha \to 1$, then the classical explicit or implicit Euler method $y_{n+1} - y_n = hf(y_n)$ resp. $y_{n+1} - y_n = hf(y_{n+1})$ is given. Compared with linear multistep methods, the sum of divided differences becomes longer and longer. For multistep methods the condition $\rho(1) = 0$ of the characteristic polynomial is necessary to reach order one of consistency. For the Grünwald–Letnikov method (4.3) the following result holds (see (3.11) and (3.19))

$$\rho(1) = \hat{K}_{0,n+1}^\alpha, \tag{4.5}$$

where $\hat{K}_{0,n+1}^\alpha = O(h^{1+\alpha})$ when $h \to 0$ $(n \to \infty)$.

Now the problem is to implement the Grünwald–Letnikov method. When the explicit or implicit method is applied to (4.1) we get the numerical solution $\{y_{n+1}\}_{n=0,1,\ldots,N}$ approximating the true solution $y(\tau)$ in the grid points (4.2) in the iterative way

$$y_{n+1} = \sum_{\nu=1}^{n+1} c_\nu^\alpha y_{n+1-\nu} + r_{n+1}^\alpha y_0 + h^\alpha f(y_n) \quad \text{or} \quad = h^\alpha f(y_{n+1}). \tag{4.6}$$

The result of Lemma 2.1 about order one of approximation relates to the case where the true values $y(\tau_{n+1-\nu})$ are used on the right-hand side of the scheme. In this case we refer later to the truncation error of the method. But we are interested in the global error which is the sum of the truncation and the propagation error. The global error is estimated by the sum over the truncation errors in all the previous steps with damping factors. Computing the first approximations $y_1, y_2, \ldots$ with a short sum, the error is relatively high and is propagated. Therefore it is necessary to create an efficient run-up method for the starting values to improve the Grünwald–Letnikov scheme. In the case of a homogeneous initial value the situation is better. In Section 6 the relevant error estimates are studied in more detail.

For the investigation of the stability properties of the Grünwald–Letnikov scheme (4.3) a special form of the discrete Gronwall lemma [30, p. 14], which can be proved by induction, is very useful.

Lemma 4.1. *Assume that $\{\xi_n\}$, $\{\rho_n\}$ and $\{\eta_n\}$ are nonnegative sequences and*

$$\xi_n = \rho_n + \sum_{k=0}^{n-1} \eta_k \xi_k \quad \textit{for } n \ge 0. \tag{4.7}$$

Then it holds that

$$\xi_n = \rho_n + \sum_{k=0}^{n-1} \rho_k \eta_k \prod_{j=k+1}^{n-1} (1 + \eta_j) \quad \textit{for } n \ge 0. \tag{4.8}$$

This lemma and the following corollary are also valid in the case when Eqs. (4.7), (4.8) and (4.10) are replaced by inequalities. If it is applied to the Grünwald–Letnikov scheme, then from (4.3) with $h = 0$ we have

$$y_{n+1} = \sum_{\nu=1}^{n+1} c_\nu^\alpha y_{n+1-\nu} + r_{n+1}^\alpha y_0 \quad \text{for } n \ge 0. \tag{4.9}$$

Corollary 4.1. *The sequence $\{y_n\}$ from (4.9) satisfies for $n \ge 0$ the following relations*

$$|y_{n+1}| = \sum_{\nu=1}^{n+1} r_\nu^\alpha c_{n+1-\nu}^\alpha \prod_{j=\nu+1}^{n} (1 + c_{n+1-j}^\alpha) + r_{n+1}^\alpha |y_0|, \tag{4.10}$$

$$|y_{n+1}| \le \exp(1) \sum_{\nu=1}^{n+1} c_\nu^\alpha r_{n+1-\nu}^\alpha + r_{n+1}^\alpha |y_0|, \tag{4.11}$$

$$|y_{n+1}| \le \exp(1) + r_{n+1}^\alpha |y_0|. \tag{4.12}$$

Proof. Since c_ν^α and r_{n+1}^α are positive, the values y_{n+1} remain positive if $y_0 > 0$, and negative if $y_0 < 0$. Therefore, in Eq. (4.9) the values y_ν can be replaced by their absolute values $|y_\nu|$. Set $\xi_n = |y_n|$, $\rho_n = r_n^\alpha |y_0|$, $\eta_n = c_n^\alpha$, which satisfy the assumption of Lemma 4.1, then the result (4.10) follows.

Regarding (3.5), (3.16) and (3.17), especially $r_\nu^\alpha \le 1$, the product in (4.10) is estimated by

$$\prod_{j=\nu+1}^{n} (1 + c_{n+1-j}^\alpha) \le \prod_{j=0}^{n} (1 + c_{n+1-j}^\alpha) \le \exp(S_{0,n+1}^\alpha) \le \exp(1) \tag{4.13}$$

and the sum by

$$\sum_{\nu=1}^{n+1} r_\nu^\alpha c_{n+1-\nu}^\alpha \le S_{0,n+1}^\alpha \le 1, \tag{4.14}$$

which proves the result (4.11) and (4.12). □

5. Stability investigation

We begin with the asymptotic stability. Consider the finite difference equation

$$y_{n+1} = \sum_{\nu=1}^{n+1} \beta_\nu y_{n+1-\nu}, \quad n \ge 0, \tag{5.1}$$

with arbitrary initial value y_0 and solution $\{y_n\}_{n\ge0}$. The finite difference equation is called stable if there exists a constant K such that

$$|y_n| \le K \quad \text{for all } n \ge 0. \tag{5.2}$$

When the Grünwald–Letnikov scheme (4.3) is applied to $D_R^\alpha y(t) = 0$ or $D_*^\alpha y(t) = 0$ (the case when $h \to 0$) with initial value $y(\tau_0) = y_0$ for any y_0 and $0 < \alpha < 1$, then the finite difference (5.1) follows with $\beta_\nu = c_\nu^\alpha$ $(0 \le \nu \le n)$ and $\beta_{n+1} = c_{n+1}^\alpha + r_{n+1}^\alpha$, where the correction term $r_{n+1}^\alpha y_0$ is necessary in the Caputo case. The Grünwald–Letnikov scheme (4.3) is called *asymptotically stable*, if there exists a constant K such that condition (5.2) holds for any arbitrary initial value y_0.

Theorem 5.1. *The explicit and implicit Grünwald–Letnikov methods (4.3) are asymptotically stable.*

Proof. Using properties (3.15)–(3.17) from Lemma 3.2, the asymptotic stability will be deduced. In the Riemann–Liouville case, where $y_{n+1} = \sum_{\nu=1}^{n+1} c_\nu^\alpha y_{n+1-\nu}$ (without correction term), it yields immediately

$$|y_{n+1}| \le S_{0,n+1}^\alpha |y_0| \le |y_0|. \tag{5.3}$$

In the Caputo case, where $y_{n+1} = \sum_{\nu=1}^{n+1} c_\nu^\alpha y_{n+1-\nu} + r_{n+1}^\alpha y_0$ (with correction term), from Corollary 4.1 and (3.17) it follows

$$|y_{n+1}| \le \exp(1) + r_{n+1}^\alpha |y_0| \le \exp(1) + |y_0|, \tag{5.4}$$

and therefore the asymptotic stability. □

The absolute stability behavior of methods is investigated when they are applied to convenient *test equations*, where $0 < \alpha < 1$. The following fractional differential equations are proposed and the true solutions are given using the Mittag-Leffler function:

$$D_R^\alpha y(t) = \lambda y(t), \qquad D_R^{\alpha-1} y(t)|_0 = b_1 \tag{5.5}$$

$$y(t) = b_1 t^{\alpha-1} E_{\alpha,\alpha}(\lambda t^\alpha) = b_1 t^{\alpha-1} \sum_{\nu=1}^{\infty} \frac{(\lambda t^\alpha)^\nu}{\Gamma(\alpha\nu + \alpha)}$$

$$D_*^\alpha y(t) = \lambda y(t), \qquad y(0) = y_0 \tag{5.6}$$

$$y(t) = y_0 E_\alpha(\lambda t^\alpha) = y_0 \sum_{\nu=0}^{\infty} \gamma_{0,\nu}^\alpha (\lambda t^\alpha)^\nu$$

$$D_*^\alpha y(t) = \lambda (y(t) + v_0), \qquad y(0) = 0 \tag{5.7}$$

$$y(t) = -v_0 + v_0 E_\alpha(\lambda t^\alpha) = v_0 \sum_{\nu=1}^{\infty} \gamma_{0,\nu}^\alpha (\lambda t^\alpha)^\nu.$$

Concerning stability $\lambda < 0$ is assumed and concerning error discussion both cases $\lambda < 0$ and $\lambda > 0$ are considered. We concentrate on the inhomogeneous Caputo type test equation (5.6), where the solution $y(t)$ satisfies the monotony condition (see Fig. 2.1)

$$|y(t+\delta)| \le |y(t)| \le |y(0)| \quad \text{for all } t \text{ and } \delta > 0. \tag{5.8}$$

The question, whether the numerical solution $\{y_n\}_{n\ge 0}$ can preserve this property $|y_{n+1}| \le |y_n|$ for $n \ge 0$, is difficult to answer, because of the correction term. Therefore correspondingly to the asymptotic stability we demand the boundedness of the solution.

Definition 5.1. The Grünwald–Letnikov method is called absolute stable for step size h, if applied to the test equation (5.6) with $\lambda < 0$ there exists a constant K such that condition (5.2) holds for any arbitrary initial value y_0.

Theorem 5.2. *The Grünwald–Letnikov method is absolute stable in the explicit case if the step size h satisfies*

$$|\alpha + \lambda h^\alpha| \le \alpha, \tag{5.9}$$

and in the implicit case without any step size restriction.

Proof. The application of the Grünwald–Letnikov method (4.3) to the test equation (5.6) yields

$$y_{n+1} = (\alpha + \lambda h^\alpha)\, y_n + \sum_{\nu=2}^{n+1} c_\nu^\alpha y_{n+1-\nu} + r_{n+1}^\alpha y_0, \tag{5.10}$$

$$y_{n+1} = (1 - \lambda h^\alpha)^{-1} \left(\sum_{\nu=1}^{n+1} c_\nu^\alpha y_{n+1-\nu} + r_{n+1}^\alpha y_0 \right), \tag{5.11}$$

in the explicit and implicit cases, respectively. In the explicit case the step size condition (5.9) is assumed, and in the implicit case $|1-\lambda h^\alpha|^{-1} \le 1$ is satisfied without any step size restriction. Therefore in both cases the estimate follows

$$|y_{n+1}| \le \sum_{\nu=1}^{n+1} c_\nu^\alpha |y_{n+1-\nu}| + r_{n+1}^\alpha |y_0|, \tag{5.12}$$

and further, using Corollary 4.1 with the inequality in (4.8) the condition (5.2). □

Remarks. In the case of the homogeneous test equation (5.7) the same behavior is given for the shifted solution $w(t) = y(t) + v_0$ and the same stability property can be proved for the shifted approximation $w_n = y_n + v_0$. The application of (4.3) delivers the same equations as (5.10) and (5.11), where the y_ν are replaced by w_ν and $r_{n+1}^\alpha y_0$ by $(1 - S_{0,n+1}^\alpha) v_0$. Under the same assumption as in Theorem 5.2 we derive from the modified equations (5.10) and (5.11)

$$|w_{n+1}| \le \sum_{\nu=2}^{n+1} c_\nu^\alpha |w_{n+1-\nu}| + (1 - S_{0,n+1}^\alpha) v_0 \tag{5.13}$$

and prove by induction $|w_{n+1}| \le |w_0| = v_0$.

In the case of the test equation (5.5) but with the initial condition $y(0) = y_0$, where the true solution is not known, the result of Theorem 5.2 also holds. Namely for Riemann–Liouville the correction term $r_{n+1}^\alpha y_0$ is canceled in (5.10)–(5.12), and again the boundedness of the approximate solution follows by induction.

If $\alpha = 1$ in (5.9), then the condition for the absolute stability of the explicit Euler method follows. Regarding $\lambda < 0$ the restriction (5.9) is equivalent to $|\lambda| h^\alpha \le 2\alpha$, which remembers the rule of thumb $|\lambda| h \le 1$ in the classical case. Consider $\lambda = -100$: If $\alpha = 1$ then $h \le 0.02$, if $\alpha = 0.8$ then $h \le 0.005$, and if $\alpha = 0.5$ then $h \le 0.0001$.

6. Error analysis

We consider the explicit and implicit Grünwald–Letnikov method (5.10) and (5.11) applied to the test equation (5.6) for arbitrary λ and derive asymptotic error representations, where the rule of thumb

$$|\lambda| h^\alpha < 1 \tag{6.1}$$

is used. Inserting the true values $y(\tau_\nu)$ into the right-hand side of (5.10) and (5.11), it is denoted by

$$\hat{y}_{n+1} = (\alpha + \lambda h^\alpha)\, y(\tau_n) + \sum_{\nu=2}^{n+1} c_\nu^\alpha y(\tau_{n+1-\nu}) + r_{n+1}^\alpha y_0, \tag{6.2}$$

$$\hat{y}_{n+1} = (1 - \lambda h^\alpha)^{-1} \left(\sum_{\nu=1}^{n+1} c_\nu^\alpha y(\tau_{n+1-\nu}) + r_{n+1}^\alpha y_0 \right), \tag{6.3}$$

and therefore the *truncation error* by $q_{n+1} = y(\tau_{n+1}) - \hat{y}_{n+1}$ and the *propagation error* by $p_{n+1} = \hat{y}_{n+1} - y_{n+1}$. The *global error* $e_{n+1} = y(\tau_{n+1}) - y_{n+1}$ is split into truncation error and propagation error, i.e., $e_{n+1} = q_{n+1} + p_{n+1}$.

Theorem 6.1. *The explicit and implicit Grünwald–Letnikov methods are applied to (5.6) assuming condition (6.1). Then the truncation error satisfies the asymptotic expansion*

$$q_{n+1} = y_0 \left(\hat{K}^{\alpha}_{0,n+1} + \sum_{\mu=1}^{\infty} \gamma^{\alpha}_{0,\mu} K^{\alpha}_{\mu,n+1} \lambda^{\mu} h^{\mu\alpha} \right) \tag{6.4}$$

in the explicit case and

$$q_{n+1} = y_0 \sum_{\mu=0}^{\infty} \gamma^{\alpha}_{0,\mu} \hat{K}^{\alpha}_{\mu,n+1} \lambda^{\mu} h^{\mu\alpha} \tag{6.5}$$

in the implicit case, where the coefficients $\gamma^{\alpha}_{0,\mu}$, $K^{\alpha}_{\mu,n+1}$ and $\hat{K}^{\alpha}_{\mu,n+1}$ are already given in (3.3), (3.10) and (3.11).

Proof. The true values $y(\tau_\nu)$ in (6.2) and (6.3) are expanded using the representation of the Mittag-Leffler function $E_\alpha(\lambda\tau^{\alpha}_{\nu})$ from (5.6)

$$\hat{y}_{n+1} = y_0(\alpha + \lambda h^{\alpha}) \sum_{k=0}^{\infty} \gamma^{\alpha}_{0,k} n^{k\alpha} (\lambda h^{\alpha})^k + y_0 \sum_{\nu=2}^{n+1} c^{\alpha}_{\nu} \sum_{k=0}^{\infty} \gamma^{\alpha}_{0,k} (n+1-\nu)^{k\alpha} (\lambda h^{\alpha})^k + y_0 r^{\alpha}_{n+1}, \tag{6.6}$$

$$\hat{y}_{n+1} = y_0 (1 - \lambda h^{\alpha})^{-1} \left(\sum_{\nu=1}^{n+1} c^{\alpha}_{\nu} \sum_{k=0}^{\infty} \gamma^{\alpha}_{0,k} (n+1-\nu)^{k\alpha} (\lambda h^{\alpha})^k + r^{\alpha}_{n+1} \right). \tag{6.7}$$

Expanding $(1 - \lambda h^{\alpha})^{-1} = 1 + \lambda h^{\alpha} + \cdots$ and arranging the terms by power of λh^{α}, the evaluation reads in the explicit and implicit cases

$$\hat{y}_{n+1} = y_0 \left(\hat{L}^{\alpha}_{0,n+1} + \gamma^{\alpha}_{0,1} L^{\alpha}_{1,n+1} \lambda h^{\alpha} + \gamma^{\alpha}_{0,2} L^{\alpha}_{2,n+1} (\lambda h^{\alpha})^2 + \cdots \right) \tag{6.8}$$

and

$$\hat{y}_{n+1} = y_0 \left(\hat{L}^{\alpha}_{0,n+1} + \gamma^{\alpha}_{0,1} \hat{L}^{\alpha}_{1,n+1} \lambda h^{\alpha} + \gamma^{\alpha}_{0,2} \hat{L}^{\alpha}_{2,n+1} (\lambda h^{\alpha})^2 + \cdots \right), \tag{6.9}$$

respectively. Compare it with the expansion of the true solution

$$y(\tau_{n+1}) = y_0 \left(1 + \gamma^{\alpha}_{0,1} (n+1)^{\alpha} \lambda h^{\alpha} + \gamma^{\alpha}_{0,2} (n+1)^{2\alpha} (\lambda h^{\alpha})^2 + \cdots \right), \tag{6.10}$$

then using the error coefficients $K^{\alpha}_{\mu,n+1}$ and $\hat{K}^{\alpha}_{\mu,n+1}$ from (3.10) and (3.11) the results (6.4) and (6.5) follow. □

Corollary 6.1. *The explicit and implicit Grünwald–Letnikov method are applied to (5.7) assuming condition (6.1). Then the truncation error satisfies the asymptotic expansion (6.4) and (6.5), respectively, where the first term $\hat{K}^{\alpha}_{0,n+1}$ is canceled and y_0 is replaced by v_0.*

Proof. The same way is pursued as in the previous proof: Replace in (6.2), (6.3), (6.6) and (6.7) the last term $r^{\alpha}_{n+1} y_0$ by $\lambda h^{\alpha} v_0$. In (6.6) and (6.7) replace y_0 by v_0 and let the expansion of the Mittag-Leffler function begin with $k = 1$. Then the expansions of $\hat{y}_{n+1}$ and $y(\tau_{n+1})$ are deduced as in (6.9) and (6.10), where y_0 is replaced by v_0 and the first terms without a power of λh^{α} are canceled. □

Remarks. Concerning the expansion of the truncation error (6.4) and (6.5) we emphasize the following. The behavior of the individual schemes for computing y_k is shown when $h \to 0$ (and k is fixed). The behavior of the scheme for computing y_{n+1} at the point $t = (n+1)h$ is shown when $h \to 0$ ($n \to \infty$). The error coefficients $K^{\alpha}_{\mu,n+1}$ and $\hat{K}^{\alpha}_{\mu,n+1}$ depend on $n+1 = \frac{t}{h}$, and therefore on h. In Lemma 3.3 it is proved that the coefficients $K^{\alpha}_{\mu,n+1}$ and $\hat{K}^{\alpha}_{\mu,n+1}$ satisfy $O(h^{1-(\mu-1)\alpha})$ when $h \to 0$ ($n \to \infty$) for $\mu \geq 0$. Therefore, each term of the expansion satisfies $O(h^{1+\alpha})$. Using $\sum_{\mu=0}^{\infty} \gamma^{\alpha}_{0,\mu} \leq \frac{4}{\alpha}$ the truncation error itself satisfies

$$q_{n+1} = O(h^{1+\alpha}) \quad (h \to 0). \tag{6.11}$$

Further, regarding (3.12) and Table 3.3 we notice that the coefficients $\gamma^{\alpha}_{0,\mu}$ rapidly tend to zero when $\mu \to \infty$. The assumption of condition (6.1) can be released.

Now let us consider the individual scheme for computing the value y_k, where k is fixed. From (6.4) and (6.5) when $h \to 0$ it follows that $q_k \to y_0 \hat{K}^{\alpha}_{0,k}$ in the case of an inhomogeneous initial value. The coefficient $\hat{K}^{\alpha}_{0,n+1}$, which dominates the truncation error, is independent of h and has a negative value. Thus for special values of h there can arise some extinction with negative and positive values in the expansion. Further, we do not have consistency in the case of an inhomogeneous initial value. From Table 3.1 we know for $\alpha = 0.8$ the values $\hat{K}^{\alpha}_{0,1} = -0.0178$, $\hat{K}^{\alpha}_{0,2} = -0.0051$, $\hat{K}^{\alpha}_{0,3} = -0.0015$, which express the size of the truncation error of the Grünwald–Letnikov scheme (4.3) in the first three steps. Therefore, we can assume that the error q_1 in the first step is the largest one. In the case of a homogeneous initial value (Corollary 6.1) the situation concerning the truncation error in the individual steps is better. The main error terms depend on h and satisfy $O(h^\alpha)$.

In the limit case $\alpha \to 1$, where the Euler method results, the first error coefficients in (6.4) and (6.5) become zero (see (3.29)).

Now the discussion of the propagation error $p_{n+1} = \hat{y}_{n+1} - y_{n+1}$ and the global error $e_{n+1} = q_{n+1} + p_{n+1}$ is pursued.

Theorem 6.2. *The explicit and implicit Grünwald–Letnikov methods are applied to the test equation (5.6), where for $\lambda < 0$ in the explicit case the stability condition (5.9) is assumed. Then the propagation error satisfies for $\lambda < 0$*

$$|p_{n+1}| \le \sum_{\nu=1}^{n+1} c_\nu^\alpha |e_{n+1-\nu}| \tag{6.12}$$

and for $\lambda > 0$

$$|p_{n+1}| \le (c_1^\alpha + \lambda h^\alpha)|e_n| + \sum_{\nu=2}^{n+1} c_\nu^\alpha |e_{n+1-\nu}|, \tag{6.13}$$

$$|p_{n+1}| \le (1 - \lambda h^\alpha)^{-1} \sum_{\nu=1}^{n+1} c_\nu^\alpha |e_{n+1-\nu}|. \tag{6.14}$$

Proof. Comparing (5.10), (5.11) with (6.2), (6.3) the propagation error of the explicit and implicit method satisfies

$$p_{n+1} = (\alpha + \lambda h^\alpha)e_n + \sum_{\nu=2}^{n+1} c_\nu^\alpha e_{n+1-\nu}, \tag{6.15}$$

$$p_{n+1} = (1 - \lambda h^\alpha)^{-1} \sum_{\nu=1}^{n+1} c_\nu^\alpha e_{n+1-\nu}, \tag{6.16}$$

respectively, which implies the estimates (6.12)–(6.14). □

Remarks. The result (6.12) accentuates the stability of the Grünwald–Letnikov method caused by the strong damping factors c_ν^α in the fractional binomial evaluation. The additional terms in (6.13), (6.14) reflect the behavior for $\lambda > 0$. Further, the errors in the past are more and more damped, which means that the Grünwald–Letnikov sum can be truncated. This is called *short-memory* effect [6, p. 203].

Theorem 6.3. *The explicit and implicit Grünwald–Letnikov methods are applied to the test equation (5.6), where if $\lambda < 0$ in the explicit case the stability condition (5.9) is assumed. Then the global error satisfies*

$$|e_{n+1}| \le C \sum_{\nu=1}^{n} c_\nu^\alpha |q_{n+1-\nu}| + |q_{n+1}|, \tag{6.17}$$

where

$$C \le \exp(1). \tag{6.18}$$

If $\lambda > 0$ in (5.6), then (6.17) holds, where in the explicit and implicit cases, respectively,

$$C \le \exp(1 + \lambda h^\alpha), \tag{6.19}$$

$$C \le (1 - \lambda h^\alpha)^{-1} \exp((1 - \lambda h^\alpha)^{-1}). \tag{6.20}$$

Proof. Regarding $|e_{n+1}| \le |p_{n+1}| + |q_{n+1}|$ and using the results (6.12)–(6.14) on the propagation error $|p_{n+1}|$, the following estimates of the global error follow

$$\lambda < 0 : |e_{n+1}| \le \sum_{\nu=1}^{n} c_\nu^\alpha |e_{n+1-\nu}| + |q_{n+1}|, \tag{6.21}$$

$$\lambda > 0 : |e_{n+1}| \le (c_1^\alpha + \lambda h^\alpha)|e_n| + \sum_{\nu=2}^{n} c_\nu^\alpha |e_{n+1-\nu}| + |q_{n+1}|, \tag{6.22}$$

$$\lambda > 0 : |e_{n+1}| \le (1 - \lambda h^\alpha)^{-1} \sum_{\nu=1}^{n} c_\nu^\alpha |e_{n+1-\nu}| + |q_{n+1}|. \tag{6.23}$$

Using Corollary 4.1, especially (4.11), the result of Theorem 6.3 is deduced. □

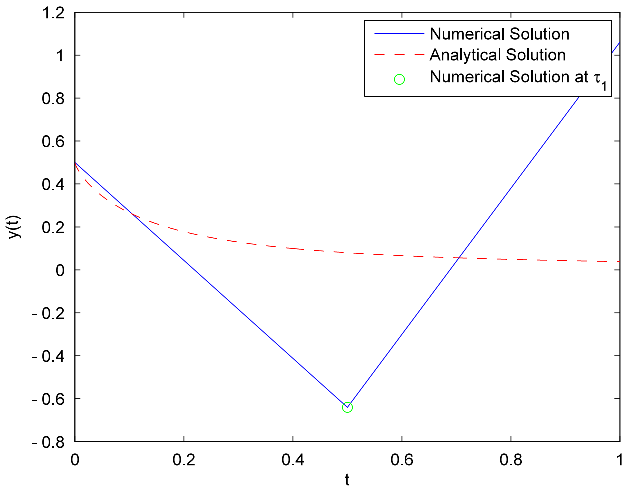

Fig. 7.1. Explicit method for $h = 0.5$.

Remarks. The global error is estimated by the sum of the truncation error of the current step and all other previous steps provided with the strong damping coefficients c_ν^α. In (6.17) we have on the one hand $q_{n+1}, c_1^\alpha q_n$ and on the other hand $c_{n-1}^\alpha q_2, c_n^\alpha q_1$ and know that $q_{n+1} = O(h^{1+\alpha})$ and $c_{n+1}^\alpha = O(h^{1+\alpha})$ for $h \to 0, n \to \infty$ (see (6.11) and Lemma 3.2). In the intermediate terms $c_\nu^\alpha q_{n+1-\nu}$ both effects have influence. Regarding (3.14), (6.11), $(n+1)h = t$ and $\nu(n+1-\nu) \geq n$ it follows that

$$c_\nu^\alpha q_{n+1-\nu} = O\left(h^{1+\alpha}\right) \quad (h \to 0, n \to \infty). \tag{6.24}$$

The estimate (6.17) includes $n+1$ such terms, therefore the asymptotic behavior of

$$\sum_{\nu=1}^{n} \left(\frac{1}{\nu(n+1-\nu)}\right)^{1+\alpha} \tag{6.25}$$

has to be studied in detail. The order of convergence is expected to be one, in accordance with Lemma 2.1.

When the Grünwald–Letnikov scheme is applied to the test equation (5.7) with homogeneous initial value, the first term in the expansion (6.4) and (6.5) of the truncation error is canceled, which yields $q_k = O(h^\alpha)$ for each k. Making the step size smaller the error in the first steps will become smaller. If possible, a problem with inhomogeneous initial value should be transformed into a problem with homogeneous initial value.

Further, the maximal value of the global error over all steps $e_M = \max_\nu |e_\nu|$ is in the size of the truncation error $|q_1|$ in the first step. Therefore it is necessary to construct improved approximations y_k in the first few steps by extrapolation techniques or by using other methods to improve the accuracy of the method. The construction of such a run-up method for the Grünwald–Letnikov scheme is not yet completely solved.

7. Numerical experiments

Numerical experiments for the test equation (5.6) are presented, where the values $\lambda = -4, y_0 = 0.5, \alpha = 0.8$ and $\alpha = 0.5$, respectively, and the interval $[0, 1]$ are chosen. The explicit and implicit Grünwald–Letnikov methods are applied with different step sizes h and figures of the true and numerical solutions are given. The stability condition (5.9) or $|\lambda|h^\alpha \leq 2\alpha$ implies that the explicit method is absolute stable, if the step size satisfies $h \leq 0.318$ in the case of $\alpha = 0.8$, and $h \leq 0.0625$ in the case of $\alpha = 0.5$. The global error $e_\nu = y(\tau_\nu) - y_\nu$ is calculated after the first step $e_A = |e_1|$, at the end $e_B = |e_{N+1}|$, where $(N+1)h = 1$, and as the maximum over all steps $e_M = \max\{|e_\nu|, 1 \leq \nu \leq N+1\}$. The results are given in tables. The abbreviation $\mathrm{E} - k$ denotes 10 to the power $-k$.

(1) *The case* $\alpha = 0.8$.

The explicit method is unstable for $h = 0.5$. The global errors for different h are given:

(2) *The case* $\alpha = 0.5$.

The explicit method is unstable for $h = 0.1$. The global errors for different h are given:

These experiments verify the theoretical results. The error e_A after the first step is equal to the truncation error $|q_1|$, where the first term $\hat{K}_{0,1}^\alpha$ in the expansion (6.4) and (6.5) is independent of h and $y_0|\hat{K}_{0,1}^\alpha|$ is given as 8.9E−3 and 3.2E−2 in the case of $\alpha = 0.8$ and $\alpha = 0.5$, respectively (see Table 3.4). Therefore e_A tends to these values when $h \to 0$, but not monotonically, because in (6.4) and (6.5) there can arise some extinction with negative and positive values. The maximum value of the

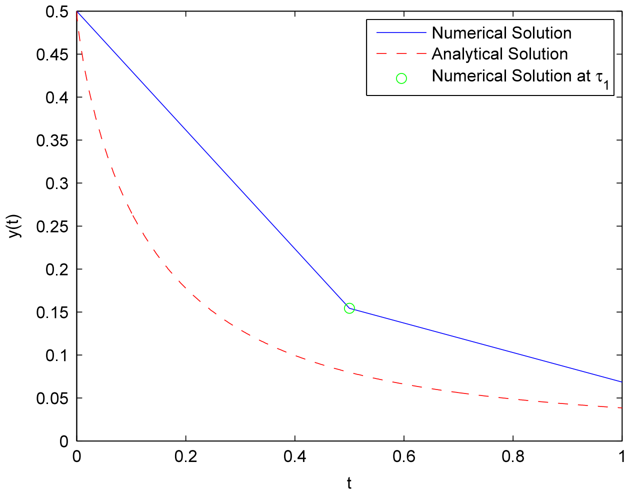

Fig. 7.2. Implicit method for $h = 0.5$.

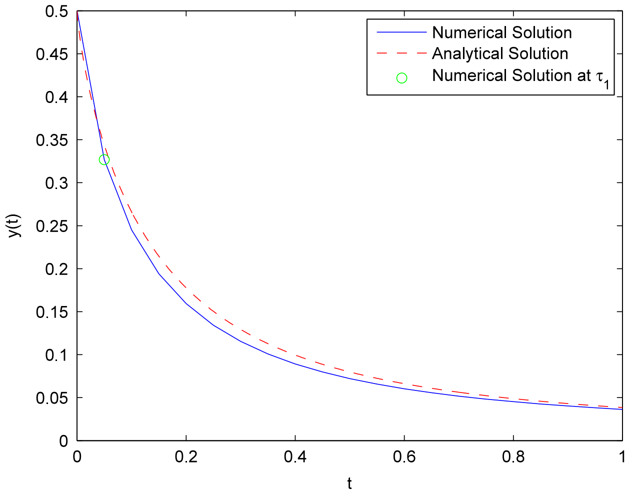

Fig. 7.3. Explicit method for $h = 0.05$.

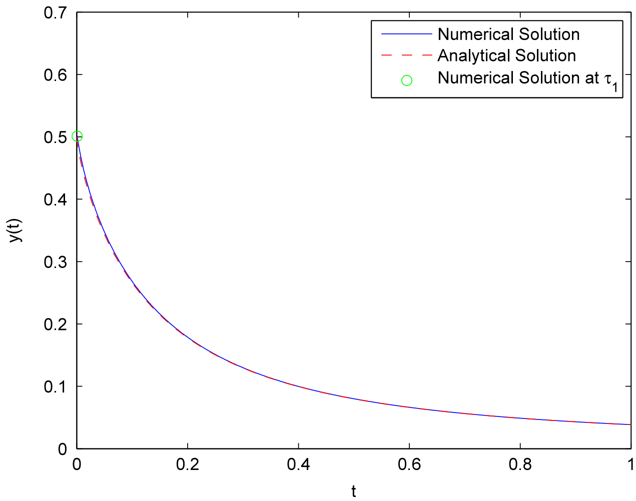

Fig. 7.4. Explicit method for $h = 0.001$.

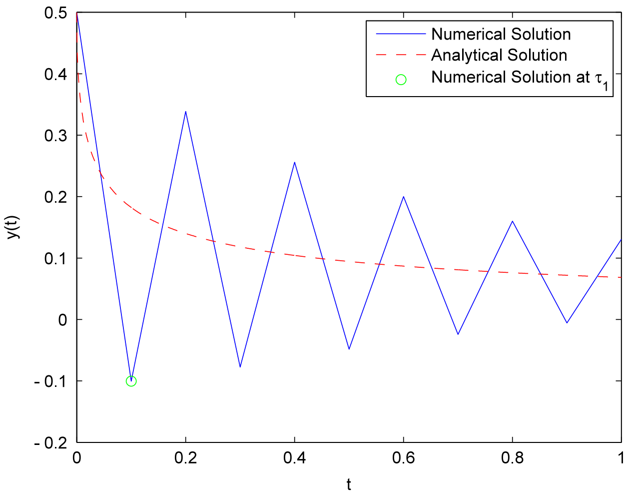

Fig. 7.5. Explicit method for $h = 0.1$.

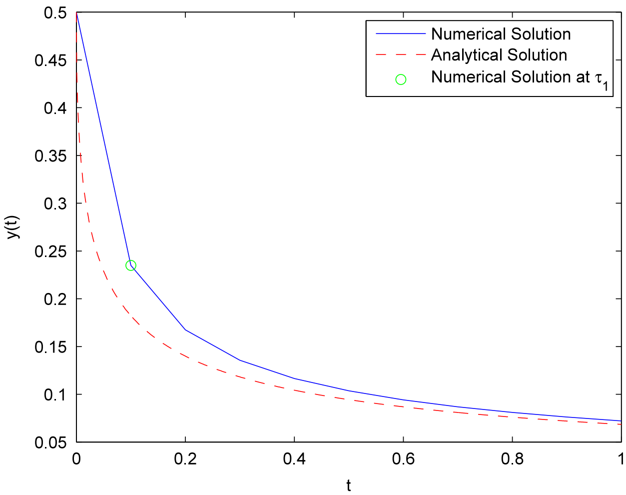

Fig. 7.6. Implicit method for $h = 0.1$.

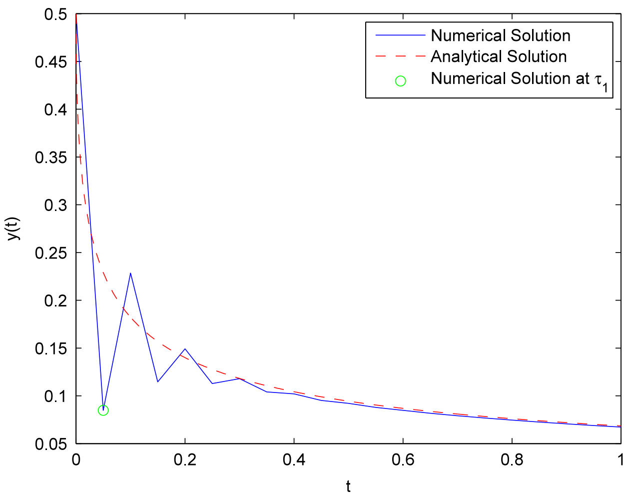

Fig. 7.7. Explicit method for $h = 0.05$.

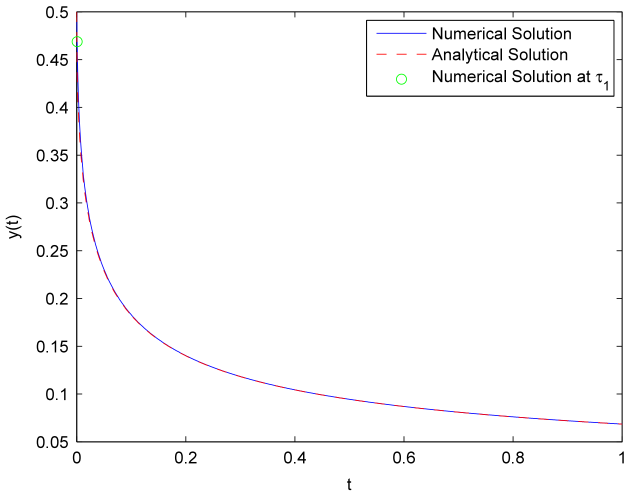

Fig. 7.8. Explicit method for $h = 0.001$.

Table 7.1
Explicit method.

h	0.1	0.05	0.02	0.01	0.005	0.001	0.0001
e_A	7.4E−2	1.7E−2	5.5E−3	9.2E−3	9.9E−3	9.4E−3	9.0E−3
e_M	7.4E−2	2.1E−2	5.5E−3	9.2E−3	9.9E−3	1.0E−2	9.7E−3
e_B	4.5E−3	2.3E−3	8.7E−4	3.8E−4	1.4E−4	3.4E−5	4.9E−5

Table 7.2
Implicit method.

h	0.1	0.05	0.02	0.01	0.005	0.001	0.0001
e_A	4.5E−2	2.9E−2	1.7E−2	1.3E−2	1.1E−2	9.4E−3	9.0E−3
e_M	4.5E−2	2.9E−2	1.8E−2	1.3E−2	1.1E−2	1.0E−2	9.7E−2
e_B	5.2E−3	2.6E−3	1.1E−3	6.1E−4	3.5E−4	1.3E−4	5.9E−5

Table 7.3
Explicit method.

h	0.05	0.02	0.01	0.005	0.001	0.0001
e_A	1.4E−1	4.3E−2	3.3E−3	1.7E−2	3.3E−2	3.4E−2
e_M	1.4E−1	4.3E−2	3.4E−3	1.7E−2	3.3E−2	3.4E−2
e_B	1.1E−3	3.8E−4	1.5E−4	4.4E−5	1.6E−5	1.1E−5

Table 7.4
Implicit method.

h	0.1	0.05	0.02	0.01	0.005	0.001
e_A	5.3E−2	5.2E−2	4.8E−2	4.5E−2	4.2E−2	3.6E−2
e_M	5.3E−2	5.2E−2	4.8E−2	4.5E−2	4.2E−2	3.6E−2
e_B	3.6E−3	1.9E−3	8.2E−4	4.5E−4	2.6E−4	7.6E−5

global error e_M is in the size of e_A. Further, we observe that the method is convergent. The values of the implicit method seem to be more smooth. Altogether, the Grünwald–Letnikov method is a very simple method which delivers qualitatively right approximations. But it is necessary to construct better approximations in the first steps to improve the accuracy of the method. Such a run-up method and further numerical experiments for a larger class of test equations are studied in a forthcoming paper (Figs. 7.1–7.8, Tables 7.1–7.4).

8. Conclusions

In a sense the Grünwald–Letnikov method is an extension of the Euler method. The coefficients are fractional order binomial coefficients, which are recursively defined and positive. The scheme proceeds iteratively but the sum becomes longer and longer. The fractional binomial coefficients act as damping factors producing stability and good error behavior for the Grünwald–Letnikov method. A correction term is necessary in the case of an inhomogeneous initial value, and this term causes some perturbation. In the case of a homogeneous initial value the accuracy seems to be higher than that for the case of a inhomogeneous initial value. The numerical experiments confirm the stability and convergence properties as well as the error estimates. The Grünwald–Letnikov method reproduces the qualitatively right behavior of the solution.

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References

[1] K. Diethelm, The Analysis of Fractional Differential Equations, Springer, Berlin, 2010.
[2] A.A. Kilbas, H.M. Srivastava, J.J. Trujillo, Theory and Applications of Fractional Differential Equations, in: North-Holland Mathematics Studies, vol. 204, Elsevier, Amsterdam, 2006.
[3] V. Kiryakova, Generalized Fractional Calculus and Applications, in: Pitman Research Notes in Math., vol. 301, Longman, Harlow, 1994.
[4] K.S. Miller, B. Ross, An Introduction to the Fractional Calculus and Fractional Differential Equations, Wiley, New York, 1993.
[5] K.B. Oldham, J. Spanier, The Fractional Calculus, Academic Press, New York, London, 1974.
[6] I. Podlubny, Fractional Differential Equations. An Introduction to Fractional Derivatives, Fractional Differential Equations, to Methods of their Solution and Some of their Applications, Academic Press, San Diego, CA, 1999.
[7] S.G. Samko, A.A. Kilbas, O.I. Marichev, The Fractional Integrals and Derivatives. Theory and Applications, Gordon and Breach, Amsterdam, 1993.
[8] L. Boyadjiev, R. Scherer, Fractional extensions of the temperature field problem in oil strata, Kuwait J. Sci. Engrg. 31 (2) (2004) 15–32.
[9] F. Mainardi, The fundamental solutions for the fractional diffusion-wave equation, Appl. Math. Lett. 9 (1996) 23–28.
[10] R.K. Saxena, S.L. Kalla, On the solution of certain fractional kinetic equations, Appl. Math. Comput. 199 (2008) 504–511.
[11] M. Cui, Compact finite difference method for the fractional diffusion equation, J. Comput. Phys. 228 (2009) 7792–7804.
[12] K. Diethelm, N.J. Ford, A.D. Freed, Detailed error analysis for a fractional Adams method, Numer. Algorithms 36 (2004) 31–52.
[13] K. Diethelm, J.M. Ford, N.J. Ford, M. Weilbeer, Pitfalls in fast numerical solvers for fractional differential equations, J. Comput. Appl. Math. 186 (2006) 482–503.
[14] R. Du, W.R. Cao, Z.Z. Sun, A compact difference scheme for the fractional diffusion-wave equation, Appl. Math. Model. 34 (2010) 2998–3007.
[15] P. Kumar, O.P. Agrawal, Numerical scheme for the solution of fractional differential equations of order greater than one, J. Comput. Nonlinear Dyn. 1 (2006) 178–185.
[16] P. Kumar, O.P. Agrawal, An approximate method for numerical solution of fractional differential equations, Signal Process. 86 (2006) 2602–2610.
[17] D.A. Murio, Stable numerical evaluation of Grünwald–Letnikov fractional derivatives applied to a fractional IHCP, Inverse Probl. Sci. Eng. 17 (2009) 229–243.
[18] I. Podlubny, A. Chechkin, T. Skovranek, Y. Chen, B.M. Vinagre Jara, Matrix approach to discrete fractional calculus. II: partial fractional differential equations, J. Comput. Phys. 228 (2009) 3137–3153.
[19] R. Scherer, S.L. Kalla, L. Boyadjiev, B. Al-Saqabi, Numerical treatment of fractional heat equations, Appl. Numer. Math. 58 (2008) 1212–1223.
[20] Z.Z. Sun, X.N. Wu, A fully discrete difference scheme for a diffusion-wave system, Appl. Numer. Math. 56 (2006) 193–209.
[21] C. Tadjeran, M.M. Meerschaert, A second-order accurate numerical method for the two-dimensional fractional diffusion equation, J. Comput. Phys. 220 (2007) 813–823.
[22] V. Daftardar-Gejji, S. Bhalekar, Solving fractional diffusion-wave equations using a new iterative method, Fract. Calc. Appl. Anal. 11 (2008) 193–202.
[23] M. Caputo, Linear models of dissipation whose Q is almost frequency independent II, Geophys. J. R. Astron. Soc. 13 (1967) 529–539.
[24] M. Caputo, Elasticity and Dissipation, Zanichelli, Bologna, Italy, 1969.
[25] R.L. Bagley, P.J. Torvik, A theoretical basis for the application of fractional calculus to viscoelasticity, J. Rheol. 27 (1983) 201–210.
[26] K. Diethelm, N.J. Ford, Numerical solution of the Bagley–Torvik equation, BIT 42 (2002) 490–507.
[27] Y. Ben Nakhi, S.L. Kalla, Some boundary value problems of temperature fields in oil strata, Appl. Math. Comput. 146 (2003) 105–119.
[28] L. Boyadjiev, O. Kamenov, S.L. Kalla, On the Lauwerier formulation of the temperature field problem in oil strata, Int. J. Math. Math. Sci. 2005 (2005) 1577–1588.
[29] I.S. Gradshteyn, I.M. Ryzhik, Tables of Integrals, Series, and Products, 4th ed., Academic Press, New York, 1980.
[30] A. Quateroni, A. Valli, Numerical Approximation of Partial Differential Equations, Springer, Berlin, 1997.