A note on a predictor–corrector method for ordinary fractional differential equations

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Abstract

In this note, we take a second look at a predictor–corrector method which was introduced in a paper by Diethelm, Ford and Freed in 2004 for solving initial value problems for fractional differential equations. One purpose of the present text is the application of a discrete weakly singular Gronwall type inequality to avoid in the main results possible restrictions of the interval of interest for the independent variable. In addition, we present an expansion of the solution which allows, under minimal smoothness conditions, best possible convergence rates for the considered numerical scheme for all fractional orders less than one.

1 Introduction

In the following, we consider a predictor–corrector method introduced by Diethelm, Ford and Freed for solving initial value problems for fractional differential equations, cf. [5] and also [3, Appendix C]. For applications of their results, see e.g., [20, 27]. In the present note, we extent the results in [5] (a) by using a special weakly singular discrete Gronwall inequality and (b) by considering an expansion of the solution which allows best possible convergence rates under minimal smoothness conditions for all fractional orders less than one.

The outline of the paper is as follows. The following section introduces the problem and provides some basics. In Section 3, details of the considered predictor–corrector method are given, where in fact the product rectangle rule and the product trapezoidal rule serve as predictor and corrector, respectively. In Section 4, we employ an expansion assumption on the solution of the considered problem. In addition, we recall some basic error estimates for the two underlying quadrature methods which can be applied directly to the terms occurring in the considered expansion of the solution. In Section 5, we consider a weakly singular discrete Gronwall inequality which is needed to proceed with an estimation of the accumulated error. Meanwhile, it is shown that the considered discrete Gronwall inequality can be derived from a continuous analog. In the concluding section, we present an expansion of the solution which belongs to the class of solutions considered in our basic assumption presented in Section 4, provided that the considered fractional differential equation is sufficiently smooth.

2 Preliminaries

2.1 Fractional integration and differentiation

As a preparation, we recall basic definitions and properties of fractional integration and the Caputo fractional derivative. For any $\beta > 0$, the *Riemann–Liouville fractional integral operator*

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I^β is given by

$$(I^\beta u)(t) = \frac{1}{\Gamma(\beta)} \int_0^t (t-s)^{\beta-1} u(s)\, ds \quad \text{for } 0 \le t \le T,$$

where $u : [\,0,T\,] \to \mathbb{R}$ is an integrable function, and Γ denotes Euler's gamma function. We have, e.g.,

$$I^\beta \frac{t^q}{\Gamma(q+1)} = \frac{t^{q+\beta}}{\Gamma(q+\beta+1)} \quad \text{for } q > -1. \tag{2.1}$$

Other basic properties are as follows (see, e.g., Gorenflo and Vessella [14]):

- $(I^1 u)(t) = \int_0^t u(s)\, ds$, where $u : [\,0,T\,] \to \mathbb{R}$ is an integrable function.
- $(I^\beta u)' = I^\beta u'$ for $u \in C^1[\,0,T\,],\ u(0) = 0$.
- Semigroup property: $I^{\beta+\gamma} = I^\beta I^\gamma$ on $L^1(0,T)$ for $\beta, \gamma > 0$.

For the second identity see, e.g., [11, p. 3] or [17, Corollary 2.2]. We next recall the *Caputo fractional derivative operator*. For $0 < \alpha < 1$, it is given by

$$D^\alpha = I^{1-\alpha} D, \tag{2.2}$$

where D denotes the differentiation operator, i.e., $Du := u'$ for $u \in C^1[\,0,T\,]$. Basic properties are as follows:

- $D^\alpha \frac{t^q}{\Gamma(q+1)} = \frac{t^{q-\alpha}}{\Gamma(q-\alpha+1)}$ for $q \ge 1$.
- $I^\alpha D^\alpha u = u - u(0)$ for $u \in C^1[\,0,T\,]$.
- $D^\alpha I^\alpha u = u$ for $u \in C^1[\,0,T\,], u(0) = 0$.

There exist a variant of the Caputo fractional derivative, cf. [24, Section 2.4], or [3, Definition 3.2], which allows to extent the domain of definition:

$$D^\alpha u = D^\alpha_{\text{RL}}(u - u(0)) \quad \text{for } u \in u(0) + I^\alpha(C[\,0,T\,]), \tag{2.3}$$

where $D^\alpha_{\text{RL}} := D I^{1-\alpha}$ denotes the Riemann–Liouville fractional differential operator.

Both representations (2.2) and (2.3) coincide for $u \in C^1[\,0,T\,]$. However, (2.3) is more appropriate in the context of the fractional differential equations considered below, since equivalence to a Volterra integral equation, cf. (3.1) below, can easily be derived then. Further extensions of the domain of definitions in (2.2) and (2.3) are possible but not needed here. Note that for the extended version (2.3), we still have $D^\alpha u \in C[\,0,T\,]$ due to the semigroup property of fractional integration.

2.2 Initial value problems for fractional differential equations

Throughout this paper, let $0 < \alpha < 1$ and $f : [\,0,T\,] \times \mathbb{R} \to \mathbb{R}$ be a given function, if not further specified. For given $y_0 \in \mathbb{R}$, we consider the following initial value problem for a fractional differential equation:

$$D^\alpha y = f(t,y) \quad \text{for } 0 \le t \le T, \qquad y(0) = y_0, \tag{2.4}$$

with D^α as in (2.3). For applications, see, e.g., the references given in the introduction of [10].

Example 2.1. For $q > 0$ and $0 < \alpha < 1$, the solution of the initial value problem

$$D^\alpha y = \tfrac{t^q}{\Gamma(q+1)} \quad \text{for } \; 0 \le t \le T, \quad y(0) = 0,$$

is given by $y(t) = \frac{t^{q+\alpha}}{\Gamma(q+\alpha+1)}$ for $0 \le t \le T$, cf. the basic properties of the Caputo fractional derivative considered above.

As a preparation for the next example, we recall the classical one-parametric *Mittag-Leffler function* $E_\alpha : \mathbb{C} \to \mathbb{C}$ ($\alpha > 0$) which is given by

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}, \quad z \in \mathbb{C}.$$

This in particular means $E_1 = \exp$. For an introduction to Mittag-Leffler functions and their numerical computation, see, e.g., [12, 13].

Example 2.2. For $\lambda > 0$ and $0 < \alpha < 1$, the solution of the initial value problem

$$D^\alpha y = \lambda y \text{ on } [\,0, T\,], \quad y(0) = y_0,$$

is given by $y(t) = y_0 E_\alpha(\lambda t^\alpha)$ for $0 \le t \le T$, cf. e.g., [3, Theorem 6.11]. In fact:

$$D^\alpha y = \lambda y \text{ on } [\,0, T\,], \quad y(0) = y_0 \Longleftrightarrow y - y_0 = \lambda I^\alpha y \Longleftrightarrow y = (\mathrm{id} - \lambda I^\alpha)^{-1} y_0.$$

By considering the Neumann series for the quasinilpotent operator λI^α and the semigroup property of fractional integration, e.g., on $L^1(0,T)$, we obtain

$$y = \sum_{n=0}^{\infty} \lambda^n I^{\alpha n} y_0 = y_0 \sum_{n=0}^{\infty} \lambda^n \frac{t^{\alpha n}}{\Gamma(\alpha n + 1)} = y_0 \sum_{n=0}^{\infty} \frac{(\lambda t^\alpha)^n}{\Gamma(\alpha n + 1)} = y_0 E_\alpha(\lambda t^\alpha). \qquad \triangle$$

3 Predictor–corrector method based on product rectangle and trapezoidal rule

Fractional integration of the initial value problem (2.4) leads to the following (equivalent) nonlinear, weakly singular Volterra integral equation of second kind on $C[\,0, T\,]$,

$$y = y_0 + I^\alpha f(\cdot, y(\cdot)) \quad \text{on } [\,0, T\,],$$

i.e.,

$$y(t) = y_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} f(s, y(s))\, ds, \quad 0 \le t \le T. \tag{3.1}$$

This representation is the starting point of the predictor–corrector method considered below.

For the quadrature of weakly singular Volterra integrals $(I^\alpha u)(t)$, we make use of the product rectangle rule and the product trapezoidal rule which are recalled next. As a preparation, consider on the interval $[\,0, T\,]$ equidistant grid points

$$t_n = nh \quad \text{for } \; n = 0, 1, \ldots, N, \quad \text{with } \; h = \frac{T}{N}. \tag{3.2}$$

This notation is used throughout the paper without further notice.

3.1 Product rectangle rule

The *product rectangle rule* for the numerical quadrature of $(I^\alpha u)(t_n)$ is of the form

$$h^\alpha \sum_{j=0}^{n-1} b_{n-j} u(t_j) = (I^\alpha u)(t_n) + \tau_n^*(h,u), \qquad n = 1,2,\ldots,N,$$

with weights

$$b_n = \frac{1}{\Gamma(\alpha+1)}\{ n^\alpha - (n-1)^\alpha \} \quad \text{for } n = 1,2,\ldots, \tag{3.3}$$

and $\tau_n^*(h,u)$ denotes the quadrature error of the method at t_n with respect to the function u. The product rectangle rule is obtained by replacing in the weakly singular integral $(I^\alpha u)(t_n)$ the function u on the interval $[\, t_j, t_{j+1} \,]$ by the constant term $u(t_j)$ $(j = 0,1,\ldots,n-1)$, and the resulting integrand including the weakly singular kernel is computed exactly.

For convergence results on the product rectangle rule for solving weakly singular Volterra integral equations of the first kind, see [8]. It is an immediate consequence of the definition in (3.3) that

$$b_n = \mathcal{O}(n^{\alpha-1}) \quad \text{as } n \to \infty. \tag{3.4}$$

Estimates of the quadrature error $\tau_n^*(h,u)$ related with the product rectangle rule may be found in Proposition 4.6 below.

3.2 Product trapezoidal rule

The *product trapezoidal rule* for the numerical quadrature of $(I^\alpha u)(t_n)$ is of the form

$$h^\alpha \sum_{j=1}^{n} a_{n-j} u(t_j) + \widetilde{a}_n u(0) = (I^\alpha u)(t_n) + \tau_n(h,u), \quad n = 1,2,\ldots,N. \tag{3.5}$$

The nonnegative coefficients $a_0, a_1, \ldots$ and $\widetilde{a}_1, \widetilde{a}_2, \ldots$ in (3.5) are given by

$$a_n = \frac{1}{\Gamma(\alpha+2)}\{ (n+1)^{\alpha+1} - 2n^{\alpha+1} + (n-1)^{\alpha+1} \},\ n = 1,2,\ldots,\ a_0 = \frac{1}{\Gamma(\alpha+2)}, \tag{3.6}$$

$$\widetilde{a}_n = \frac{1}{\Gamma(\alpha+2)}\{ (n-1)^{\alpha+1} - n^{\alpha+1} + (\alpha+1)n^\alpha \}, \quad n = 1,2,\ldots\,. \tag{3.7}$$

In addition, $\tau_n(h,u)$ denotes the quadrature error of the method at t_n with respect to the function u. The product trapezoidal rule is obtained by replacing in the weakly singular integral $(I^\alpha u)(t_n)$ the function u on the interval $[\, t_j, t_{j+1} \,]$ by the polynomial of up to first degree that interpolates u at the grid points t_j and t_{j+1} $(j = 0,1,\ldots,n-1)$. The resulting integrand including the weakly singular kernel is computed exactly then.

For convergence results on the product trapezoidal rule for solving weakly singular Volterra integral equations of the first kind, see [8, 9, 23, 25]. There holds

$$a_n = \mathcal{O}(n^{\alpha-1}), \qquad \widetilde{a}_n = \mathcal{O}(n^{\alpha-1}) \quad \text{as } n \to \infty, \tag{3.8}$$

which is left as an exercise. Relevant estimates of the quadrature error $\tau_n(h,u)$ related with the product trapezoidal rule are given in Proposition 4.7 below.

3.3 Predictor–corrector method

Let $0 < \alpha < 1$. We consider the following predictor–corrector method (PCM) for solving the fractional initial value problem (2.4): for $n = 1, 2, \ldots, N$, let

$$y_n = y_0 + h^\alpha \big(\widetilde{a}_n f(0, y_0) + \sum_{j=1}^{n-1} a_{n-j} f(t_j, y_j) + a_0 f(t_n, y_n^{\mathrm{P}}) \big), \tag{3.9}$$

where

$$y_n^{\mathrm{P}} = y_0 + h^\alpha \sum_{j=0}^{n-1} b_{n-j} f(t_j, y_j). \tag{3.10}$$

This means that y_n^{P} and y_n are computed by the product rectangle rule (the predictor) and the product trapezoidal rule (the corrector), respectively. In other terms, we are dealing with a predictor–corrector method for solving the given fractional differential equation, with a fractional variant of the explicit Euler scheme serving as predictor, and a fractional version of the implicit one-step Adams–Moulton method performs as corrector. For an introduction of those classes for nonfractional ODEs, see, e.g., [22].

4 Error analysis

4.1 A first error estimate for the method

Assumption 4.1. Let $0 < \alpha < 1$. In addition, let $f : [\,0, T\,] \times \mathbb{R} \to \mathbb{R}$ satisfy a global Lipschitz condition with respect to the second argument, uniformly in t, i.e.,

$$|\, f(t, u) - f(t, v) \,| \le L |u - v| \quad \text{for } \ u, v \in \mathbb{R}, \ t \in [\,0, T\,], \tag{4.1}$$

with some finite constant $L > 0$. We suppose that a unique solution of the initial value problem (2.4) exists on the considered interval $[\,0, T\,]$. $\triangle$

The Lipschitz condition (4.1) implies uniqueness of the solution, cf. e.g., [4, Theorem 3.3]. Existence of a solution can be guaranteed at least on a sufficiently short range of the independent variable, if f is a continuous function; see, e.g., [3, Theorems 6.1 and 6.5] for details.

In what follows, for given $h = \frac{T}{N}$, we denote by

$$e_n = y_n - y(t_n), \quad n = 0, 1, \ldots, N, \tag{4.2}$$

the errors of the predictor–corrector method at the grid points. We next present a first estimate of the quadrature error of the predictor–corrector method.

Theorem 4.2. *Let the propositions of Assumption 4.1 be satisfied. For the errors (4.2) of the predictor–corrector method (3.9)–(3.10), we have*

$$|\, e_n \,| \le C h^\alpha \sum_{j=1}^{n-1} (n-j)^{\alpha-1} |\, e_j \,| + r_n, \quad \textit{with } \ r_n = \mathcal{O}(\tau_n(h, u)) + h^\alpha \mathcal{O}(\tau_n^*(h, u)),$$

uniformly for $n = 1, 2, \ldots, N$, where $C > 0$ denotes some constant, and $u(t) := f(t, y(t))$ for $0 \le t \le T$.

Proof. We start with the error estimation of the corrector. Utilizing the initial condition $y(0) = y_0$, from (3.9) and (3.5) we obtain

$$
\begin{aligned}
|e_n| &\le h^\alpha \sum_{j=1}^{n-1} a_{n-j} |f(t_j, y_j) - f(t_j, y(t_j))| + h^\alpha a_0 |f(t_n, y_n^{\mathrm{P}}) - f(t_n, y(t_n))| + |\tau_n(h,u)| \\
&\le h^\alpha L \sum_{j=1}^{n-1} a_{n-j} |e_j| + h^\alpha L a_0 |y_n^{\mathrm{P}} - y(t_n)| + |\tau_n(h,u)|.
\end{aligned}
$$

The error of the predictor can be estimated as follows:

$$
\begin{aligned}
|y_n^{\mathrm{P}} - y(t_n)| &\le h^\alpha \sum_{j=1}^{n-1} b_{n-j} |f(t_j, y_j) - f(t_j, y(t_j))| + |\tau_n^*(h,u)| \\
&\le h^\alpha L \sum_{j=1}^{n-1} b_{n-j} |e_j| + |\tau_n^*(h,u)|.
\end{aligned}
$$

We thus arrive at

$$
|e_n| \le h^\alpha L \max\{L a_0 T^\alpha, 1\} \sum_{j=1}^{n-1} (a_{n-j} + b_{n-j}) |e_j| + \mathcal{O}(\tau_n(h,u)) + h^\alpha \mathcal{O}(\tau_n^*(h,u)).
$$

The statement of the theorem now follows from the asymptotics (3.4) and (3.8) of the quadrature weights. ◻

4.2 A solution representation

4.2.1 Basic assumption

As a preparation, for $0 < \lambda < 1$ and $q \in \mathbb{N}_0$, we introduce the spaces

$$
\begin{aligned}
&C^{q,\lambda}[\,0,T\,] = \{\, u \in C^q[\,0,T\,] \mid \exists\, c \ge 0 : |u^{(q)}(s) - u^{(q)}(t)| \le c|s-t|^\lambda \,\}, \\
&C_0^{q,\lambda}[\,0,T\,] := \{\, u \in C^{q,\lambda}[\,0,T\,] \mid u(0) = u'(0) = \cdots = u^{(q)}(0) = 0 \,\},
\end{aligned}
$$

where $C^0[\,0,T\,] := C[\,0,T\,]$.

Assumption 4.3. Let $0 < \alpha < 1$. The solution $y : [\,0,T\,] \to \mathbb{R}$ of $D^\alpha y = f(t,y)$ for $0 \le t \le T,\ y(0) = y_0$, admits a power function expansion of the form

$$
y(t) = y_0 + c_1 t^{\beta_1} + c_2 t^{\beta_2} + \cdots + c_r t^{\beta_r} + \psi_*, \tag{4.3}
$$

with remainder $\psi_* \in I^\alpha(C_0^{1,\alpha}[\,0,T\,]), r \ge 0$, certain coefficients $c_1, c_2, \ldots, c_r \in \mathbb{R}$, and powers that satisfy either $\beta_j = \alpha$ or $2\alpha \le \beta_j < 2\alpha + 1$ for $j = 1, 2, \ldots, r$.

As a consequence of Assumption 4.3, the function $D^\alpha y$ has a power function expansion of the form

$$
f(t, y(t)) = d_0 + d_1 t^{\gamma_1} + d_2 t^{\gamma_2} + \cdots + d_r t^{\gamma_r} + \varphi_*, \tag{4.4}
$$

with remainder $\varphi_* \in C_0^{1,\alpha}[\,0,T\,], r \ge 0$, certain coefficients $d_0, d_1, \ldots, d_r \in \mathbb{R}$, and powers that satisfy $\alpha \le \gamma_j < \alpha + 1$ for $j = 1, 2, \ldots, r$. The expansion (4.4) is the basic ingredient for the numerical analysis considered below.

Example 4.4. For Example 2.1, the conditions of Assumption 4.3 are satisfied, if $q \geq \alpha$ holds. The solution arising in Example 2.2 also satisfies this assumption, with $r = \lceil \frac{1}{\alpha} \rceil + 1$, where $\lceil x \rceil$ denotes the smallest integer larger than or equal to x, and, in addition, $\beta_j = j\alpha$ for $j = 1, 2, \dots, r$.

Remark 4.5. The assumption on the remainder ψ in Assumption 4.3 can be expressed in terms of Hölder spaces. In fact, we have

$$I^\alpha(C_0^{1,\alpha}[\,0,T\,]) = \begin{cases} C_0^{1,2\alpha}[\,0,T\,] & \text{for } \alpha < \frac{1}{2}, \\ C_0^{2,2\alpha-1}[\,0,T\,] & \text{for } \alpha > \frac{1}{2}. \end{cases} \tag{4.5}$$

Note that the case $\alpha = \frac{1}{2}$ is excluded in (4.5). The representation (4.5) can be derived from a seminal paper by Hardy and Littlewood, see [15, Theorems 14, 19 and 20 and their proofs]. Related results may also be found in monographs by Samko, Kilbas and Marichev [24, Theorem 3.1] and Brunner [1, Theorem 8.1.5] and a paper by Li and Cai [19, Theorem 1.7].

4.2.2 The powers in the solution expansion (4.3) for smooth f

For sufficiently smooth functions f, representations (4.3) with exponents of the form

$$\beta_j = k_j + \ell_j \alpha \tag{4.6}$$

and a certain smooth remainder function ψ_* are available, where k_j and ℓ_j are nonnegative integers, not simultaneously vanishing. Below we give some references to the existing literature.

- For a comprehensive treatment of this topic, see Lie, Xie and Zhang [18]. In that paper, the considered intervals for the powers β_j and the degree of smoothness of the remainder function ψ_* differ from those considered in Assumption 4.3.
- In [21], Lubich has shown that an analytic function f allows a representation $y(t) = Y(t, t^\alpha)$, with a function Y that is analytic in a neighborhood of the origin.
- For related results, see Diethelm, Ford and Freed [5], and Daftardar-Gejji, Sukale and Bhalekar [2].

In the appendix, see Section 6, it is shown that for f sufficiently smooth, Assumption 4.3 is exactly satisfied, with exponents that are of the form (4.6). In particular, it turns out that for $\frac{1}{\alpha} \notin \mathbb{N}$, the case $\beta_j = 1$ may be excluded from the expansion. Note that for $\alpha > \frac{1}{2}$, the case $\beta_j = 1$ in (4.6) violates the conditions made in Assumption 4.3.

4.3 Error estimates for the quadrature error

Next we take a closer look at the quadrature errors of the functions appearing in the representation (4.3). For this purpose, we recall some results by Diethelm, Ford and Freed presented in [5] on the quadrature errors of the two product integration methods under consideration; cf. also [3, Appendix C]. We recall the notation from (3.2).

Proposition 4.6 (quadrature error, product rectangle rule)**.** *Let* $0 < \alpha < 1$.

(a) For $u \in C^1[\,0,T\,]$ *we have*

$$\tau_n^*(h,u) = \mathcal{O}(h) \quad \textit{as} \ \ h \to 0 \quad \text{uniformly in } n = 1, 2, \dots, N.$$

(b) For $0 < \gamma < 1$, there holds

$$\tau_n^*(h, t^\gamma) = \mathcal{O}(t_n^{\gamma+\alpha-1} h) \quad \textit{as} \;\; h \to 0 \quad \text{uniformly in } n = 1, 2, \ldots, N.$$

Proof. See [5, Theorem 2.4]. Part (a) also follows from Eggermont [8, proof of Theorem 6.2].

Proposition 4.7 (quadrature error, product trapezoidal rule)**.** *Let $0 < \alpha < 1$.*
(a) For $u \in C^{1,\alpha}[\,0, T\,]$ we have

$$\tau_n(h, u) = \mathcal{O}(h^{\alpha+1}) \quad \textit{as} \;\; h \to 0 \quad \text{uniformly in } n = 1, 2, \ldots, N.$$

(b) For $0 < \gamma < 1$, there holds

$$\tau_n(h, t^\gamma) = \mathcal{O}(t_n^{\alpha-1} h^{\gamma+1}) \quad \textit{as} \;\; h \to 0 \quad \text{uniformly in } n = 1, 2, \ldots, N.$$

(c) For $1 < \gamma < \alpha + 1$, there holds

$$\tau_n(h, t^\gamma) = \mathcal{O}(t_n^{\gamma+\alpha-2} h^2) \quad \textit{as} \;\; h \to 0 \quad \text{uniformly in } n = 1, 2, \ldots, N.$$

Proof. This follows from [5, Theorem 2.5]. □

We note that Propositions 4.6 and 4.7 imply $\tau_n^*(h, t^\gamma) = \mathcal{O}(t_n^{\alpha-1} h)$ for any $\gamma > 0$ and $\tau_n(h, t^\gamma) = \mathcal{O}(t_n^{\alpha-1} h^{\alpha+1})$ for any $\gamma \geq \alpha$, respectively. Below, we utilize those two facts.

As a consequence of Theorem 4.2 and the error representations in Propositions 4.6 and 4.7, we obtain the following corollary. Notice that the quadrature errors $\tau_n^*(h, u)$ and $\tau_n(h, u)$ of the considered product integration rules are linear with respect to the function u, respectively.

Corollary 4.8. *Let the representation (4.3) hold. For the errors of the predictor–corrector method (3.9)–(3.10), we have*

$$|e_n| \leq C h^\alpha \sum_{j=1}^{n-1} (n-j)^{\alpha-1} |e_j| + \mathcal{O}(t_n^{\alpha-1} h^{\alpha+1}), \quad n = 1, 2, \ldots, N, \tag{4.7}$$

uniformly for n, with some constant $C > 0$ which is independent of h.

5 A weakly singular Gronwall inequality

The further treatment of estimate (4.7) requires a special discrete Gronwall type inequality. As a preparation, we consider a suitable (non-discrete) weakly singular Gronwall inequality with a weakly singular inhomogeneity. Such kind of inequalities with constant inhomogeneities or, more general, non-decreasing inhomogeneities are the subject of some research papers or monographs, see, e.g., [1, Lemma 3.1.13] or [7]. Our version deals with an inhomogeneity that has a power-type weak singularity at the origin, cf. Henry [16, Exercise 4, p. 190]. This result may be also easily derived from [26, proofs of corollaries 1 and 3], where an inductive argument is used. See also [28] and the references therein. Below, we use an ordered Banach space argument.

Theorem 5.1. *Let $0 < \alpha < 1$ and $\eta, c > 0$. Then there exists some finite constant $c_1 > 0$ such that for each $\varepsilon \in L^1(0,T)$ satisfying*

$$\varepsilon(t) \le \eta t^{\alpha-1} + c \int_0^t (t-s)^{\alpha-1} \varepsilon(s)\, ds \quad \text{a. e. on } (0,T),$$

there holds

$$\varepsilon(t) \le c_1 \eta t^{\alpha-1} \quad \text{a. e. on } (0,T),$$

where a. e. means almost everywhere.

Proof. We consider a Neumann series expansion of the quasinilpotent operator I^α on $L^1(0,1)$. By using the semigroup property of fractional integration, for $c_2 = c\Gamma(\alpha)$ we obtain the identity

$$(\text{id} - c_2 I^\alpha)^{-1} = \sum_{n=0}^{\infty} c_2^n I^{n\alpha} \text{ on } L^1(0,T). \tag{5.1}$$

This implies, on the one hand, that $\text{id} - c_2 I^\alpha$ is *inverse positive* in the ordered Banach space sense, i.e., for $u \in L^1(0,T)$ we have

$$u - c_2 I^\alpha u \ge 0 \text{ a. e.} \implies u \ge 0 \text{ a. e.} \tag{5.2}$$

From (5.1), in addition it follows that the second-kind linear integral equation

$$F(t) = \eta t^{\alpha-1} + c_2 \int_0^t (t-s)^{\alpha-1} F(s)\, ds, \quad t > 0,$$

is solved by the function

$$F(t) = \eta \Gamma(\alpha) t^{\alpha-1} E_{\alpha,\alpha}(c_2 t^\alpha), \quad t > 0, \tag{5.3}$$

where the analytic *two-parametric Mittag-Leffler function* $E_{\alpha,\beta} : \mathbb{C} \to \mathbb{C}$ $(\alpha, \beta > 0)$ is given by $E_{\alpha,\beta}(z) = \sum_{n=0}^\infty \frac{z^n}{\Gamma(\alpha n + \beta)}$, $z \in \mathbb{C}$. From representation (5.3) it follows that $F(t) \le c_1 \eta t^{\alpha-1}$ for $0 < t \le T$, where c_1 denotes some finite constant. Consideration of $u = F - \varepsilon$ in (5.2) finally implies $\varepsilon \le F \le c_1 \eta t^{\alpha-1}$ on $(\,0, T\,]$. □

We note that the representation (5.3) in the proof above can also be derived easily, e.g., from [12, representations (4.23), (4.45)].

We next present a discrete version of Theorem 5.1. This result may also be found in [6], where it is verified by an inductive argument.

Theorem 5.2 (Weakly singular discrete Gronwall type inequality)**.** *Let c_1 and c_2 be two positive constants. Let N, h and t_n be as in (3.2), and let $v_1, v_2, \ldots, v_N \ge 0$ be given. If*

$$v_n \le c_1 h^\alpha \sum_{j=1}^{n-1} (n-j)^{\alpha-1} v_j + c_2 t_n^{\alpha-1} h^{\alpha+1} \quad \textit{for } n = 1, 2, \ldots, N \tag{5.4}$$

is satisfied, then for some constant c_3 which only depends on c_1, c_2, we have

$$v_n \le c_3 t_n^{\alpha-1} h^{\alpha+1} \quad \textit{for } n = 1, 2, \ldots, N. \tag{5.5}$$

Proof. We apply the generalized Gronwall inequality from Theorem 5.1 with a suitable step function, i.e., $\varepsilon(t) \equiv v_n$ on the interval $(t_{n-1}, t_n]$ for $n = 1, 2, \ldots, N$. For n fixed and any $t_{n-1} < t \le t_n$ we then have, by assumption,

$$\varepsilon(t) = v_n \le c_1 h^\alpha \sum_{j=1}^{n-1} (n-j)^{\alpha-1} v_j + c_2 t_n^{\alpha-1} h^{\alpha+1}.$$

For any $1 \le j \le n-1$, there holds

$$\begin{aligned} h^\alpha (n-j)^{\alpha-1} v_j &\le 2^{1-\alpha} h^\alpha (n-j+1)^{\alpha-1} v_j = 2^{1-\alpha} \int_{t_{j-1}}^{t_j} (t_n - t_{j-1})^{\alpha-1} \varepsilon(s)\, ds \\ &\le 2^{1-\alpha} \int_{t_{j-1}}^{t_j} (t-s)^{\alpha-1} \varepsilon(s)\, ds, \end{aligned}$$

and thus

$$\begin{aligned} \varepsilon(t) &\le c_2 t_n^{\alpha-1} h^{\alpha+1} + c_1 2^{1-\alpha} \int_0^{t_{n-1}} (t-s)^{\alpha-1} \varepsilon(s)\, ds \\ &\le c_2 t^{\alpha-1} h^{\alpha+1} + c_1 2^{1-\alpha} \int_0^t (t-s)^{\alpha-1} \varepsilon(s)\, ds. \end{aligned}$$

The statement of the corollary is now a direct consequence of Theorem 5.1. □

As a consequence of Theorem 5.2 and the error representation in Corollary 4.8, we obtain the following main result of the present paper.

Corollary 5.3. *Let the conditions stated in Assumption 4.1 be satisfied, and let the solution representation (4.3) hold. Then for the error of the predictor–corrector method (3.9)–(3.10), we have*

$$|e_n| = \mathcal{O}(t_n^{\alpha-1} h^{\alpha+1}) \quad \textit{uniformly in } n = 1, 2, \ldots, N \qquad (h \to 0). \tag{5.6}$$

Notice that (5.6) means $|e_n| = \mathcal{O}(h^{2\alpha})$ near the origin, and $|e_n| = \mathcal{O}(h^{\alpha+1})$ away from the origin.

6 Appendix: An expansion of the solution

In this section, we present an expansion of the solution of (2.4). For preparatory discussions, we refer back to Section 4.2.

Theorem 6.1. *For some $T_0 > 0$ and some $\eta > 0$, let $f : [\,0, T_0\,] \times [\,y_0 - \eta, y_0 + \eta\,] \to \mathbb{R}$ be $(m+1)$-times continuously differentiable, with m being the smallest integer satisfying $m\alpha \ge 1$. Then for some $0 < T \le T_0$ small enough, we have the expansion*

$$y(t) = y_0 + c_1 t^\alpha + c_2 t^{2\alpha} + \cdots + c_{m+1} t^{(m+1)\alpha} + e t^{\alpha+1} + (I^\alpha \varphi_*)(t), \quad 0 \le t \le T, \tag{6.1}$$

where $c_1, c_2, \ldots, c_{m+1}, e \in \mathbb{R}$ denote suitable coefficients, and $\varphi_* \in C_0^{1,\alpha}[0,T]$. Here, $y : [\,0, T\,] \to \mathbb{R}$ denotes the (unique) solution of the initial value problem (2.4). In the case $m\alpha = 1$, we may set $e = 0$.

Proof. For functions of the form (6.1), with φ_* replaced by φ, and with the notation

$$p(t) = \sum_{\beta \in \mathcal{A}_\alpha} c_\beta t^\beta, \qquad \mathcal{A}_\alpha := \{\, \alpha, 2\alpha, \ldots, m\alpha, \alpha+1, (m+1)\alpha \,\}, \tag{6.2}$$

the initial value problem (2.4) takes the following form,

$$\varphi = f(\cdot, y_0 + p + I^\alpha \varphi) - D^\alpha p. \tag{6.3}$$

As a further preparation, we consider a Taylor expansion of order m of the function f at $(0, y_0)$,

$$f(t,y) = Y_m(t,y) + R_m(t,y), \qquad Y_m(t,y) = \sum_{k,\ell \ge 0,\, k+\ell \le m} c_{k\ell} t^\ell (y - y_0)^k, \tag{6.4}$$

with suitable coefficients $c_{k\ell} \in \mathbb{R}$, and $R_m(t,y)$ denotes the corresponding Taylor remainder. Below, it turns out that a representation (6.3) can be obtained by performing the following three steps.

- Step 1: We first determine p introduced in (6.2) by using the Taylor polynomial in (6.4): determine the coefficients c_β $(\beta \in \mathcal{A}_\alpha)$ of the function p such that power functions t^β with

$$\beta \in -\alpha + \mathcal{A}_\alpha = \{\, 0, \alpha, 2\alpha, \ldots, (m-1)\alpha, 1, m\alpha \,\} \tag{6.5}$$

  are eliminated from the difference function $Y_m(\cdot, y_0 + p) - D^\alpha p$. This results in a representation of the form

$$Y_m(\cdot, y_0 + p) - D^\alpha p =: q, \quad \text{with } \ q \in \operatorname{span}\{\, t^\beta \mid \beta \ge \alpha + 1 \,\}, \tag{6.6}$$

  which means $q \in C_0^{1,\alpha}[\,0, T\,]$ for any $T > 0$.

- Step 2: We then consider the mapping properties of the operator

$$S\psi := f(\cdot, y_0 + p + \psi) - D^\alpha p. \tag{6.7}$$

  More specifically, we show that $S\psi \in C_0^{1,\alpha}[\,0,T\,]$ for $\psi \in C_0^{1,\alpha}[\,0,T\,]$, if $\|\, \psi \,\|_\infty$ and $T > 0$ are sufficiently small, where $\|\cdot\|_\infty$ denotes the maximum norm of a continuous function. Here and in what follows, such smallness restrictions are always made to guarantee that $f(\cdot, y_0 + p + \psi)$ is well-defined, with one exception at the end of the present proof; there, smallness is required to satisfy a contraction condition.

- Step 3: Finally, we show that the fixed point equation

$$\varphi = f(\cdot, y_0 + p + I^\alpha \varphi) - D^\alpha p \quad \text{on } [\,0, T\,] \tag{6.8}$$

  has a solution $\varphi = \varphi_* \in C_0^{1,\alpha}[\,0,T\,]$, where $T > 0$ is sufficiently small.

(a) First, we consider step 1 in more detail and show that the coefficients c_β for $\beta \in -\alpha + \mathcal{A}_\alpha$, cf. (6.5), can be uniquely determined in increasing order of β.

• For this purpose, we first take a closer look at the Taylor polynomial introduced in (6.4). From identity (2.1) and an application of the multinomial theorem to the powers p^k, it follows that the function $Y_m(\cdot, y_0 + p)$ can be written as a linear combination of power functions of the form

$$\Big(\prod_{\beta \in \mathcal{A}_\alpha} c_\beta^{k_\beta} \Big) t^{\ell + \sum_{\beta \in \mathcal{A}_\alpha} k_\beta \beta} \quad \text{for } \ \ell, k_\beta \in \mathbb{N}_0, \quad k = \sum_{\beta \in \mathcal{A}_\alpha} k_\beta \le m - \ell, \tag{6.9}$$

where $\mathbb{N}_0 := \{\, 0, 1, 2, \ldots \,\}$. Notice that the coefficients of the linear combination of terms considered in (6.9) do not depend on c_β $(\beta \in \mathcal{A}_\alpha)$.

• In (6.9), the powers $\ell + \sum_{\beta\in\mathcal{A}_\alpha} k_\beta\beta$ either belong to $-\alpha + \mathcal{A}_\alpha$ or to $\{\,\beta \mid \beta \ge \alpha + 1\,\}$. Terms with powers belonging to the latter set may be assigned to the function q.

• For $\beta_* \in -\alpha + \mathcal{A}_\alpha$ fixed, we next consider the elimination of the power function t^{β_*} in $Y_m(\cdot, y_0 + p) - D^\alpha p$. This in fact corresponds to the determination of the coefficient $c_{\beta_*+\alpha}$. For this purpose we take a closer look at those power functions in (6.9) whose exponents satisfy the identity $\ell + \sum_{\beta\in\mathcal{A}_\alpha} k_\beta\beta = \beta_*$. The case $k_\beta = 0$ means that c_β in the product in (6.9) has no impact. The other case, $k_\beta \ge 1$, necessarily implies $\beta \le \beta_*$. As a result, the coefficient $c_{\beta_*+\alpha}$, being part of the coefficient of t^{β_*} appearing in $D^\alpha p$, can be determined such that all power functions t^{β_*} occurring in $Y_m(\cdot, y_0 + p) - D^\alpha p$ annihilate.

• We finally note that the case $\ell = 1$, $k = 0$ results in a multiple of the monomial $t = t^1$. It can be eliminated if the Taylor coefficient $c_{01} = \frac{\partial f}{\partial t}(0, y_0)$ from (6.4) vanishes or $m\alpha = 1$ holds.

(b) We next consider step 2 introduced above in more detail, and for this purpose let $\psi \in C_0^{1,\alpha}[\,0, T\,]$ be arbitrary but fixed, with $\|\,\psi\,\|_\infty$ and $T > 0$ sufficiently small. Starting point is again the Taylor expansion (6.4). From a multinomial expansion of the powers $(p + \psi)^k$ and the relation $t^\beta C_0^{1,\alpha}[\,0, T\,] \subset C_0^{1,\alpha}[\,0, T\,]$ for $\beta \ge \alpha$, it follows that $(p+\psi)^k = p^k + r_{1,k}(\psi)$ for some $r_{1,k}(\psi) \in C_0^{1,\alpha}[\,0, T\,]$. This yields

$$Y_m(\cdot, y_0 + p + \psi) = Y_m(\cdot, y_0 + p) + r_1(\psi),$$

with $r_1(\psi) \in C_0^{1,\alpha}[\,0, T\,]$ appropriately chosen. Representation (6.6) then gives

$$D^\alpha p = Y_m(\cdot, y_0 + p + \psi) + q + r_1(\psi), \tag{6.10}$$

with q as in (6.6).

It remains to be verified that the function $R_m(\cdot, y_0{+}p{+}\psi)$ belongs to $C_0^{1,\alpha}[\,0, T\,]$. This follows from a careful consideration of the three terms on the right-hand side of the identity

$$\tfrac{d}{dt} R_m(\cdot, y) = \frac{\partial}{\partial t} R_m(\cdot, y) + \frac{\partial}{\partial y} R_m(\cdot, y)p' + \frac{\partial}{\partial y} R_m(\cdot, y)\psi',$$

where $y = y_0 + p + \psi$. We omit the simple but tedious details, only noting that the inclusion

$$\{\, g \in C^1(0,T] \mid g'(t) = \mathcal{O}(t^{\alpha-1}) \text{ as } t \to 0 \,\} \subset C^{0,\alpha}[\,0, T\,]$$

and estimates of the form

$$\frac{\partial^r}{\partial t^{r_1}\partial y^{r_2}} R_m(t, y) = \mathcal{O}(t^{m+1-r} + |y - y_0|^{m+1-r}), \quad r_1,\, r_2 \ge 0,\ r = r_1 + r_2 \le 2,$$

are applied repeatedly. Note that T has to be chosen sufficiently small to guarantee $|(p + \psi)(t)| \le \eta$ for each $0 \le t \le T$. This completes step 2.

(c) We next consider step 3 introduced above, i.e., in the space $C_0^{1,\alpha}[\,0, T\,]$ we are seeking for a fixed point of the composition operator $\Phi := S \circ I^\alpha$. The following items (i)–(iii) provide some preparations.

(i) As a framework for fixed point theory, we consider the Banach space

$$C_0^1[\,0, T\,] := \{\, \varphi \in C^1[\,0, T\,] \mid \varphi(0) = \varphi'(0) = 0 \,\}, \tag{6.11}$$

equipped with the norm $C_0^1[\,0, T\,] \ni \varphi \mapsto \|\,\varphi'\,\|_\infty$.

(ii) We next list some more properties of the fractional integration operator I^α:

$$\| (I^\alpha \varphi)' \|_\infty \le \tfrac{T^\alpha}{\Gamma(\alpha+1)} \| \varphi' \|_\infty \quad \text{for } \varphi \in C_0^1[0,T], \tag{6.12}$$

$$I^\alpha : C_0^1[0,T] \to C_0^{1,\alpha}[0,T]. \tag{6.13}$$

Property (6.13) follows from [14, Theorem 4.1.4 for $p = \infty$]); cf. also [19, Theorem 1.7], or [24, Theorem 3.1].

(iii) The operator S satisfies a Lipschitz condition, i.e.,

$$\| (S\psi_1)' - (S\psi_2)' \|_\infty \le L \| \psi_1' - \psi_2' \|_\infty \quad \text{for } \psi_1, \psi_2 \in \mathcal{B}(\varrho) \cap C_0^{1,\alpha}[0,T], \tag{6.14}$$
$$\mathcal{B}(\varrho) := \{ \varphi \in C_0^1[0,T] \mid \| \varphi' \|_\infty \le \varrho \},$$

where $T > 0$ and ϱ are chosen sufficiently small, and $L > 0$ denotes some constant which depends on ϱ. The verification of (6.14) is again straightforward; we only note that at some steps of the verification, estimates of the form

$$| \psi(t) | \le t \| \psi' \|_\infty \quad \text{for } 0 \le t \le T, \quad \psi \in C_0^1[0,T], \tag{6.15}$$

are needed. Further details are left to the reader. Notice that from (6.15) it follows that $\| \psi' \|_\infty$ sufficiently small implies $\| \psi \|_\infty$ sufficiently small.

The statements in the items (i)–(iii) allow us to complete step 3. From the two estimates (6.12) and (6.14), it follows that Φ has the following mapping property,

$$\Phi = S \circ I^\alpha : \mathcal{B}(\varrho) \to \mathcal{B}(\varrho), \tag{6.16}$$

and it is moreover a contraction operator with respect to the norm of $C_0^1[0,T]$, provided that $T > 0$ is chosen sufficiently small. Thus, the operator Φ has a unique fixed point in $\mathcal{B}(\varrho)$. From the mapping property stated in step 2, it follows that this fixed point necessarily belongs to $C_0^{1,\alpha}[0,T]$. This completes the proof of the theorem. □

Remark 6.2. Note that the solution representation (6.1) contains a monomial t if only if $\frac{1}{\alpha}$ is an integer. This in particular means that for $\alpha > \frac{1}{2}$, the monomial t is not part of the solution representation. This is of vital significance for the convergence rate obtained for the numerical method considered in this paper,

Acknowledgement

I would like to thank J.-F. Pietschmann (TU Chemnitz) for pointing out reference [26] to me.

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