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Analysis of New Type of Second-order Fractional Linear Multi-step Method with Improved Stability

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ABSTRACT: We present and investigate a new type of implicit fractional linear multi-step method of order two for fractional initial value problems. The method is obtained from the second-order superconvergence of the Grünwald-Letnikov approximation of the fractional derivative at a non-integer shift point. The method coincides with the backward difference method of order two for the classical initial value problem when the order of the derivative is one. The weight coefficients of the proposed method are obtained from the Grünwald weights and are hence computationally efficient compared with that of the fractional backward difference formula of order two. The stability properties are analyzed and it is shown that the stability region of the method is larger than that of the fractional Adams-Moulton method of order two and the fractional trapezoidal method. Numerical results and illustrations are presented to justify the analytical theories.

Keywords: Grünwald approximation; Generating functions; Fractional Adams-Moulton methods; Backward difference method; Super-convergence; Stability regions.

تحليل نوع جديد من الطريقة الكسرية الخطية متعددة الخطوات من الدرجة الثانية مع استقرار محسّن

حنيفة محمد ناصر و خديجة الحسني

الملخص: نقدم في هذا البحث نوع جديد من الطريقة الضمنية الكسرية الخطية متعددة الخطوات من الدرجة الثانية لمشاكل القيمة الأولية الكسرية. يتم الحصول على الطريقة من التقارب الفائق ذو الدرجة الثانية لتقريب جرنوالد للمشتقه الكسريه عند نقطة إزاحة ذات قيمة غير صحيحة. وقد تبين ان هذه الطريقة تتطابق مع طريقة الاختلاف العكسي من الرتبة الثانية لمسئله القيمة الأولية الكلاسيكية عندما يكون ترتيب المشتقه واحدًا. يتم الحصول على معاملات الوزن للطريقة المقترحة من أوزان جرنوالد ، وبالتالي فهي فعالة من الناحية الحسابية مقارنة بمعادلة الفرق الجزئي المتخلف من الدرجة الثانية. تم تحليل خصائص الثبات وتبين أن منطقة الاستقرار للطريقة المقترحة أكبر من منطقة الاستقرارلطريقة أدمز-مولتن الكسرية من الدرجة الثانية وطريقة شبه المنحرف الجزئية. وقد تم عرض النتائج العددية والرسوم التوضيحية لتبرير النظريات التحليلية .

الكلمات المفتاحية: تقريبات جرنوالد، الدالة المولدة ، طرق أدمز-مولتن الكسرية ، طريقة الاختلاف العكسي ، التقارب الفائق ، منطقة الاستقرار.

1. Introduction

Consider the fractional initial value problem (FIVP)

$$ {}_{t_0}^{C}D_t^{\beta} y(t) = f(t, y(t)), \quad t \ge t_0, \quad 0 < \beta \le 1, \qquad (1) $$
$$ y(t_0) = y_0, $$

where ${}_{t_0}^{C}D_t^{\beta}$ is the left Caputo fractional derivative operator of order β defined in Section 2, $f(t,y)$ is a bounded function satisfying the Lipschitz condition in the second argument y guaranteeing a unique solution to the problem [1]. There is no loss in considering the fractional order in the interval $\beta \in (0,1]$. For, when $1 < \beta \le n = \lceil \beta \rceil$, with appropriate initial conditions, the FIVP (1) can be formulated as a system of FIVP of order $0 < \beta/n \le 1$, just as in the case of classical initial value problems (IVPs) with higher integer order derivatives [2].
Fractional calculus, despite its long history, has only recently gained a place in science, engineering, artificial intelligence, and many other fields [3-6].

In the recent past, many numerical methods have been developed for solving (1) approximately. We are interested in the numerical methods of the type commonly known as the fractional linear multi-step methods (FLMMs).

The basic numerical method of FLMM type of consistency order one for (1) is obtained from the Grünwald-Letnikov form for the fractional derivative [7,8]. The weight coefficients for this basic FLMM are the *Grünwald weights* obtained from the series of the generating function $\omega_1(z) = (1-z)^{\beta}$.
Lubich [9] introduced a set of higher-order FLMMs as convolution quadrature methods for the Volterra integral equation (VIE) obtained by reformulating (1) (See also eg. [1]). The quadrature coefficients are obtained from the fractional-order power of a rational polynomial of the generating polynomials for the linear multi-step method (LMM) of classical initial value problems (IVPs). As a particular subfamily of these FLMMs, the fractional backward difference formulas (FBDFs) were also proposed by Lubich in [10]. Another particular form of FLMM type is the fractional trapezoid method of order 2.

Many researchers have utilized these formulations to construct variations of the FLMMs (see eg. [11] and the references therein). Galeone and Garrappa [12] studied some implicit FLMMs generalizing the Adams-Moulton methods for classical IVPs. Galeone and Garrappa [13] and Garrappa [14] have also investigated a set of explicit FLMMs generalizing the Adams-Bashforth methods.
In this paper, we propose and analyze a new type of FLMM of order 2. The method is computationally efficient and has improved stability. We also present algorithms to solve linear and non-linear FIVPs using the proposed FLMM. We also compare the method with other known FLMMs of order 2 and show that the presented method outweighs the other methods in terms of stability and/or computational efficiency.

We classify the previously known FLMMs into subclasses based on the form of their generating functions which indicate that our FLMM presented here falls into a new subclass not encountered in the past literature.

This paper is organized as follows. In Section 2, the preliminaries and previous relevant works are summarized. In Section 3, the new FLMM of order 2 is introduced along with a computational algorithm. Numerical examples for testing the method are given in Section 4. In Section 5, the stability of the method is analyzed. In Section 6, the new method is compared with other FLMMs and Section 7 draws some conclusions.

2. Preliminaries

For a sufficiently smooth function $y(t)$ defined for $t \ge t_0$, the left Riemann-Liouville (RL) fractional derivative of order $0 < \beta \le 1$ is defined by (see eg. [20])

$$ {}_{t_0}^{RL}D_t^{\beta} y(t) = \frac{1}{\Gamma(1-\beta)} \frac{d}{dt} \int_{t_0}^{t} \frac{y(\tau)}{(t-\tau)^{\beta}} d\tau, \quad 0 < \beta \le 1, \qquad (2) $$

where $\Gamma(\cdot)$ is the Euler-Gamma function.
The left Caputo fractional derivative of order $\beta > 0$ is defined as

$$ {}_{t_0}^{C}D_t^{\beta} y(t) = \frac{1}{\Gamma(1-\beta)} \int_{t_0}^{t} \frac{y'(\tau)}{(t-\tau)^{\beta}} d\tau, \quad 0 < \beta \le 1. \qquad (3) $$

In addition to the above two definitions, the Grünwald-Letnikov(GL) definition is useful for numerical approximations of fractional derivatives.

$$ {}_{t_0}^{GL}D_t^{\beta} y(t) = \lim_{h \to 0} \frac{1}{h^{\beta}} \sum_{k=0}^{\infty} g_k^{(\beta)} y(t-kh), \qquad (4) $$

where $g_k^{(\beta)} = (-1)^k \frac{\Gamma(\beta+1)}{\Gamma(\beta-k+1)k!}$ are the *Grünwald weights* and are the coefficients of the series expansion of the *Grünwald generating function*

$$\omega_1(z) = (1-z)^\beta = \sum_{k=0}^{\infty} g_k^{(\beta)} z^k.$$

The coefficients $g_k^{(\beta)}$ can be successively computed by the recurrence relation

$$g_0^{(\beta)} = 1, \qquad g_k^{(\beta)} = \left(1 - \frac{\beta+1}{k}\right) g_{k-1}^{(\beta)}, \quad k = 1,2,\dots . \tag{5}$$

For theoretical purposes, the function $y(t)$ is zero-extended for $t < t_0$, hence the infinite summation in (4). Practically, the upper limit of the sum is $n = \lceil (t - t_0)/h \rceil$.
The three definitions are equivalent under homogeneous initial conditions [8].

2.1 Fractional linear multi-step methods

Among the several numerical methods to solve (1), we list the numerical methods that fall under the category of FLMM.

The fundamental and widely investigated numerical approximation scheme is the Grünwald-Letnikov method (also called the *fractional backward Euler method*) obtained by replacing the fractional derivative operator in (1) with its GA operator δ_h^β of order one [8].

$$\delta_h^\beta y(t) := \frac{1}{h^\beta} \sum_{k=0}^{\infty} g_k^{(\beta)} y(t - kh) = f(t, y) + O(h). \tag{6}$$

By choosing the discretization step h appropriately to align the discrete points $t - kh$ with the endpoints of the problem domain $[0, T]$ and assuming zero extension for the unknown function $y(t)$ for $t < 0$, the infinite sum in (6) is reduced to a finite sum. Dropping the first order error term, choosing $h = T/N, N \in \mathbb{N}$, and denoting

$$t_n = nh, \quad y_n \approx y(t_n) \quad \text{and} \quad f_n = f(t_n, y_n), \tag{7}$$

equation (6) gives the GL scheme

$$\sum_{k=0}^{n} g_k^{(\beta)} y_{n-k} = h^\beta f_n, \quad n = 1,2,\dots,N.$$

A shifted GL approximation of (6) is given by replacing k by $k - r$ and a shifted GL scheme is then given by

$$\sum_{k=0}^{n} g_k^{(\beta)} y_{n-k+r} = h^\beta f_n, \quad n = 1,2,\dots,N, \tag{8}$$

where r is the shift. The shifted scheme is also of the first order when the shift r is an integer. However, at $r = \beta/2$, the scheme (8) gives super-convergence of order 2 [15].

$$\delta_{h,\beta/2}^\beta y(t) := \frac{1}{h^\beta} \sum_{k=0}^{\infty} g_k^{(\beta)} y(t - (k - \beta/2)h) = f(t, y) + O(h^2). \tag{9}$$

However, this super-convergence scheme introduces an additional difficulty in dealing with values of the function y at points not aligned with the grid points [15]. In Section 3, we modify this super-convergence scheme to construct a new scheme of order 2.

A general way to approximate the FIVP (1) is to replace the fractional derivative by the form with general weights w_k as

$$\Omega_h^\beta y(t) := \frac{1}{h^\beta} \sum_{k=0}^{\infty} w_k y(t - kh), \tag{10}$$

where the weights w_k are to be determined for a desired order of consistency. Thus, Grunwald-type approximation schemes for the FIVP have the form expressed in conformance with the classical backward difference form (BDF) as

$$\sum_{k=0}^{n} w_k y_{n-k} = h^\beta f_n, \quad n = 1,2,\dots, \tag{11}$$

where w_k are coefficients in the expansion of some appropriate generating function $w(z)$.
In Lubich [10], the weights w_k in (11) are chosen as the coefficients of the series expansion of the generating function

$$w(z) = \left(\frac{\rho(1/z)}{\sigma(1/z)}\right)^\beta, \tag{12}$$

where ρ, σ are the generating polynomials of the LMM for classical IVP.
It is enough to consider generating functions in the form

$$\delta(\xi) = \left(\frac{a(\xi)}{b(\xi)}\right)^\beta \frac{p(\xi)}{q(\xi)}, \tag{13}$$

where $a, b, p,$ and q are polynomials, and $\xi = 1/z$ [10].

The generating function of an FLMM completely characterizes the approximation scheme, its stability, and the order of consistency through the following theorems.

Theorem 1 [16, 17, 18]. *The order of an FLMM with generating function $\delta(\xi)$ is p if and only if*

$$\frac{1}{x^{\beta}}\delta(e^{-x}) = 1 + O(x^{p}). \tag{14}$$

Moreover, the approximation corresponding to $\delta(\xi)$ satisfies, with D_t^{β} denoting the RL fractional derivative,

$$\delta_h^{\beta} y(t) = D_t^{\beta} y(t) + h^{p} a_p(\beta) D_t^{\beta+p} y(t) + h^{p+1} a_{p+1}(\beta) D_t^{\beta+p+1} y(t) + \ldots,$$

where $y(t)$ is assumed to be sufficiently smooth.

Theorem 2 *[10] The stability region of an FLMM with generating function $\delta(\xi)$ is given by*

$$S = \{\delta(\xi) : |\xi| > 1\}. \tag{15}$$

2.2. Subclasses of FLMMs

We classify the FLMMs in the literature into subclasses. This classification suggests that the proposed FLMM in this paper belongs to a new subclass.

1. *The fractional trapezoid subclass:* The fractional trapezoidal method of order 2 (FT2) obtained from the trapezoidal rule for the ODE has the generating function [10]

$$\delta_{FT2}(\xi) = \left(2\frac{1-\xi}{1+\xi}\right)^{\beta}. \tag{16}$$

It is the only method known so far in the form $\delta(\xi) = \left(\frac{a(\xi)}{b(\xi)}\right)^{\beta}$ with $\deg b(\xi) \geq 1$.

2. *The FBDF subclass:* The fractional backward difference formula (FBDF) [13] obtained from the BDF for classical ODE has generating function of the form $\delta(\xi) = (a(\xi))^{\beta}$. For orders $1 \leq m \leq 6$, a set of six FBDF methods have been obtained with polynomials corresponding to the generating polynomials of the BDF of order m given by $a(\xi) = \sum_{k=1}^{m} \frac{1}{k}(1-\xi)^{k}$. The second order FBDF2, for example, is given by [10]

$$\delta_{FBDF2}(\xi) = \left(\frac{3}{2} - 2\xi + \frac{1}{2}\xi^{2}\right)^{\beta}. \tag{17}$$

3. *Fractional Adams subclass:* The fractional Adams methods have the generating functions of the form $\delta(\xi) = \frac{(1-\xi)^{\beta}}{q(\xi)}$, where the polynomial $q(\xi)$ is determined to have order p of consistency for the method [11—14]. When $q(0) = 0$, the method is explicit and is called fractional Adams-Bashforth methods [13,14] while $q(0) \neq 0$ gives implicit methods which are called fractional Adams-Moulton methods (FAMs)[12]. The second order FAM method is given by the generating function.

$$\delta_{FAM1}(\xi) = \frac{(1-\xi)^{\beta}}{(1-\frac{\beta}{2}) + \frac{\beta}{2}\xi}. \tag{18}$$

4. *Rational polynomial subclass:* In [19], a classical LMM type of approximation is proposed to obtain a class of FLMMs by approximating the generating function of the FBDF methods by rational polynomials in the form $\delta(\xi) = \frac{p(\xi)}{q(\xi)}$. This approach, however, reduces the order of the methods and requires higher degree polynomials p and q, to achieve orders close to the order of FBDF considered.

3. A new fractional linear multi-step method

We present the main result of constructing an FLMM of order 2 which belongs to a new subclass. We need the following lemma from the Taylor series expansion.

Lemma 1 *Let $y(t) \in C^1[a,b]$ and $y''(t)$ exists. Then, for $\mu \in (a,b)$ and $h > 0$, we have*

$$y(t+\mu h) = (1+\mu)y(t) - \mu y(t-h) + O(h^2). \tag{19}$$

The fractional derivative of the FIVP (1) (assuming with no loss $t_0 = 0$ and $y(t_0) = 0$) is replaced by the approximation with super convergence (9) of order 2. This gives, at $t = t_n$,

$$\delta^{\beta}_{h,\beta/2} y(t_n) = \frac{1}{h^\beta}\sum_{k=0}^{\infty} g_k^{(\beta)} y(t_{n-k+\beta/2}) = f(t_n, y(t_n)) + O(h^2). \tag{20}$$

Since $\beta/2$ is not an integer for $0 < \beta \le 1$, the point $t_{n-k+\beta/2}$ in (20) is not aligned with the discrete points in the computational domain $\{t_m, m = 0,1,\dots,N\}$. Using Lemma 1 with $t = t_{n-k}$ and $\mu = \beta/2$, we replace $y(t_{n-k+\beta/2})$ by (19).

$$\frac{1}{h^\beta}\sum_{k=0}^{\infty} g_k^{(\beta)} \left[\left(1+\frac{\beta}{2}\right) y(t_{n-k}) - \frac{\beta}{2} y(t_{n-k-1})\right] = f(t_n, y(t_n)) + O(h^2). \tag{21}$$

With the notations in (7), we obtain the new implicit FLMM approximation scheme

$$\Delta^{\beta}_{h,\beta/2} y_n := \sum_{k=0}^{n} g_k^{(\beta)} \left[\left(1+\frac{\beta}{2}\right) y_{n-k} - \frac{\beta}{2} y_{n-k-1}\right] = h^\beta f_n, \quad n = 1,2,\cdots, \tag{22}$$

where the function values y_{n-k} and y_{n-k+1} are properly aligned with the grid points in the computational domain.
Theorem 3 *The generating function of the new implicit FLMM is given by*

$$\delta(\xi) = (1-\xi)^\beta p(\xi), \tag{23}$$

where $p(\xi) = \left(1+\frac{\beta}{2}\right) - \frac{\beta}{2}\xi$. Moreover, the generating function satisfies

$$\frac{1}{x^\beta}\delta(e^{-x}) = 1 + O(x^2)$$

confirming order 2 consistency.

Proof. The sum on the left side of (21) is manipulated, with $p_0 = 1 + \beta/2$ and $p_1 = -\beta/2$, as follows:

$$\begin{aligned}\sum_{k=0}^{\infty} g_k^{(\beta)}(p_0 y_{n-k} + p_1 y_{n-k-1}) &= p_0 \sum_{k=0}^{\infty} g_k^{(\beta)} y_{n-k} + p_1 \sum_{k=0}^{\infty} g_k^{(\beta)} y_{n-k-1} \\ &= p_0 \sum_{k=0}^{\infty} g_k^{(\beta)} y_{n-k} + p_1 \sum_{k=1}^{\infty} g_{k-1}^{(\beta)} y_{n-k} = \sum_{k=0}^{\infty}\left(p_0 g_k^{(\beta)} + p_1 g_{k-1}^{(\beta)}\right) y_{n-k},\end{aligned} \tag{24}$$

where we have set $g_{-1}^{(\beta)} = 0$. The weights

$$w_k = p_0 g_k^{(\beta)} + p_1 g_{k-1}^{(\beta)}, \quad k = 0,1,\dots \tag{25}$$

are the coefficients of the generating function

$$\delta(\xi) = p_0(1-\xi)^\beta + p_1\xi(1-\xi)^\beta = (1-\xi)^\beta(p_0 + p_1\xi).$$

Moreover, we have

$$\frac{1}{x^\beta}\delta(e^{-x}) = 1 - \frac{\beta(3\beta+5)}{24}x^2 + O(x^3)$$

which, by Theorem 1, confirms the order 2 consistency of the method.

The generating function for the new FLMM is of the form (23) and is different from those subclasses listed in subsection 2.2. Therefore, it can be considered to belong to a new subclass in the family of FLMMs.
The notion of super-convergence and nodal alignment have been applied for space fractional diffusion equations in [15] and [20]. The fractional Adam-Moulton method (FAM1) [12] of order 2 derived from fractional Newton-Gregory functions and Taylor series expansion methods, can also be derived from the super-convergence of the Grünwald approximation in the form

$$\frac{1}{h^\beta}\sum_{k=0}^{\infty} g_k^{(\beta)} y(t_{n-k}) = f_{n-\beta/2} + O(h^2)$$

by replacing the right-hand side with the respective second-order approximations

$$f_{n-\beta/2} = \left(1-\frac{\beta}{2}\right) f_n + \frac{\beta}{2} f_{n-1} + O(h^2). \tag{26}$$

The generating function for the FAM1 is thus given by (18).
Dimitrov et al. [21] formulated an order 2 scheme with super-convergence from asymptotic expansions of the super-convergence. However, the non-aligned points of super-convergence have not been re-aligned in their work.
To the knowledge of the authors, the application of super-convergence of Grünwald approximation for time-fractional differential equations with re-alignments of the super-convergence point has not appeared before in the literature. The following theorem relates the proposed FLMM scheme (22) with the FBDF of order 2 by Lubich [10] and the FAM1 of order 2 by Galeone and Garrappa [12].

Theorem 4 *When* $\beta \to 1$,

1. the new FLMM converges to the BDF2 method of order 2 for the classical ODE by generating polynomial $\delta(\xi) = \frac{3}{2} - 2\xi + \frac{1}{2}\xi^2$.
2. the FAM1 converges to the fractional trapezoid method of order 2 with generating function $\delta(\xi) = 2\frac{1-\xi}{1+\xi}$.

Proof. Immediate by substituting $\beta = 1$ in (18) and (16) respectively.

3.1. Implementation

Here, we give two algorithms to compute the approximate solutions for the FIVP for linear and non-linear cases respectively using the new FLMM.
For brevity, we use the following notations: For a sequence $a = \{a_k\}$, the vector slice $[a_i, a_i + 1, \dots, a_j]$ is denoted by $a_{i:j}$. The convolution of two vectors a, b of size $n + 1$ is denoted by $a * b = \sum_{k=0}^{n} a_k b_{n-k}$.
We reformulate the new FLMM scheme (22) with (24) and (25) as

$$\sum_{k=0}^{n} w_k y_{n-k} = w_{0:n} * y_{0:n} = w_0 y_n + w_{1:n} * y_{0:n-1} = h^\beta f_n. \tag{27}$$

In the case of linear FIVP, we have $f(t, y) = \lambda y(t) + s(t)$ for some constant λ and function $s(t)$. The scheme (27) for this case, with $s_n = s(t_n)$, is then

$$w_0 y_n + w_{1:n} * y_{0:n-1} = h^\beta(\lambda y_n + s_n)$$

which gives

$$y_n = \frac{1}{w_0 - \lambda h^\beta}\left[h^\beta s_n - w_{1:n} * y_{0:n-1}\right], \quad n = 1,2,\dots .$$

Algorithm 1 is given for the linear FIVP.

Algorithm 1 (For linear FIVP)

1. Define $s(t)$ (for $f(t, y) = \lambda y + s(t)$).
2. Input β, λ, h, and N.
3. Define g with $g_0 = 1$, $g_n = \left(1 - \frac{\beta+1}{n}\right) g_{n-1}, \quad n = 1,2, \dots, N$.
4. Define $p = [1 + \beta/2, -\beta/2]$. $w_{0:N} == \{p * g_{k-1:k}, k = 0,1, \dots, N\}$.
5. Define array $\boldsymbol{y} = \{y_k, k = 0,1, \dots, N\}$ and set $y_0 = 0$.
6. For $n = 1,2, \dots, N$
$$y_n = \frac{1}{w_0 - \lambda h^\beta}\left[h^\beta s(t_n) - w_{1:n} * y_{0:n-1}\right].$$
7. Return $\boldsymbol{y}$.

For non-linear FIVP, the non-linear equation (27) in y_n needs to be solved for the unknown y_n. The Newton-Raphson method numerically solves this with an initial seed $y_{n,0} = y_{n-1}$. Algorithm 2 is given for the non-linear FIVP.

Algorithm 2 (For non-linear FIVP)

1. Define $f(t, y), f_y(t, y)$.
2. Input β, h, and N.
3. Define g with $g_0 = 1$, $g_n = \left(1 - \frac{\beta+1}{n}\right) g_{n-1}, n = 1,2, \dots, N$.
4. Define $p = [1 + \beta/2, -\beta/2]$. $w_{0:N} = \{p * g_{k-1:k}, k = 0,1, \dots, N\}$.
5. Define array $\boldsymbol{y} = \{y_k, k = 0,1, \dots, N\}$ and set $y_0 = 0$.
6. $Tolerence = 10^{-15}, Error = 10^8$.
7. For $n = 1,2, \dots, N$
   $x_0 \leftarrow y_{n-1}$.
   $c_n = w_{1:n} * y_{0:n-1}$.
   $Error > Tolerance$
   $F = w_0 x_0 - h^\beta f(t_n, x_0) + c_n$.
   $JF = w_0 - h^\beta f_y(t_n, x_0)$.
   $y_n = x_0 - \frac{F}{JF}$.
   $Error = |y_n - x_0|$.
   $x_0 \leftarrow y_n$.
8. return $\boldsymbol{y}$.

Table 1. Computational order of the new FLMM for example 1.

	$\beta = 0.4$		$\beta = 0.8$		$\beta = 1.0$	
M	Max. Error	Order	Max Error	Order	Max Error	Order
8	6.533e-03	–	1.803e-02	–	2.538e-02	–
16	1.882e-03	1.79544	5.319e-03	1.76094	7.569e-03	1.74543
32	5.052e-04	1.89743	1.449e-03	1.87619	2.078e-03	1.86499
64	1.309e-04	1.94874	3.783e-04	1.93741	5.448e-04	1.93116
128	3.330e-05	1.97438	9.665e-05	1.96858	1.395e-04	1.96533
256	8.400e-06	1.98720	2.443e-05	1.98427	3.530e-05	1.98261
512	2.109e-06	1.99360	6.140e-06	1.99213	8.879e-06	1.99130
1024	5.285e-07	1.99680	1.539e-06	1.99606	2.227e-06	1.99564
2048	1.323e-07	1.99840	3.853e-07	1.99803	5.575e-07	1.99782
4096	3.309e-08	1.99920	9.640e-08	1.99902	1.395e-07	1.99891

Table 2. Computational order of the new FLMM for example 2.

	$\beta = 0.4$		$\beta = 0.8$		$\beta = 1.0$	
M	Max. Error	Order	Max Error	Order	Max Error	Order
8	1.698e-01	–	7.835e-02	–	6.985e-02	–
16	2.779e-02	2.61128	1.978e-02	1.98599	1.769e-02	1.98155
32	6.648e-03	2.06349	5.060e-03	1.96667	4.466e-03	1.98563
64	1.663e-03	1.99866	1.286e-03	1.97645	1.122e-03	1.99286
128	4.186e-04	1.99047	3.245e-04	1.98628	2.812e-04	1.99660
256	1.052e-04	1.99271	8.155e-05	1.99260	7.037e-05	1.99836
512	2.638e-05	1.99566	2.044e-05	1.99616	1.760e-05	1.99920
1024	6.605e-06	1.99764	5.117e-06	1.99804	4.402e-06	1.99960
2048	1.653e-06	1.99877	1.280e-06	1.99901	1.101e-06	1.99980
4096	4.133e-07	1.99938	3.202e-07	1.99950	2.752e-07	1.99990

4. Numerical tests

We used the new FLMM to compute approximate solutions of the FIVP (1) with a linear and a non-linear source function $f(t,y)$ in the time interval $[0,1]$.

Example 1:

$$ {}^{C}D_0^{\beta} y(t) = \frac{\Gamma(m+1)}{\Gamma(m+1-\gamma)} t^{m-\gamma} - \frac{\Gamma(m)}{\Gamma(m-\gamma)} t^{m-1-\gamma} + \lambda y(t) + t^m - t^{m-1}, $$

$y(0) = 0,$

where $\lambda = -1$ and we set $m = 5$. The exact solution is given by $y(t) = t^m - t^{m-1}$.

Example 2:

$$ {}^{C}D_0^{\beta} y(t) = \frac{\Gamma(2\beta+5)}{\Gamma(\beta+5)} t^{\beta+4} - \frac{240}{\Gamma(6-\beta)} t^{(5-\beta)} + (t^{2\beta+4} - 2t^5)^2 - y(t)^2, $$

$y(0) = 0,$

with exact solution $y(t) = t^{2\beta+4} - 2t^5$.

The problems are solved for fractional order values $\beta = 0.4, 0.8$ and 1.0. The computational domain for both problems are $\{t_n = n/M, n = 0,1,\cdots,M\}$ and step size $h = 1/M$, where M is the number of subintervals of the problem domain $[0,1]$. The problems were solved for $M = 2^j, j = 3,4,\ldots,12$.
The computational order of the new FLMM method is computed by the formula

$$ p_{j+1} = \log(E_{j+1}/E_j)/\log(h_{j+1}/h_j) $$

where E_j, h_j are the merror and the step size for $M = 2^j$.

Tables 1 and 2 list the maximum errors and computational orders for Examples 1 and 2 respectively for various grid sizes $M = 8,16,\dots,4096$. The computational orders confirm the theoretical order 2 of the new FLMM.

5. Analysis of linear stability

For the analysis of the stability of an FLMM, we have the following preparations. The analytical solution to the test problem

$$ {}^{C}D_t^{\beta} y(t) = \lambda y(t), \quad y(0) = y_0 $$

is given by $y(t) = E_\beta(\lambda t^\beta) y_0$, where $E_\beta(\cdot)$ is the Mittag-Leffler function

$$ E_\beta(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(\beta k + 1)}. $$

The analytical solution $y(t)$ of the test problem is stable in the sense that it vanishes in the $\beta\pi$-angled region

$$ \Sigma_\beta = \left\{ \xi \in \mathbb{C} : |\arg(\xi)| > \frac{\beta\pi}{2} \right\}, $$

where the angle $\beta\pi/2$ is measured from the positive real axis.
The analytical unstable region is thus the infinite wedge $\{\xi \in \mathbb{C} : |\arg(\xi)| \le \frac{\beta\pi}{2}\} = \mathbb{C}\backslash\Sigma_\beta$.

For the numerical stability of FLMM, we have the following criteria:

Definition 1 *Let S be the numerical stability region of an FLMM. For an angle, α, define the sector*

$$ S(\alpha) = \{\xi : |\pi - \arg(\xi)| < \alpha\}, $$

where the angle α is measured from the negative real axis.
The FLMM is said to be

1. $A(\alpha)$-stable if $S(\alpha) \subseteq S$.
2. A-stable if it is $A(\pi - \beta\pi/2)$-stable. That is, $\Sigma_\beta \subseteq S$.
3. unconditionally stable if it is $A(0)$-stable. That is if the negative real line $(-\infty, 0) \subseteq S$.

We analyze the stability of the new FLMM through its stability region $S = \{\delta(\xi) = (1-\xi)^\beta p(\xi) : |\xi| > 1\} = \mathbb{C}\backslash S^c$, where $S^c = \{\delta(\xi) = (1-\xi)^\beta p(\xi) : |\xi| \le 1\}$ is the unstable region.

Theorem 5 *The unstable region S^c is bounded and symmetric about the real axis. Moreover, For $0 < \beta \le 1$, if the imaginary part of ξ, $\Im(\xi) > 0$, then the real part $\Re(\delta(\xi)) > 0$ and $\Im(\delta(\xi)) < 0$.*

Proof. For the boundedness of S^c, we see that for $|\xi| \le 1$,

$$ |\delta(\xi)| \le (1 + |\xi|)^\beta \left[\left(1 + \frac{\beta}{2}\right) + \frac{\beta}{2}|\xi| \right] \le 2^\beta(1+\beta) < \infty. $$

For the symmetry about the real axis, we immediately see that $\delta(\bar{\xi}) = \overline{\delta(\xi)}$.
For $\xi = e^{i\theta}$, we have

$$ 1 - \xi = \left(e^{-\frac{i\theta}{2}} - e^{\frac{i\theta}{2}} \right) e^{\frac{i\theta}{2}} = 2i\sin\frac{\theta}{2} e^{\frac{i\theta}{2}} = 2\sin\frac{\theta}{2} e^{i(\frac{\theta}{2} - \frac{\pi}{2})} =: be^{i\phi}, $$

where $\phi \equiv \phi(\theta) = \frac{\theta}{2} - \frac{\pi}{2}$ and $b \equiv b(\theta) = 2\sin\frac{\theta}{2} = 2\cos\phi > 0$ for $0 < \theta < 2\pi$.
Now, writing $\delta(\xi) = (1-\xi)^\beta + \beta/2(1-\xi)^{\beta+1}$, we have for the real part of $\delta(\xi)$,

$$ \Re(\delta(\xi)) = b^\beta[\cos\beta\phi + \beta\cos\phi\cos(\beta+1)\phi] =: b^\beta g(\theta) \quad (28) $$

where, with some trigonometric manipulations,

$$ g(\theta) = \left(1 + \frac{\beta}{2}\right)\cos\beta\phi + \frac{\beta}{2}\cos(\beta+2)\phi. $$

Now,

$$g'(\theta) = -\beta\left(1+\frac{\beta}{2}\right)[\sin\beta\phi + \sin(\beta+2)\phi]\phi' = -\frac{1}{2}\beta(2+\beta)\sin(\beta+1)\phi\cos\phi > 0,$$

because, for $0<\theta<\pi$, $\phi \in (-\pi/2, 0)$ where $\cos\phi > 0$ and $(\beta+1)\phi \in [-\frac{(\beta+1)\pi}{2}, 0]$ in the quadrants III and IV for $0<\beta\le 1$ where $\sin(\beta+1)\phi < 0$.

Hence, $g(\theta)$ is increasing with $g(0) = \cos(\beta\pi/2) > 0$. Thus, $g(\theta) > 0$ for $0<\theta<\pi$. It then follows from the symmetry that $\Re(\delta(\xi)) = \Re(\delta(\bar{\xi})) > 0$.
For the imaginary part of $\delta(\xi)$,

$$\Im(\delta(\xi)) = b^{\beta}[\sin\beta\phi + \beta\cos\phi\sin(\beta+1)\phi] =: b^{\beta}h(\theta) < 0, \tag{29}$$

because, when $0<\theta<\pi$, we see that ϕ and $\beta\phi$ are in the quadrant IV where $\cos\phi > 0$ and $\sin\beta\phi < 0$, and $(\beta+1)\phi$ is in the quadrants III and IV where $\sin(\beta+1)\phi < 0$. This gives $\Im(\delta(\xi(\theta)) < 0$ for $0<\theta<\pi$. When $\pi<\theta<2\pi$, we again see that ϕ and $\beta\phi$ are in quadrant I where $\cos\phi > 0$ and $\sin\beta\phi > 0$, and $(\beta+1)\phi$ is in the quadrants I and II where $\sin(\beta+1)\phi > 0$. This gives $\Im(\delta(\xi(\theta)) > 0$ for $\pi<\theta<2\pi$. and the proof is completed.

Theorem 5 tells us that the new FLMM is $A(\frac{\pi}{2})$-stable for $0<\beta\le 1$. We have a stronger result.

Theorem 6 *The FLMM in (22) is A-stable for* $0<\beta\le 1$.

Proof. From (28) and (29), the tangent at $\theta \in [0,\pi]$ on the stability region boundary $\{\delta(\xi): |\xi| = 1\}$ is $h(\theta)/g(\theta)$ with its derivative given by

$$\frac{d}{d\theta}\frac{h(\theta)}{g(\theta)} = \frac{\beta(\beta+1)(\beta+2)\cos^2\phi}{2(g(\theta))^2} > 0.$$

Thus, the tangent is monotonically increasing in $[0,\pi]$ with minimum at $\theta = 0$,

$$(h/g)(0) = -\tan(\beta\pi/2).$$

Therefore, from the symmetry, the unstable region is contained in the wedge $\{\xi: |\arg(\xi)| \le \frac{\beta\pi}{2}\} = \mathbb{C}\backslash\Sigma_{\beta}$ meaning that the new FLMM is *A*-stable.

The *A*-stability confirms that, for $0<\beta\le 1$, our new FLMM is $A(\pi/2)$-stable and hence unconditionally stable.

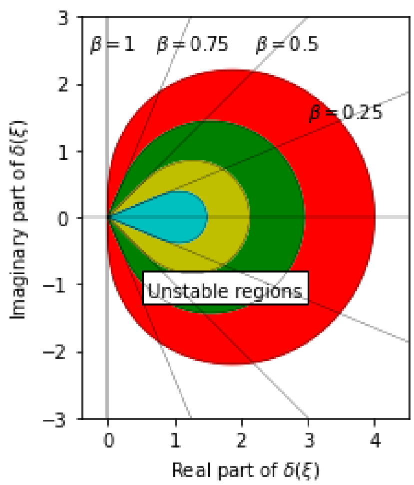


Figure 1. Unstable regions and *A*-stable tangent boundaries for the new FLMM in (23).

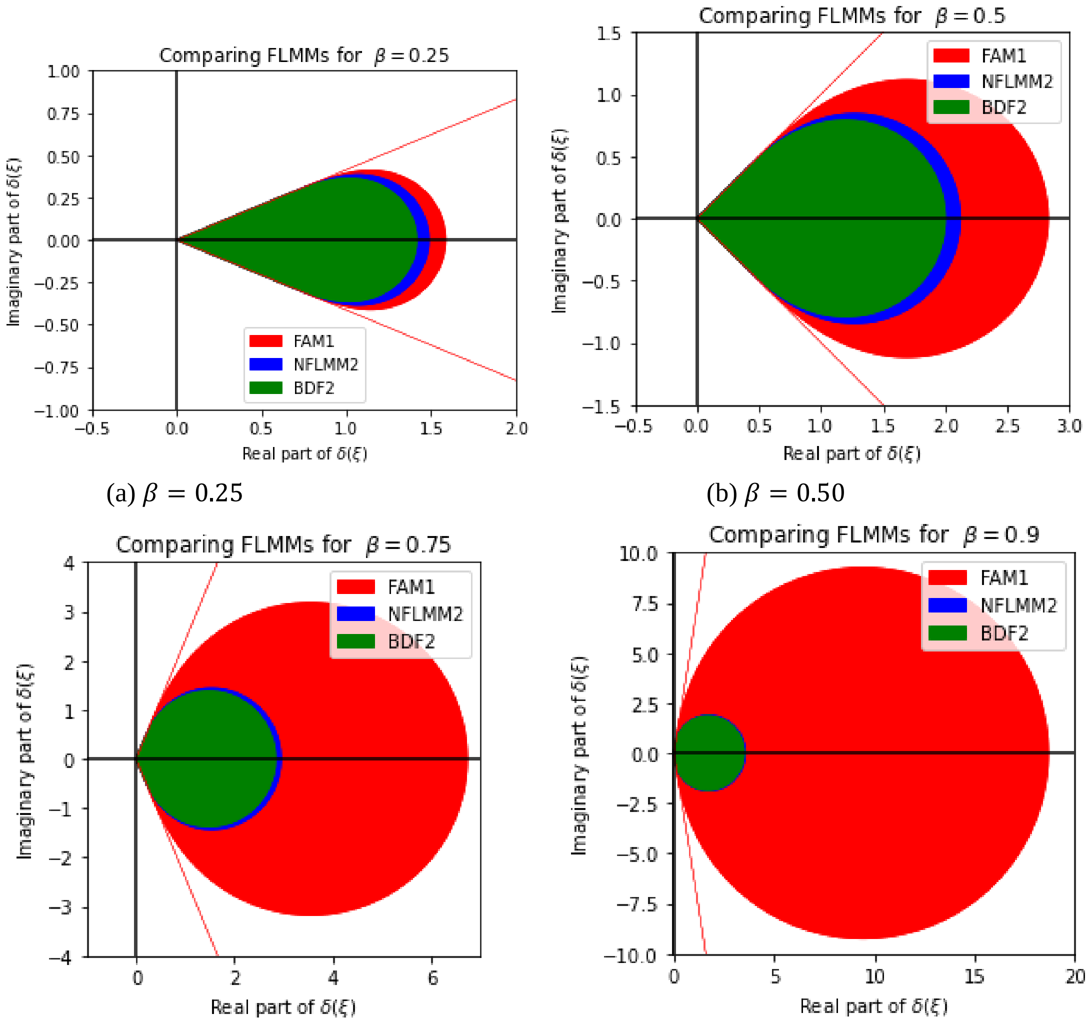
In Figure 1, the unstable regions and the A-stable tangent boundaries of the new FLMM given by the generating function (23) for fractional order values $\beta = 0.25, 0.5, 0.75, 1$ are shown. Note that the unstable region for a generating function $\delta(\xi)$ is given by the graph (see also (15))

$$S^c = \{\delta(\xi) : |\xi| \leq 1\}.$$

6. Comparison of stability regions

We compare the stability regions of previously established implicit FLMMs of order 2 with our new FLMM which we now denote by NFLMM2 for want of an abbreviation.

For this, we consider the Lubich's fractional backward difference method FBDF2 [10], the fractional Adams-Moulton method FAM1 [6] and the fractional Trapezoid rule [10, 22] given by their respective generating functions in (17), (18) and (16).



(a) $\beta = 0.25$ (b) $\beta = 0.50$

(c) $\beta = 0.75$ (d) $\beta = 0.90$

Figure 2. Comparing the unstable regions of FAM1, NFLMM2 and FBDF2 for various β.

In Figure 2, the unstable regions for these FLMMs and our NFLMM2 are shaded for various values of β. Note that the straight lines in the figures depict the boundary of the stability region of the FT2 method in which the left sides of the lines are the stability region which also corresponds to the boundary of the analytical stability regions Σ_β. The unstable regions of FT2 are not shaded for clarity.

The advantage of our NFLMM2, in terms of the unstable regions (UR), is that the UR of the NFLMM2 is smaller than that of the FAM1 and is very much closer to the UR of the FBDF2. Also, the UR of the FT2 is the largest among all the URs.

We note this from the observation that the unstable regions (see also the figures in Figure 2) satisfy the ordering

$$\delta_{FBDF2}(-1) < \delta_{NFLMM2}(-1) < \delta_{FAM1}(-1) < \delta_{FT2}(-1) = +\infty.$$

The computational costs of all the FLMMs of order 2 in the general form (11) are the same. Therefore, the efficiency of the methods is measured by the computational cost of the weights w_k in (11).

The weights w_k of NFLMM2 have the simplest computational effort as they involve only a linear combination of the Grünwald weights $g_k^{(\beta)}$ given in (25) which can be recursively computed by (5) with only one previous weight.

In contrast, the weights of FBDF2 require computations using Miller's formula (see eg. [12]) with two previous weights.

The weights of FAM1 require more effort as its generating function involves a rational function. However, in this case, the right-hand side of the FAM1 scheme has the form (26) with almost the same computational effort as NFLMM2. Nevertheless, the right-hand side of this scheme requires two coefficients and two values of the function $f(t, y)$ requiring an additional memory [6].
Finally, computing the weights for FT2 needs more effort as it requires the first n coefficients of its generating function and FFT [12].

7. Conclusion

We proposed and analyzed a new FLMM of order two for FIVPs that falls under a new subclass of FLMM. The new FLMM is as A-stable as the other known order two methods. However, the proposed method has a larger stability region than that of the FAM1 and FT2 methods. The computational cost of the NFLMM2 is better than that of the FBDF2 method, whereas the FAM1 requires an additional memory requirement in its iterations. Hence, the proposed method can be considered competitive with the other methods of order 2 in terms of stability and/or computational cost.

Conflict of interest

The authors declare no conflict of interest.

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