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New fractional linear multi-step methods of order four with improved stabilities

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Abstract

We present two implicit fractional linear multi-step methods (FLMM) of order four for fractional initial value problems. These FLMMs are of a new type that has not appeared before in the literature. The methods are obtained from the second order super-convergence of the Grünwald-Letnikov approximation of the fractional derivative at a non-integer shift point, taking advantage of the fact that the error coefficients of this super-convergence vanish not only at first order, but also at the third order terms.

The weight coefficients of the methods are obtained from the Grünwald weights and hence computationally efficient compared with that of the fractional backward difference formula method of order four.

The stability regions of the proposed methods are larger than that of the fractional Adams-Moulton method and the fractional backward difference formula method. Numerical results and illustrations are presented to justify results.

Keywords: Lubich generating functions. super convergence. $A(\alpha)$-stability. fractional Adams-Moulton methods. fractional backward difference methods.

1 Introduction

Consider the fractional initial value problem (FIVP)

$$ {}_0^C D_t^\beta y(t) = f(t, y(t)), \quad t \geq 0, \quad 0 < \beta \leq 1, \tag{1a} $$

$$ y(0) = y_0, \tag{1b} $$

where ${}_0^C D_t^\beta$ is the left Caputo fractional derivative operator defined in Section 2, $f(t, y)$ is a source function satisfying the Lipschitz condition in the second argument y guaranteeing a unique solution to the problem (DIETHELM, 2010).

Fractional calculus and fractional differential equations, despite their long history, have only recently gained places in science, engineering, artificial intelligence and many other fields.

Many numerical methods have been developed in the recent past for solving (1) approximately. We are interested in the numerical methods of type commonly known as fractional liner multi-step methods (FLMM).

Lubich (LUBICH, 1985) introduced a set of higher order FLMMs as convolution quadratures for the Volterra integral equation (VIE) obtained by reformulating (1) (See also eg. (DIETHELM, 2010)). The quadrature coefficients are obtained from the fractional order power of the rational polynomial of the generating functions of linear multi-step method (LMM) for ordinary differential equations (ODEs). As a particular subfamily of these FLMMs, the fractional backward difference formulas (FBDFs) were also proposed by Lubich in (LUBICH, 1986). Other forms of FLMM are the fractional trapezoidal method of order 2 and the fractional Adams methods.

In this work, we propose two fourth order implicit FLMMs of new type that does not come under the subfamilies of FLMMs listed in Section 2. The weight coefficients of the methods are obtained from the simple Grünwald weights and has an improved stability region compared to the previously known FLMMs of order four.

2 Prelimineries

For a sufficiently smooth function $y(t)$ defined for $t \geq t_0$, the left Riemann-Liouville (RL) fractional derivative of order $\beta > 0$ is defined by (see eg. (PODLUBNY, 1999))

$$ {}_{t_0}D_t^\beta y(t) = \frac{1}{\Gamma(m-\beta)} \frac{d^m}{dx^m} \int_{t_0}^{t} \frac{y(\tau)}{(t-\tau)^{\beta-m+1}} d\tau, \quad m-1 < \beta \leq m, \tag{2} $$

where $m = \lceil \beta \rceil$ – the smallest integer larger than or equal to β.

The left Caputo fractional derivative of order $\beta > 0$ is defined as

$$ {}_{t_0}^C D_t^\beta y(t) = \frac{1}{\Gamma(m-\beta)} \int_{t_0}^{t} \frac{y^{(m)}(\tau)}{(t-\tau)^{\beta-m+1}} d\tau, m-1 < \beta \leq m, \tag{3} $$

where $y^{(m)}$ is the m-th derivative of y.

Often, for practical reasons, the integer ceiling m of the fractional order β is considered to be one or two. In this paper, we investigate the case of $0 < \beta \leq 1$ when $m = 1$. Further, there is no loss in generality in the assumptions $t_0 = 0$ and $y(0) = 0$.

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

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

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* $W_1(z) = (1-z)^\beta = \sum_{k=0}^{\infty} g_k^{(\beta)} z^k$. The coefficients can be successively computed by the recurrence relation

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

For theoretical purposes, the function $y(t)$ is zero extended for $t < 0$ and hence the infinite summation in the GL formulation (4). Practically, the upper limit of the sum is $n = [t/h]$, where $[\cdot]$ is the integer part function.

The three definitions in (2)–(4) are equivalent under homogeneous derivative conditions at the initial point (PODLUBNY, 1999).

2.1 Numerical approximations of fractional derivatives

For numerical approximation of the fractional derivative, the GL definition is commonly used by dropping the limit in (4) giving the Grunwald Approximation (GA) for a fixed step h (OLDHAM; SPANIER, 1974).

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

A more general Grünwald type approximation is given by the shifted Grunwald approximation (SGA) (MEERSCHAERT; TADJERAN, 2004).

$$\delta_{h,r}^\beta y(t) = \frac{1}{h^\beta} \sum_{k=0}^{\infty} g_k^{(\beta)} y(t - (k-r)h), \tag{7}$$

where r is the shift parameter.

For an integer shift r, the SGA is of order one consistency (MEERSCHAERT; TADJERAN, 2004). However, it is shown in (NASIR; GUNAWARDANA; ABEYRATHNA, 2013) that the SGA gives a second order approximation at a non-integer shift $r = \beta/2$ displaying super convergence.

$$\delta_{h,\beta/2}^\beta y(t) = {}_0^{GL}D_t^\beta y(t) + O(h^2). \tag{8}$$

Some higher order Grünwald type approximations with shifts have been presented in (GUNARATHNA; NASIR; DAUNDASEKERA, 2019) with the weight coefficients obtained from some generating functions in an explicit form according to the order and shift requirements.

2.2 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.

Lubich (LUBICH, 1986) presented and studied numerical approximation methods for the FIVP (1) through some convolution quadrature for the equivalent Volterra integral equation of the FIVP.

An analogous equivalent formulation for the FIVP is also given in (GALEONE; GARRAPPA, 2008) in the classical LMM form

$$\sum_{k=0}^{s} w_{n,k}^{(\beta)} y_k + \sum_{k=0}^{n} w_k^{(\beta)} y_{n-k} = h^\beta f_n, \tag{9}$$

where $w_k^{(\beta)}$ are the coefficients of the series expansion of the generating function $w(\xi) = \left(\frac{\rho(1/\xi)}{\sigma(1/\xi)}\right)^{\beta}$ with (ρ, σ) are the generating polynomials of the LMM for ODEs and $w_{n,k}^{(\beta)}$ are starting weights to compensate the reduction of order of convergence for certain class of solution functions having singular derivatives at the initial point.

This FLMM have some subclasses in the literature with generating functions of the following general forms:

1. **Fractional Trapezoidal rule:** The fractional trapezoidal method of order 2 (FT2) obtained from the trapezoidal rule for the ODE has the generating function

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

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

2. **Fractional backward difference formula:** The fractional backward difference formula (FBDF) obtained from the BDF for ODE has the generating functions of the form $\delta(\xi) = (a(\xi))^{\beta}$.

   For orders $1 \leq m \leq 6$, a set of 6 FDBFm methods have been obtained in (LUBICH, 1986) with polynomials corresponding to the generating polynomials of the BDF of order m given by
   $w_m(\xi) = \left(\sum_{k=1}^{m} \frac{1}{k}(1-\xi)^k\right)^{\beta}$.

3. **Fractional Adams methods:** The fractional Adams methods have the generating functions of the form $\delta(\xi) = \frac{(a(\xi))^{\beta}}{q(\xi)}$, where the polynomial $a(\xi)$ is one of the polynomials in FBDF methods and $q(\xi)$ is determined to have a specified order of consistency for the method. Often, $a(\xi) = 1-\xi$ (see (GALEONE; GARRAPPA, 2006),(GALEONE; GARRAPPA, 2008),(GALEONE; GARRAPPA, 2009),(GARRAPPA, 2009)). However, other polynomials in the FBDF have also appeared in the literature (BONAB; JAVIDI, 2020),(HERIS; JAVIDI, 2018).

   When $q_0 = 0$, the method is explicit and is called fractional Adams-Bashforth methods (FABs) (GALEONE; GARRAPPA, 2009; GARRAPPA, 2009). $\sigma_0 \neq 0$ gives implicit methods called fractional Adams-Moulton methods (FAMs).

4. A new type of second order FLMM is proposed in this journal by the present authors having generating function $\delta(\xi) = (1-\xi)^{\beta} p(\xi)$.

5. **Rational approximation:** In (ACETO; MAGHERINI; NOVATI, 2015), a classical LMM type of approximation is proposed to obtain a class of FLMMs by rational approximations of the FBDF generating functions. These methods have generating functions in the rational polynomial form $\delta(\xi) = \frac{p(\xi)}{q(\xi)}$.

3 New FLMMs of order four

We present the main result of constructing two new FLMMs of order 4.

The fractional derivative in (1a) is replaced by the super convergence approximation (8) of order two. This gives at $t = t_n$, with the error coefficient of order 2:

$$\delta^{\beta}_{h,\beta/2}y(t_n) = \frac{1}{h^{\beta}}\sum_{k=0}^{\infty} g_k^{(\beta)} y(t_n - (k-\beta/2)h) = {}_0D_t^{\beta}y(t_n) + a_2h^2\, {}_0D_t^{2+\beta}y(t_n) + O(h^4)$$
$$= (I + a_2h^2D^2)f(t_n, y(t_n)) + O(h^4), \qquad (10)$$

where $a_2 \equiv a_2(\beta) = \frac{\beta}{24}$ and $D^2 = d^2/dx^2$ is the second differential operator.

Note that the super-convergence approximation diminishes all the odd order terms of h^1, h^3, etc.

Now, we perform two approximation on the super-convergence equation (8).

First, since $k - \beta/2$ is not integer for $0 < \beta \leq 1$, the point $t_n - (k-\beta/2)h$ is not aligned with the discrete points of the computational domain $\{t_m, m = 0, 1, ..., N\}$.

We approximate this non-aligned function value by an order 4 approximation using function values at the nodal points

$$y\left(t_n - \left(k - \frac{\beta}{2}\right)h\right) = b_0y(t_{n-k}) + b_1y(t_{n-k+1}) + b_2y(t_{n-k+2}) + b_3y(t_{n-k+3}) + O(h^4), \qquad (11)$$

where $t_{n-m} = t_n - mh$ and

$$b_0 = \frac{1}{48}(\beta+2)(\beta+4)(\beta+6), \qquad b_1 = -\frac{1}{16}\beta(\beta+4)(\beta+6)$$
$$b_2 = \frac{1}{16}\beta(\beta+2)(\beta+6), \qquad b_3 = -\frac{1}{48}\beta(\beta+2)(\beta+4).$$

Next, the differential operator D^2 is approximated by the order 2 backward difference approximation given by

$$D^2g(x) = \frac{1}{h^2}(2g(x) - 5g(x-h) + 4g(x-2h) - g(x-3h)) + O(h^2)$$

which gives for the function $f(t_n, y(t_n)) =: F(t_n)$

$$h^2D^2F(t_n) = (2F(t_n) - 5F(t_n - h) + 4F(t_n - 2h) - F(t_n - 3h)) + O(h^4). \qquad (12)$$

Substituting (11) and (12) in (8), dropping the error term $O(h^4)$, choosing $h = T/N, N \in \mathbb{N}$, and denoting $t_k = kh$, $y_k \approx y(t_k)$ and $f_k = f(t_k, y_k)$, for $k = 0, 1, ..., N$, we obtain a new implicit FLMM approximation scheme of order 4:

$$\sum_{k=0}^{n} g_k^{(\beta)} \left(b_0y_{n-k} + b_1y_{n-k-1} + b_2y_{n-k-2} + b_3y_{n-k-3}\right)$$
$$= h^{\beta}[f_n + a_2(2f_n - 5f_{n-1} + 4f_{n-2} - f_{n-3})], \quad n = 1, 2, ..., N. \qquad (13)$$

Again, the second differential operator D^2 can also be approximated by the order 2 difference formula

$$D^2g(x) = \frac{1}{h^2}(3g(x-h) - 8g(x-2h) + 7g(x-3h)) - 2g(x-4h) + O(h^2)$$

which gives for the function $f(t_n, y(t_n)) =: F(t_n)$

$$h^2 D^2 F(t_n) = (3F(t_n - h) - 8F(t_n - 2h) + 7F(t_n - 3h)) - 2F(t_n - 4h) + O(h^4). \quad (14)$$

Substituting (11) and (14) in (8), we obtain another new implicit FLMM approximation scheme of order 4:

$$\sum_{k=0}^{n} g_k^{(\beta)} \left(b_0 y_{n-k} + b_1 y_{n-k-1} + b_2 y_{n-k-2} + b_3 y_{n-k-3}\right)$$
$$= h^\beta [f_n + a_2(3f_{n-1} - 8f_{n-2} + 7f_{n-3} - 2f_{n-4})], \quad n = 1, 2, ..., N. \quad (15)$$

The coefficients in the new FLMMs (13) and (15) are linear combinations of the Grünwald weights $g_k^{(\beta)}$ and thus does not involve any heavy computations.

Theorem 1 *The new FLMMs in* (13) *and* (15) *are consistent of order 4 and has the generating function of the form*

$$\delta(\xi) = (1 - \xi)^\beta \frac{p(\xi)}{q(\xi)}, \quad (16)$$

with $p(\xi) = b_0 + b_1\xi + b_2\xi^2 + b_3\xi^3$ *for both FLMMs, and* $q(\xi) = 1 + a_2(\beta)(2 - 5\xi + 4\xi^2 - \xi^3)$ *for* (13) *and* $q(\xi) = 1 + a_2(\beta)(3\xi - 8\xi^2 + 7\xi^3 - \xi^4)$ *for* (15).

To the best our knowledge, this form of generating functions has not been appeared in the previously known FLMMs in the literature.

4 Numerical tests

We used the proposed new FLMMs to compute approximate solutions of the non-linear FIVP

$$D^\beta y(t) = f(t, y), \quad 0 \le t \le 1, \quad 0 < \beta \le 1,$$
$$y(0) = 0.$$

where

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

The exact solution of the problems is given by $y(t) = t^{2\beta+4} - 2t^5$.

The problem was solved with fractional orders $\beta = 0.4, 0.6$ and 0.8. The computational domain of the problem is $\{t_n = n/N, n = 0, 1, ..., N\}$ and step size $h = 1/N$, where N is the number of subintervals of the problem domain $[0, 1]$. The problem was computed for $N_j = 2^j$, $j = 5, 6, ..., 11$.

The computational order of the 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 Maximum error and the step size for the computational domain size M_j.

Tables 1 and 2 list the results obtained in the computations for the proposed FLMM4.1 and FLMM4.2 respectively for $\beta = 0.4, 0.6$ and 0.6.

	$\beta = 0.4$		$\beta = 0.6$		$\beta = 0.8$	
N	Max. Error	Order	Max Error	Order	Max Error	Order
32	2.553e-05	–	1.694e-05	–	6.289e-06	–
64	1.636e-06	4.00210	1.077e-06	3.93178	3.919e-07	4.14632
128	1.036e-07	3.94879	6.791e-08	3.95412	2.446e-08	4.00795
256	6.520e-09	3.96417	4.262e-09	3.97538	1.528e-09	4.00417
512	4.089e-10	3.98062	2.670e-10	3.98764	9.547e-11	4.00182
1024	2.560e-11	3.99019	1.671e-11	3.99387	5.966e-12	4.00082
2048	1.606e-12	3.99509	1.051e-12	3.99694	3.723e-13	4.00045

Table 1: Computational order of the new FLMM4.1

	$\beta = 0.4$		$\beta = 0.6$		$\beta = 0.8$	
N	Max. Error	Order	Max Error	Order	Max Error	Order
32	1.042e-05	–	8.593e-06	–	3.657e-06	–
64	6.572e-07	3.98706	5.433e-07	3.98340	2.281e-07	4.00305
128	4.129e-08	3.99244	3.415e-08	3.99159	1.424e-08	4.00150
256	2.588e-09	3.99612	2.141e-09	3.99581	8.895e-10	4.00075
512	1.619e-10	3.99804	1.340e-10	3.99789	5.558e-11	4.00038
1024	1.013e-11	3.99856	8.385e-12	3.99825	3.473e-12	4.00030
2048	6.375e-13	3.99036	5.314e-13	3.98000	2.165e-13	4.00364

Table 2: Computational order of the new FLMM4.2

5 Stability regions and comparisons

For the analysis of stability of a FLMM, the analytical solution of the test problem ${}^{C}D^{\beta}y(t) = \lambda y(t), y(0) = y_0$ is given by $y(t) = E_{\beta}(\lambda t^{\beta})y_0$, where $E_{\beta}(\cdot)$ is the the Mittag-Leffler function

$$E_{\beta}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(\beta k + 1)}. \tag{17}$$

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

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

where the angle $\beta\pi/2$ is measured from the positive real axis of the complex plane. The analytical unstable region is thus the infinite wedge with angle $\beta\pi$ complement to the analytical stability region Σ_{β}.

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

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

$$S(\alpha) = \{z : |\arg(z) - \pi| \leq \alpha\},$$

where α is measured from the negative real axis of the complex plane. 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, the negative real line $(-\infty, 0) \subseteq S$.*

We denote our new FLMMs in (13) and (15) as NFLMM4.1 and NFLMM4.2 respectively.

We compare the stability regions of previously established implicit FLMMs of order 4 with our new FLMMs. For this, we consider the Lubich's FBDF4 (LUBICH, 1986) and the FAM3(GALEONE; GARRAPPA, 2008) given by their respective generating functions

$$\delta_{FBDF4}(\xi) = \left(\frac{25}{12} - 4\xi + 3\xi^2 - \frac{4}{3}\xi^3 + \frac{1}{4}\xi^4\right)^{\beta},$$

and

$$\delta_{FAM3}(\xi) = \frac{(1-\xi)^{\beta}}{\gamma_0 + \gamma_1\xi + \gamma_2\xi^2 + \gamma_3\xi^3},$$

where

$$\gamma_0 = 1 - \frac{5}{6}\beta + \frac{11}{48}\beta^2 - \frac{1}{48}\beta^3, \qquad \gamma_1 = \frac{31}{24}\beta - \frac{9}{16}\beta^2 + \frac{1}{16}\beta^3,$$
$$\gamma_0 = -\frac{7}{12}\beta + \frac{7}{16}\beta^2 - \frac{1}{16}\beta^3, \qquad \gamma_1 = \frac{1}{8}\beta - \frac{5}{48}\beta^2 + \frac{1}{48}\beta^3.$$

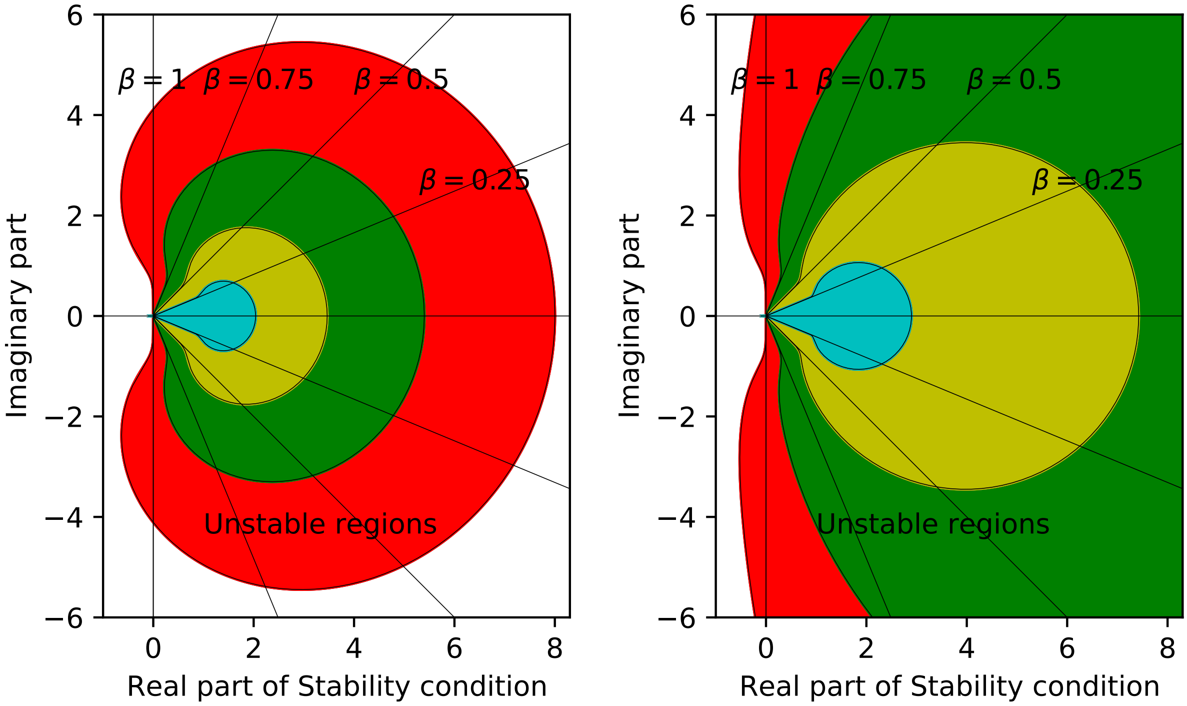
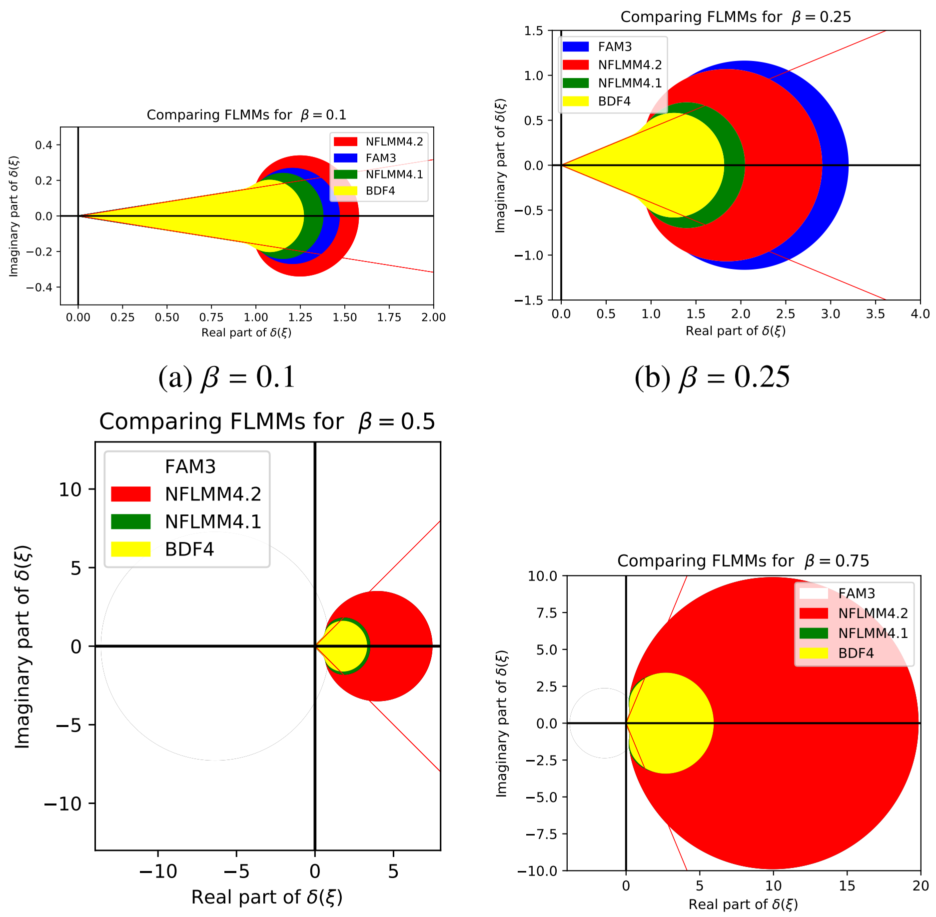


Figure 1: Unstable regions for the new FLMM4.1 and FLMM4.2

From the Dahlquist's second barrier for FLMM (see (GALEONE; GARRAPPA, 2008)), it is clear that order 4 methods are not A-stable. However, $A(\pi/2)$-stability and $A(0)$-stability could be measuring tools for comparing the FLMM methods of orders higher than 2.

In Figure 1, the unstable regions of the proposed two FLMMs for various values of β are illustrated. Here, the straight lines in the figures depicts the A-stable boundaries of the analytical stability region where the left side of the lines are the analytical stability regions Σ_β for various β values. Note that the unstable regions surpasses the A-stable boundaries for all values of β. This confirms that the methods are not A-stable.



(a) $\beta = 0.1$ (b) $\beta = 0.25$

(c) $\beta = 0.5$ $\beta = 0.75$

Figure 2: Comparing the FLMMs of order 4

As for the $A(\pi/2)$-stability, we see from the figure that the unstable regions are on the right side of the complex plane for many values of β. However, there are values of β for which the unstable region peeks in to the left side as well, for example $\beta = 1$.

We numerically computed the intervals for β where the FLMMs are $A(\pi/2)$-stable. Table 3 gives the values β^* for which the intervals $0 < \beta \leq \beta^*$ gives the $A(\pi/2)$-stability.

NFLMM4.1	FBDF4	NFLMM4.2	FAM3
0.82960	0.843895	0.8501118	0.4384471

Table 3: Upper bound β^* for $A(\pi/2)$-stability

As we see, the NFLMM4.2 has the highest interval for β for $A(\pi/2)$ stability followed by FBDF4, NFLMM4.1 and FAM3. The FAM3 has a far lower interval size in this sense.

Note also that the A(0)-stability of FAM3 is destroyed as β passes the $A(\pi/2)$-stability bound β^*. The stability region for $\beta > \beta^*$ becomes bounded and falls in the left side of the complex plane (GALEONE; GARRAPPA, 2008) displaying only conditional stability.

As, for the computational efficiency, the weights of the NFLMMs have the simplest computational effort as they involve only a linear combinations of the Grünwald coefficients $g_k^{(\beta)}$. Obviously, the weights of FBDF4 require computations by the Miller's formula with four previous weights.

6 Conclusion

We proposed two new type of FLMMs of order 4 for FIVPs. The new FLMMs are $A(\pi/2)$-stable for a larger interval of the fractional order compared with known order 4 FAM3. Moreover, the proposed methods outweighs the other methods in terms of computational cost as well.

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