Revista Eletrônica Paulista de Matemática

ISSN 2316-9664
v. 22, n. 2, set. 2022
Edição Brazilian Symposium on Fractional Calculus

A new type of fractional linear multi-step method with improved stability

Haniffa Mohamed Nasir
Sultan Qaboos University
nasirh@squ.edu.om

Khadija Al-Hasani
Sultan Qaboos University
s13639@student.squ.edu.om

Abstract

We present a new type of implicit fractional linear multi-step method (FLMM) of order two for fractional initial value problems. The method is obtained from the second order super convergence of the Grünwald-Letnikov form of the fractional derivative at a non-integer shift point in the domain. The proposed method coincides with the classical BDF method of order two for ordinary initial value problems when the fractional order of the derivative is one. The weight coefficients of the proposed method are obtained from the Grünwald weights and hence computationally efficient compared with the fractional backward difference formula of order two (FBDF2). The stability region of the FLMM is larger than that of the fractional Adams-Moulton method of order two and the fractional trapezoidal method, and is very much closer in size to the FBDF2. Numerical result and illustrations are presented to justify the claims.

Keywords: Lubich Generating functions. super convergence. A-stability. fractional Adams-Moulton methods. Trapezoidal rule.

1 Introduction

Consider the fractional initial value problem (FIVP)

$$
\begin{aligned}
{}_{0}^{C}D_{t}^{\beta} y(t) &= f(t, y(t)), \quad t \geq 0, \quad 0 < \beta \leq 1, && \text{(1a)}\\
y(0) &= y_0, && \text{(1b)}
\end{aligned}
$$

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).

The basic numerical method of FLMM type of order one for (1) is obtained from the Grünwald-Letnikov form for the fractional derivative (PODLUBNY, 1999; OLDHAM; SPANIER, 1974). The weight coefficients for this basic FLMM are the *Grünwald weights* obtained from the series of the generating function $(1 - z)^{\beta}$.

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 a second order implicit FLMM of a new type that does not come under the above mentioned subfamilies of FLMMs. The weight coefficients of the method are obtained from the simple Grünwald weights and has an improved stability region compared to the previously known FLMMs of order 2.

2 Preliminieries

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))

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

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

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

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 $\delta(\xi) = \left(\frac{a(\xi)}{b(\xi)}\right)^\beta$.

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 with polynomials corresponding to the generating polynomials of the BDF of order m given by $a(\xi) = \sum_{k=1}^{m} \frac{1}{k}(1-\xi)^k$.

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. **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.

3 A new form of FLMM

We present the main result of constructing a new FLMM of order 2.

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

$$\delta^{\beta}_{h,\beta/2}y(t_n) = \frac{1}{h^{\beta}}\sum_{k=0}^{\infty} g_k^{(\beta)} y(t_n - (k - \beta/2)h) = f(t_n, y(t_n)) + O(h^2). \tag{10}$$

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 $\{t_m, m = 0, 1, ..., N\}$. Replace it with an order 2 approximation using points in the computational domain as follows:

$$y\left(t_n - \left(k - \frac{\beta}{2}\right)h\right) = \left(1 + \frac{\beta}{2}\right)y(t_n - kh) - \frac{\beta}{2}y(t_n - (k-1)h) + O(h^2). \tag{11}$$

Dropping the error term $O(h^2)$, choosing $h = T/N, N \in \mathbb{N}$ and denoting $t_n = nh$, $y_n \approx y(t_n)$ and $f_n = f(t_n, y_n)$, we obtain the new FLMM implicit approximation scheme

$$\sum_{k=0}^{\infty} g_k^{(\beta)}\left[\left(1 + \frac{\beta}{2}\right)y_{n-k} - \frac{\beta}{2}y_{n-k-1}\right] = h^{\beta}f_n, \quad n = 1, 2, \cdots. \tag{12}$$

The coefficients in the new FLMM (12) are linear expressions of the Grünwald weights $g_k^{(\beta)}$ and thus does not involve any extra computations.

Theorem 1 *The new FLMM in* (12) *is consistent with order 2 and has the generating function*

$$\delta(\xi) = (1-\xi)^{\beta}p(\xi), \tag{13}$$

where $p(\xi) = \left(1 + \frac{\beta}{2}\right) - \frac{\beta}{2}\xi$.

Remark: When $\alpha = 1$, the new FLMM coincides with the BDF method of order 2 for ODE with the generating polynomial $\rho(t) = \frac{3}{2} - 2\xi + \frac{1}{2}\xi^2$.

4 Numerical Tests

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

$$\begin{aligned} D^{\beta}y(t) &= f(t, y), \quad 0 \leq t \leq 1, \quad 0 < \beta \leq 1, \\ y(0) &= 0. \end{aligned}$$

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 $\{t_n = n/M, n = 0, 1, \cdots, M\}$ and step size $h = 1/M$, where M is the number of subintervals of the problem domain $[0, 1]$. The problem was computed for $M_j = 2^j$, $j = 3, 4, ..., 12$.

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.

Table 1 list the results obtained in the computations.

	$\beta = 0.4$		$\beta = 0.6$		$\beta = 0.8$	
M	Max. Error	Order	Max Error	Order	Max Error	Order
8	1.698e-01	–	9.070e-02	–	7.835e-02	–
16	2.779e-02	2.61128	2.169e-02	2.06382	1.978e-02	1.98599
32	6.648e-03	2.06349	5.503e-03	1.97912	5.060e-03	1.96667
64	1.663e-03	1.99866	1.398e-03	1.97644	1.286e-03	1.97645
128	4.186e-04	1.99047	3.534e-04	1.98446	3.245e-04	1.98628
256	1.052e-04	1.99271	8.888e-05	1.99117	8.155e-05	1.99260
512	2.638e-05	1.99566	2.229e-05	1.99530	2.044e-05	1.99616
1024	6.605e-06	1.99764	5.583e-06	1.99758	5.117e-06	1.99804
2048	1.653e-06	1.99877	1.397e-06	1.99877	1.280e-06	1.99901
4096	4.133e-07	1.99938	3.494e-07	1.99938	3.202e-07	1.99950

Table 1: Computational order of the new FLMM

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

$$E_{\beta}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(\beta k + 1)}. \tag{14}$$

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

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

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 $(-\infty, 0) \subseteq S$.*

In Figure 1, the unstable regions of the new FLMM for various values of β are given along with their A-stable boundary lines. This shows that the new FLMM is A-stable for $0 < \beta \leq 1$.

We compare the stability regions of previously established implicit FLMMs of order 2 with our new FLMM (We call this NFLMM2 in this section for want of an abbreviation).

For this we consider the Lubich's FBDF2 (LUBICH, 1986), the FAM1(GALEONE; GARRAPPA, 2008) and the fractional Trapezoidal rule (FT2) (LUBICH, 1986), (GARRAPPA, 2015) given by their respective generating functions

$$\delta_{FBDF2}(\xi) = \left(\frac{3}{2} - 2\xi + \frac{1}{2}\right)^{\beta}, \quad \delta_{FAM1}(\xi) = \frac{(1-\xi)^{\beta}}{(1-\frac{\beta}{2}) + \frac{\beta}{2}\xi}$$

and

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

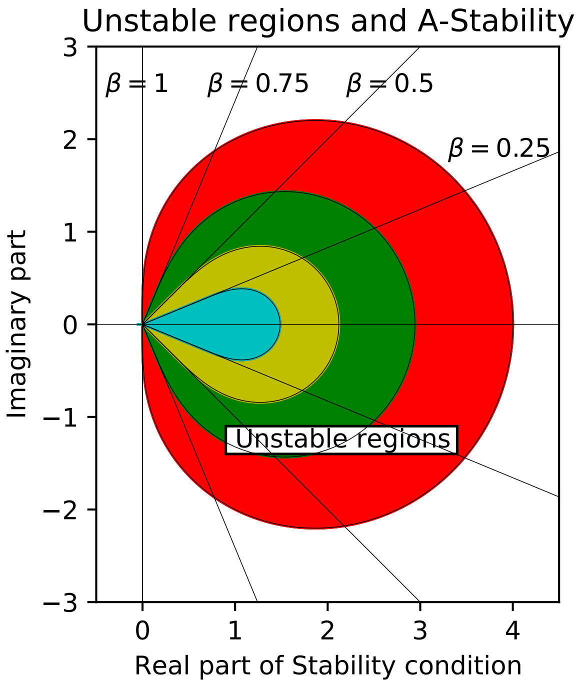


Figure 1: Unstable regions and A-stable boundaries for the new FLMM

It is known that the three methods are also A-stable (GALEONE; GARRAPPA, 2008; GARRAPPA, 2015; LUBICH, 1986). Hence, they are competitive with the NFLMM2 in this sense. Note that the straight lines in the figures depicts the boundary of the stability region of the FT2 method where the left side of the lines are the stability regions. Also note that these line correspond to the boundary of the analytical stability region Σ_{β} as well.

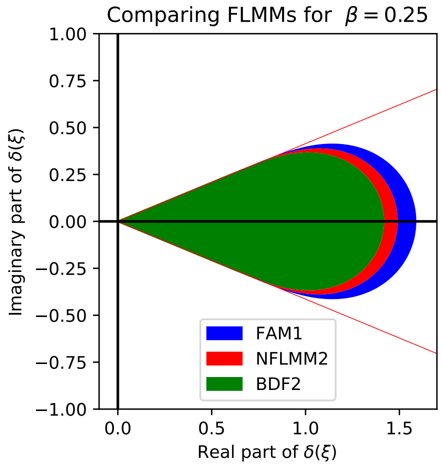
The advantage of our NFLMM2 is, in terms of the stability regions (SR), is that the SR of the NFLMM2 is larger than that of FAM1 and is very much close to the SR of the FBDF2. Also, the SR of the FT2 is smallest of all the other FLMMs having the largest unstable region.

The observation is confirmed by the relations of the longest points of the boundaries of the unstable regions (see also the figures in Figure 2)

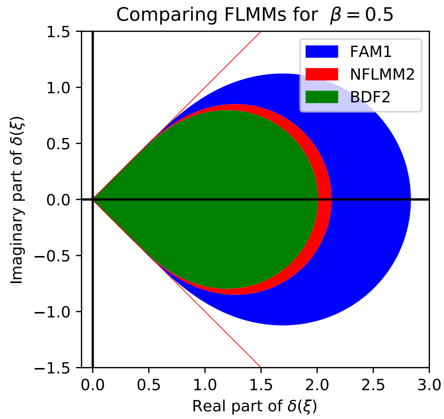
$$\delta_{FBDF2}(-1) < \delta_{NFLMM2}(-1) < \delta_{FAM1}(-1) < \delta_{FT2}(-1) = +\infty.$$

and, for $|\xi| \leq 1$, by the relations of the unstable regions

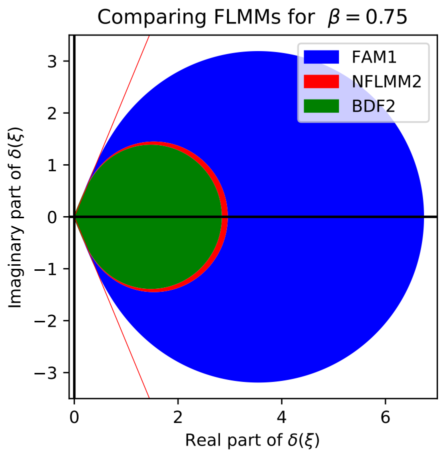
$$S_{FBDF2} \subset S_{NFLMM1} \subset S_{FAM1} \subset S_{FT2}. \tag{15}$$



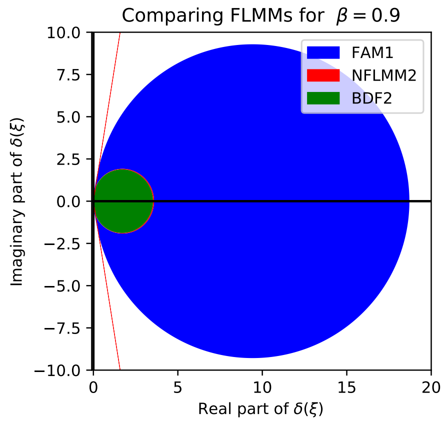
(a) $\beta = 0.25$



(b) $\beta = 0.50$



(c) $\beta = 0.75$



(d) $\beta = 0.90$

Figure 2: Comparing the FLMMs of order 2

Another interesting observation is that, as β approaches 1, the SR of FAM1 shrinks to the SR of FT2 while the SR of our NFLMM2 enlarges to the SR of FBDF2.

As, for the computational efficiency, the weights w_k of NFLMMs has the simplest computational effort for the weight coefficients w_k as they involve only a linear combinations the Grünwald coefficients $g_k^{(\beta)}$. Obviously, the weights of FBDF2 requires computation by the Miller's formula with two previous weights.

The weights of FAM1 can be computed with the same amount of computation as that of NFLMM2. However, the right hand side of FAM1 requires two function values of $f(t, y)$. The weights of FT2 need more efforts as they require the first n coefficients of its generating function and requires FFT to compute them (GARRAPPA, 2015).

6 Conclusion

We proposed a new type of FLMM of order 2 for FIVPs. The new FLMM is A-stable as the other known order 2 FLMM methods. However, the proposed method outweighs the other methods in terms of stability regions and computational cost.

References

ACETO, L.; MAGHERINI, C.; NOVATI, P. On the construction and properties of m-step methods for fdes. **SIAM Journal on Scientific Computing**, Philadelphia, v. 37, n. 2, p. A653–A675, 2015.

BONAB, Z. F.; JAVIDI, M. Higher order methods for fractional differential equation based on fractional backward differentiation formula of order three. **Mathematics and Computers in Simulation**, Amsterdam, v. 172, p. 71–89, 2020.

DIETHELM, K. **The analysis of fractional differential equations**: an application-oriented exposition using operators of caputo type. Berlin: Springer, 2010.

GALEONE, L.; GARRAPPA, R. On multistep methods for differential equations of fractional order. **Mediterranean Journal of Mathematics**, New York, v. 3, n. 3, p. 565–580, 2006.

GALEONE, L.; GARRAPPA, R. Fractional adams–moulton methods. **Mathematics and Computers in Simulation**, Amsterdam, v. 79, n. 4, p. 1358–1367, 2008.

GALEONE, L.; GARRAPPA, R. Explicit methods for fractional differential equations and their stability properties. **Journal of Computational and Applied Mathematics**, Amsterdam, v. 228, n. 2, p. 548–560, 2009.

GARRAPPA, R. On some explicit adams multistep methods for fractional differential equations. **Journal of computational and Applied Mathematics**, Amsterdam, v. 229, n. 2, p. 392–399, 2009.

GARRAPPA, R. Trapezoidal methods for fractional differential equations: theoretical and computational aspects. **Mathematics and Computers in Simulation**, Amsterdam, v. 110, p. 96–112, 2015.

GUNARATHNA, W. A.; NASIR, H. M.; DAUNDASEKERA, W. B. An explicit form for higher order approximations of fractional derivatives. **Applied Numerical Mathematics**, Amsterdam, v. 143, p. 51–60, 2019.

HERIS, M. S.; JAVIDI, M. On fractional backward differential formulas methods for fractional differential equations with delay. **International Journal of Applied and Computational Mathematics**, New York, v. 4, n. 2, p. 1–15, 2018.

LUBICH, C. Fractional linear multistep methods for abel-volterra integral equations of the second kind. **Mathematics of computation**, Providence, v. 45, n. 172, p. 463–469, 1985.

LUBICH, C. Discretized fractional calculus. **SIAM Journal on Mathematical Analysis**, Philadelphia, v. 17, n. 3, p. 704–719, 1986.

MEERSCHAERT, M. M.; TADJERAN, C. Finite difference approximations for fractional advection–dispersion flow equations. **Journal of Computational and Applied Mathematics**, Amsterdam, v. 172, n. 1, p. 65–77, 2004.

NASIR, H. M.; GUNAWARDANA, B. L. K.; ABEYRATHNA, H. M. N. P. A second order finite difference approximation for the fractional diffusion equation. **International Journal of Applied Physics and Mathematics**, San Bernardino, v. 3, n. 4, p. 237–243, 2013.

OLDHAM, K.; SPANIER, J. **The fractional calculus theory and applications of differentiation and integration to arbitrary order**. Amsterdam: Elsevier, 1974.

PODLUBNY, I. Fractional differential equations: an introduction to fractional derivatives, fractional differential equations, to methods of their solution and some of their applications. **Mathematics in Science and Engineering**, Amsterdam, v. 198, p. 41–119, 1999.