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Numerical methods for solving large-scale linear system of fractional differential equations

Lakhlifa Sadek^{a,*}

lakhifasadek@gmail.com; sadek.l@ucd.ac.ma

^aDepartment of Mathematics, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.

Abstract

We will utilize the extended block Krylov method, in which we propose two new methods to solve a large-scale linear system of fractional differential equations (LSFDEs). The first method (EBA-MML) is based on the exact solution and projection of the Mittag-Leffler function of the matrix (MML). The second method (EBA-GLM, EBA-FBDF) is based on the projection of the initial problem onto an extended block Krylov subspace to get a new problem of small size then solve it with the Grünwald-Letnikov method (GLM) or the fractional backward differentiation formula (FBDF) method and the obtained solution is used to have a low-rank approximate solution of the initial problem. We will present some theoretical results as an accurate expression of the residual and the error norms. Finally, numerical experiments are presented to confirm the strength of the new methods in terms of time.

Keywords: LSFDE, extended block Krylov subspace, MML, low-rank approximation solutions, fractional calculus, GLM, FBDF method.

2010 MSC: 65F50, 15A24, 65F10, 65F30, 15A16, 34A08, 33E12

*Corresponding author

1. Introduction

In the present paper, we consider the large-scale LSFDE on the interval $[t_0, T_f]$ of the form

$$\begin{cases} \mathcal{X}^{(\alpha)}(t) = \mathcal{A}\mathcal{X}(t) + \mathcal{B}L(t), \\ \mathcal{X}(t_0) = \mathcal{C}, \end{cases} \quad (1)$$

where

- \mathcal{A} is $n \times n$ matrix nonsingular assumed to be large and sparse.
- \mathcal{B} is $n \times s$ matrix full rank.
- 5 • $\mathcal{X}(t)$ is $n \times s$ unknown matrix function.
- α is parameter describing the order of the fractional Caputo's derivative.
- $L(t)$ is $s \times s$ matrix function,

with $s \ll n$. In particular, when $\alpha = 1$, then we obtain well-known large-scale linear system of differential equations.

10 Many real-life phenomena can be modeled by a LSFDEs [21, 25]. For instance, the mathematical models of circuits and mechanical systems involving several springs connected in series can be given by a LSFDEs. Generally, such systems are frequently encountered in chemical [18], biological [12], economics [19], psychology [2], physical and engineering applications [25], and other fields.

15 There are several methods for solving small or medium-sized LSFDEs (1) numerically that have been proposed in the literature. (See [16, 15, 13, 14, 17]).

Definition 1. [21] *The Caputo derivative with order α is*

$$\mathcal{X}^{(\alpha)}(t) = \frac{1}{\Gamma(1-\alpha)} \int_{t_0}^t \frac{\dot{\mathcal{X}}(\tau)}{(t-\tau)^\alpha} d\tau. \quad (2)$$

The exact solution of the fractional differential matrix equation (1) is given by the following result.

Theorem 2. [4, 23] Let $0 < \alpha \leq 1$, the unique solution of the fractional differential matrix equations (1) is defined by

$$\mathcal{X}(t) = E_{\alpha,1}((t-t_0)^\alpha \mathcal{A}) \mathcal{C} + \int_{t_0}^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{A}) \mathcal{B} L(\tau) d\tau, \quad (3)$$

the Mittag-Leffler function (ML) [15] is defined by means of the series

$$E_{\alpha,\beta}(z) = \sum_{j=0}^{\infty} \frac{z^j}{\Gamma(\alpha j + \beta)}, z \in \mathbb{C},$$

and Eulers gamma function is defined by the integral

$$\Gamma(z) = \int_0^{\infty} e^{-t} t^{z-1} dt, \quad \text{Re}(z) > 0.$$

However, these approaches are not suitable for large-scale LSFDEs because
 20 they take a lot of time, and a program will be blocked, and there is no method
 for large problems, so the objective of this work is to develop numerical methods
 more adapted for this kind of fractional differential equations.

In this study, we present two new methods based on extended block Krylov
 methods to solve large-scale LSFDEs. A first approach is based on the computa-
 25 tion of the exact solution by using Mittag-Leffler function projection technique.
 The second is based on the idea of solving a new problem of small size then
 consider the GLM or FBDF method.

Throughout the paper, we use the following notations. The Frobenius inner
 product of the matrices U and V is defined by $\langle U, V \rangle_F = \text{tr}(U^T V)$, where $\text{tr}(Z)$
 denotes the trace of a square matrix Z . The associated norm is the Frobenius
 norm denoted by $\|\cdot\|_F$,

$$\|\mathcal{A}\|_F^2 = \text{tr}(\mathcal{A}^T \mathcal{A}), \quad \text{and the 2-norm denoted by } \|\mathcal{A}\|_2^2 = \lambda_{\max}(\mathcal{A}^T \mathcal{A}).$$

The rest of the paper is organized as follows. In section 2, we recall the
 extended block Arnoldi process with some of its properties. In Section 3, we de-
 30 fined EBA-MML method based on extended block Krylov subspaces $\mathcal{K}_m(\mathcal{A}, \mathcal{B})$
 to approximate MML function of solution of LSFDE (1). In Section 4, we
 present a low-rank approximation solution of LSFDE (1) using projection onto

extended block Krylov subspaces $\mathcal{H}_m(\mathcal{A}, \mathcal{B})$, in other words, when we drop the initial large-scale problem, we get a small-scale problem solved by GLM (EBA-GLM) or FPDF method (EBA-FBDF). Finally, Section 5 is devoted to numerical experiments showing effectiveness of proposed methods.

2. The extended block Arnoldi algorithm

In this section, we consider the extended block Krylov subspaces associated to pair $(\mathcal{A}, \mathcal{B})$ defined as follows:

$$\mathcal{H}_m(\mathcal{A}, \mathcal{B}) = \text{range} \left\{ \mathcal{B}, \mathcal{A}^{-1}\mathcal{B}, \mathcal{A}\mathcal{B}, \mathcal{A}^{-2}\mathcal{B}, \mathcal{A}^2\mathcal{B}, \dots, \mathcal{A}^{m-1}\mathcal{B}, \mathcal{A}^{-m}\mathcal{B} \right\}.$$

The iterative Krylov-type methods, used for about 36 years, are generally more effective in large problems. Most of the iterative methods manipulate the linear system through "matrix-vector" products, which reduces memory space.

The iterative methods based on a projection technique on a block-extended Krylov subspace are more efficient and fast (the speed of convergence) based on the Petrov-Galerkin condition, (See [1, 5, 6, 10, 26, 27, 28]).

Recall extended block Arnoldi (EBA) [10, 29] algorithm applied to the pair $(\mathcal{A}, \mathcal{B})$. The EBA is described in Algorithm 1 as follows

Algorithm 1 The extended block Arnoldi algorithm (EBA)

Inputs: \mathcal{A} an $n \times n$ matrix, \mathcal{B} an $n \times s$ matrix and m an integer.

1. Compute the QR decomposition of $[\mathcal{B}, \mathcal{A}^{-1}\mathcal{B}]$, i.e., $[\mathcal{B}, \mathcal{A}^{-1}\mathcal{B}] = V_1\Lambda$;
2. Set $\mathcal{V}_0 = []$;
3. **For** $j = 1, 2, 3, \dots, m$
4. Set $V_j^{(1)} = V_j(:, 1 : s)$ and $V_j^{(2)} = V_j(:, s + 1 : 2s)$
5. $\mathcal{V}_j = [\mathcal{V}_{j-1}, V_j]$; $\widehat{V}_{j+1} = [\mathcal{A}V_j^{(1)}, \mathcal{A}^{-1}V_j^{(2)}]$;
6. **For** $i = 1, \dots, j$
7. $H_{i,j} = V_i^T \widehat{V}_{j+1}$;
8. $\widehat{V}_{j+1} = \widehat{V}_{j+1} - V_i H_{i,j}$;
9. **End For** i
10. Compute the QR decomposition of U i.e., $\widehat{V}_{j+1} = V_{j+1}H_{j+1,j}$;
11. **End For** m .

Output: $\mathcal{V}_m = [V_1, \dots, V_m]$.

Through our algorithm 1 we have the orthonormal matrix $\mathcal{V}_m = [V_1, \dots, V_m] \in \mathbb{R}^{n \times 2ms}$ verifies $\mathcal{V}_m^T \mathcal{V}_m = I_{2ms}$ and we also generate block Hessenberg matrices

50 $\overline{\mathcal{H}}_m = \mathcal{V}_{m+1}^T \mathcal{A} \mathcal{V}_m \in \mathbb{R}^{2(m+1)s \times 2ms}$ satisfying the following algebraic relations

$$\begin{aligned} \mathcal{A} \mathcal{V}_m &= \mathcal{V}_{m+1} \overline{\mathcal{H}}_m \\ &= \mathcal{V}_m \mathcal{H}_m + V_{m+1} H_{m+1,m} E_m^T, \\ \overline{\mathcal{H}}_m &= \mathcal{V}_{m+1} \begin{bmatrix} \mathcal{H}_m \\ H_{m+1,m} E_m^T \end{bmatrix}, \end{aligned}$$

and Hessenberg matrix $\mathcal{H}_m = \mathcal{V}_m^T \mathcal{A} \mathcal{V}_m = [H_{i,j}] \in \mathbb{R}^{2ms \times 2ms}$, with $H_{i,j} \in \mathbb{R}^{2s \times 2s}$. And we have the following relations

$$\mathcal{V}_m = \mathcal{V}_{m+1} \begin{bmatrix} I_{2sm} \\ 0_{2s \times 2s} \end{bmatrix},$$

and

$$\mathcal{V}_m^T \mathcal{B} = \mathcal{E}_1 \Lambda_{11} \quad \text{with} \quad \Lambda = \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ 0_{s \times s} & \Lambda_{22} \end{bmatrix},$$

where $E_m^T = [0_{2s \times 2s(m-1)}, I_{2s}] \in \mathbb{R}^{2s \times 2ms}$, Λ_{11} is the $s \times s$ matrix, and $\mathcal{E}_1 = [I_s, 0_{s \times (2m-1)s}]^T$.

3. The matrix Mittag-Leffler function approximation

For our first approach, we use this expression of $\mathcal{X}(t)$ to obtain low-rank approximate solution. We will rather consider the product $E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{A})\mathcal{B}$ for which approximation via projection method onto extended block Krylov subspace (See [20, 33]). An approximation to $E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{A})\mathcal{B}$ can be obtained as

$$E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{A})\mathcal{B} \cong \mathcal{V}_m E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{H}_m) \mathcal{E}_1 \Lambda_{11},$$

where Λ_{11} is the $s \times s$ matrix obtained from the QR decomposition

$$[\mathcal{B}, \mathcal{A}^{-1}\mathcal{B}] = \mathcal{E}_1 \Lambda_{11} = V_1 \Lambda \quad \text{with} \quad \Lambda = \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ 0_{s \times s} & \Lambda_{22} \end{bmatrix},$$

so

$$\int_{t_0}^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{A})\mathcal{B}L(\tau)d\tau \approx \mathcal{V}_m \int_{t_0}^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{H}_m) \mathcal{E}_1 \Lambda_{11} L(\tau)d\tau,$$

we assume that $\mathcal{C} = 0_{n \times s}$, we notice that if $\mathcal{C} \neq 0_{n \times s}$, then we can also approximate the first term $E_{\alpha,1}((t-t_0)^\alpha \mathcal{A})\mathcal{C}$ of (3) by \mathcal{C}_m , using a Krylov based or another method and then the approximate solution of (3) is given as

$$\mathcal{X}_m(t) = \mathcal{C}_m + \mathcal{V}_m \mathbb{X}_m(t).$$

An approximation to $\mathcal{X}(t)$ can be expressed as the product

$$\mathcal{X}_m(t) = \mathcal{V}_m \mathbb{X}_m(t), \tag{4}$$

where

$$\mathbb{X}_m(t) = \int_{t_0}^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{H}_m) \mathcal{E}_1 \Lambda_{11} L(\tau)d\tau. \tag{5}$$

55 The next result shows that the $2ms \times s$ matrix function $\mathbb{X}_m(t)$ is solution of a small-scale LSFDEs.

Theorem 3. Let $\mathbb{X}_m(t)$ be the matrix function defined by (4), then it satisfies the following small-scale LSFDE

$$\begin{cases} \mathbb{X}_m^{(\alpha)}(t) = \mathcal{H}_m \mathbb{X}_m(t) + \mathcal{E}_1 \Lambda_{11} L(t), & t \in [t_0, T_f], \\ \mathbb{X}_m(t_0) = 0_{2ms \times s}. \end{cases} \quad (6)$$

Proof 1. The proof can be easily derived from the expression (5) and theorem 2.

Theorem 4. Let $\mathcal{X}_m(t) = \mathcal{V}_m \mathbb{X}_m(t)$ be the approximation solution obtained at step m by the extended block Arnoldi algorithm and $R_m(t) = \mathcal{X}_m^{(\alpha)}(t) - \mathcal{A} \mathcal{X}_m(t) - \mathcal{B}L(t)$ is the residual associated to the approximation $\mathcal{X}_m(t)$. Then the residual $R_m(t)$ satisfies the relation

$$\|R_m(t)\|_F = \|H_{m+1,m} E_m^T \mathbb{X}_m(t)\|_F, \quad (7)$$

and for the two-norm, we have

$$\|R_m(t)\|_2 = \|H_{m+1,m} E_m^T \mathbb{X}_m(t)\|_2. \quad (8)$$

Proof 2. As a $R_m(t) = \mathcal{X}_m^{(\alpha)}(t) - \mathcal{A} \mathcal{X}_m(t) - \mathcal{B}L(t)$ and relation (4), therefore, we get

$$R_m(t) = \mathcal{V}_m \mathbb{X}_m^{(\alpha)}(t) - \mathcal{A} \mathcal{V}_m \mathbb{X}_m(t) - \mathcal{B}L(t),$$

as a

$$\mathcal{A} \mathcal{V}_m = \mathcal{V}_m \mathcal{H}_m + V_{m+1} H_{m+1,m} E_m^T,$$

and $\mathbb{X}_m(t)$ exact solution of the equation $\mathbb{X}_m^{(\alpha)}(t) = \mathcal{H}_m \mathbb{X}_m(t) + \mathcal{V}_m^T \mathcal{B}L(t)$, so

$$\begin{aligned} R_m(t) &= \mathcal{V}_m (\mathcal{H}_m \mathbb{X}_m(t) + \mathcal{V}_m^T \mathcal{B}) - (\mathcal{V}_m \mathcal{H}_m + V_{m+1} H_{m+1,m} E_m^T) \mathbb{X}_m(t) - \mathcal{B}L(t) \\ &= \mathcal{V}_m \mathcal{H}_m \mathbb{X}_m(t) + \mathcal{V}_m \mathcal{V}_m^T \mathcal{B} - \mathcal{V}_m \mathcal{H}_m \mathbb{X}_m(t) - V_{m+1} H_{m+1,m} E_m^T \mathbb{X}_m(t) - \mathcal{B}L(t) \\ &= -V_{m+1} H_{m+1,m} E_m^T \mathbb{X}_m(t), \end{aligned}$$

60 SO

$$\begin{aligned} \|R_m(t)\|_F^2 &= \text{tr} \left(R_m(t)^T R_m(t) \right) \\ &= \text{tr} \left(\mathbb{X}_m(t)^T E_m H_{m+1,m}^T V_{m+1}^T V_{m+1} H_{m+1,m} E_m^T \mathbb{X}_m(t) \right), \end{aligned}$$

and relation $V_{m+1}^T V_{m+1} = I_{2s}$ therefore, we get $\|R_m(t)\|_F^2 = \|H_{m+1,m} E_m^T \mathbb{X}_m(t)\|_F^2$,

so

$$\|R_m(t)\|_F = \|H_{m+1,m} E_m^T \mathbb{X}_m(t)\|_F.$$

To prove the expression (8) with the two-norm, let us first remark that if

$$\begin{aligned} \|R_m(t)\|_2^2 &= \lambda_{\max}\left(R_m(t)^T R_m(t)\right) \\ &= \lambda_{\max}\left(\mathbb{X}_m(t)^T E_m H_{m+1,m}^T V_{m+1}^T V_{m+1} H_{m+1,m} E_m^T \mathbb{X}_m(t)\right) \\ &= \lambda_{\max}\left(\mathbb{X}_m(t)^T E_m H_{m+1,m}^T H_{m+1,m} E_m^T \mathbb{X}_m(t)\right) \\ &= \|H_{m+1,m} E_m^T \mathbb{X}_m(t)\|_2^2, \end{aligned}$$

so

$$\|R_m(t)\|_2 = \|H_{m+1,m} E_m^T \mathbb{X}_m(t)\|_2.$$

The following result shows that the approximation $\mathcal{X}_m(t)$ is an exact solution of a perturbed fractional differential equation.

Theorem 5. *Let $\mathcal{X}_m(t)$ be the approximate solution given by (4). Then we have,*

$$\mathcal{X}_m^{(\alpha)}(t) = (\mathcal{A} - \mathcal{A}_m) \mathcal{X}_m(t) + \mathcal{B}L(t),$$

where $\mathcal{A}_m = V_{m+1} H_{m+1,m} V_m^T$.

Proof 3. By multiplying the (6) left by \mathcal{V}_m , we obtain

$$\begin{aligned} \mathcal{V}_m \mathbb{X}_m^{(\alpha)}(t)_m(t) &= \mathcal{V}_m \mathcal{H}_m \mathbb{X}_m(t) + \mathcal{V}_m \mathcal{E}_1 \Lambda_{11} L(t) \\ &= \mathcal{V}_m \mathcal{H}_m \mathbb{X}_m(t) + \mathcal{B}L(t), \end{aligned}$$

and $\mathcal{A} \mathcal{V}_m = \mathcal{V}_m \mathcal{T}_m + V_{m+1} H_{m+1,m} E_m^T$ and $\mathcal{V}_m \mathcal{E}_1 \Lambda_{11} = \mathcal{B}$ so

$$\begin{aligned} \mathcal{X}_m^{(\alpha)}(t) &= [\mathcal{A} \mathcal{V}_m - V_{m+1} H_{m+1,m} E_m^T] \mathbb{X}_m(t) + \mathcal{B}L(t) \\ &= [\mathcal{A} - V_{m+1} H_{m+1,m} E_m^T \mathcal{V}_m^T] \mathcal{X}_m(t) + \mathcal{B}L(t), \end{aligned}$$

so $\mathcal{X}_m^{(\alpha)}(t) = (\mathcal{A} - \mathcal{A}_m) \mathcal{X}_m(t) + \mathcal{B}L(t)$.

We summarize the steps of our proposed first method (EBA–MML) in the following algorithm

Algorithm 2 The EBA–MML method for solving LSFDE

Input: \mathcal{C} an $n \times s$ matrix, \mathcal{A} an $n \times n$ matrix, \mathcal{B} an $n \times s$ matrix, t_0, T_f .

1. Choose a tolerance $tol > 0$ and an integer m_{max} .
2. For $m = 1 : m_{max}$
3. Apply the EBA (Algorithm 1) to $(\mathcal{A}, \mathcal{B})$ to get the \mathcal{V}_m and \mathcal{H}_m .
4. Compute $\mathbb{X}_m(t) = \int_{t_0}^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{H}_m) \mathcal{E}_1 \Lambda_{11} L(\tau) d\tau$ we use the Matlab `ml_matrix` function in Mathworks website [35], and a quadrature method to compute the integral.
5. If $\|R_m(t)\|_F < tol$, stop.
6. The \mathcal{X}_m approximation given by $\mathcal{X}_m \approx \mathcal{V}_m \mathbb{X}_m$.
7. End

Output: \mathcal{X}_m .

70 The next result the error $e_m(t) = \mathcal{X}(t) - \mathcal{X}_m(t)$ satisfies also a LSFDE.

Theorem 6. *Let $\mathcal{X}(t)$ the exact solution of (1) and let $\mathcal{X}_m(t)$ be the approximate solution obtained at step m . The error $e_m(t)$ satisfies the following fractional differential equation*

$$\begin{cases} e_m^{(\alpha)}(t) = \mathcal{A}e_m(t) - R_m(t), \\ e_{m,0} = e_m(t_0), \end{cases} \quad (9)$$

Proof 4. *As a $\mathcal{X}^{(\alpha)}(t) = \mathcal{A}\mathcal{X}(t) + \mathcal{B}L(t)$ and $R_m(t) = \mathcal{X}_m^{(\alpha)}(t) - \mathcal{A}\mathcal{X}_m(t) - \mathcal{B}L(t)$, so*

$$\begin{aligned} e_m^{(\alpha)}(t) &= \mathcal{X}^{(\alpha)}(t) - \mathcal{X}_m^{(\alpha)}(t) \\ &= \mathcal{A}\mathcal{X}(t) + \mathcal{B}L(t) - \mathcal{A}\mathcal{X}_m(t) - \mathcal{B}L(t) - R_m(t) \\ &= \mathcal{A}e_m(t) - R_m(t). \end{aligned}$$

The next result gives the expression of the error $e_m(t)$.

Theorem 7. *The expression of the error e_m is*

$$e_m(t) = E_{\alpha,1}((t-t_0)^\alpha \mathcal{A})e_{m,0} - \int_{t_0}^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{A})R_m(\tau)d\tau, \quad t \in [t_0, T_f].$$

75 **Proof 5.** *The proof can be easily derived from the expression (9) and theorem 2.*

In this property we'll give a maximum value to the $e_m(t)$.

Theorem 8. *Then at step m of the extended block Arnoldi process, we have the following upper bound for the norm of the error,*

$$\|e_m(t)\|_2 \leq E_{\alpha,1}(t^\alpha \|\mathcal{A}\|_2) \|e_{m,0}\|_2 + \delta(t) \|H_{m+1,m}\|_2 t^\alpha E_{\alpha,\alpha+1}(t^\alpha \|A\|_2) \quad (10)$$

80 where $\delta(t) = \max_{\tau \in [0,t]} \|E_m^T \mathbb{X}_m(\tau)\|_2, \forall t \geq 0$.

Proof 6. *We have*

$$\begin{aligned} \|e_m(t)\|_2 &= \|E_{\alpha,1}(t^\alpha \mathcal{A})e_{m,0} - \int_0^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{A})R_m(\tau)d\tau\|_2 \\ &\leq \|E_{\alpha,1}(t^\alpha \mathcal{A})\|_2 \|e_{m,0}\|_2 + \delta(t) \|H_{m+1,m}\|_2 \int_0^t (t-\tau)^{\alpha-1} \|E_{\alpha,\alpha}((t-\tau)^\alpha \mathcal{A})\|_2 d\tau. \end{aligned}$$

By means of the following general formula (see [23]) concerning the integration of ML functions

$$\int_0^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}((t-\tau)^\alpha A) d\tau = t^\alpha E_{\alpha,\alpha+1}(t^\alpha A),$$

and like $\|E_{\alpha,\alpha+1}(t^\alpha A)\|_2 \leq E_{\alpha,\alpha+1}(t^\alpha \|A\|_2)$, then

$$\|e_m(t)\|_2 \leq E_{\alpha,1}(t^\alpha \|\mathcal{A}\|_2) \|e_{m,0}\|_2 + \delta(t) \|H_{m+1,m}\|_2 t^\alpha E_{\alpha,\alpha+1}(t^\alpha \|A\|_2).$$

In Figure 1, we computed the error upper bound norm by formula (10) at $T_f = 1$ and norm of the errors $e_m(T_f) = \mathcal{X}(T_f) - \mathcal{X}_m(T_f)$ vs number m of iterations, where \mathcal{X} is the exact solution and \mathcal{X}_m is the approximate solution
85 of LSFDE (1) for $\mathcal{A} = \text{tridiag}(1, -2, 1)$ matrix and \mathcal{B} were chosen as rank 2 matrix and $\alpha = 0.5$.

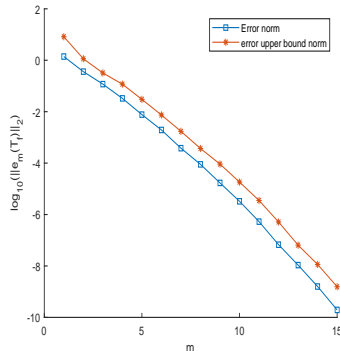


Figure 1: Norm of the errors and the corresponding bounds given by (10) in function of the number m of iterations.

4. Low-rank approximation solutions

In this section, we show how to obtain low-rank approximate solutions to the LSFDE (1) by first projecting directly the initial problem onto extended block Krylov subspaces then solve the obtained small-scale fractional differential problem. We first apply the extended block Arnoldi algorithm to the pair $(\mathcal{A}, \mathcal{B})$ to get the orthonormal matrix \mathcal{V}_m whose columns form orthonormal bases of the extended block Krylov subspaces $\mathcal{K}_m(\mathcal{A}, \mathcal{B})$. We also get the upper block Hessenberg matrix $\mathcal{H}_m = \mathcal{V}_m^T \mathcal{A} \mathcal{V}_m$. Let

$$\mathcal{X}_m(t) = \mathcal{V}_m \mathbb{Y}_m(t),$$

after the condition of orthogonality Petrov-Galerkin has the following result.

90 The next result shows that the $2ms \times s$ matrix function $\mathbb{X}_m(t)$ is solution of a small-scale LSFDEs.

Theorem 9. *Let $\mathcal{X}_m(t) = \mathcal{V}_m \mathbb{Y}_m(t)$ be the matrix function, then it satisfies the following small-scale LSFDE*

$$\begin{cases} \mathbb{Y}_m^{(\alpha)}(t) = \mathcal{H}_m \mathbb{Y}_m(t) + \mathcal{B}_m L(t) & t \in [t_0, T_f], \\ \mathbb{Y}_m(t_0) = \mathcal{V}_m^T \mathcal{C}, \end{cases} \quad (11)$$

where $\mathcal{B}_m := \mathcal{V}_m^T \mathcal{B} = \mathcal{E}_1 \Lambda_{11}$ and Λ_{11} is the $s \times s$ matrix obtained from the QR decomposition

$$[\mathcal{B}, \mathcal{A}^{-1} \mathcal{B}] = V_1 \Lambda \quad \text{with} \quad \Lambda = \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ 0_{s \times s} & \Lambda_{22} \end{bmatrix}.$$

Proof 7. As $\mathcal{X}_m(t) = \mathcal{V}_m \mathbb{Y}_m(t)$ satisfying the condition of orthogonality Petrov-Galerkin

$$\mathcal{V}_m^T R_m(t) = 0_{2ms \times s}, \quad t \in [t_0, T].$$

Then from $R_m(t) = \mathcal{X}_m^{(\alpha)}(t) - \mathcal{A} \mathcal{X}_m(t) - \mathcal{B}L(t)$, we get the LSFDE

$$\mathbb{Y}_m^{(\alpha)}(t) = \mathcal{H}_m \mathbb{Y}_m(t) + \mathcal{B}_m L(t).$$

Note that the small-scale fractional differential equation obtained (6) is the same as that given by (11). For this second approach, we need to solve this fractional differential equation by the Grünwald-Letnikov method or FBDF method.

Theorem 10. Let $\mathcal{X}_m(t) = \mathcal{V}_m \mathbb{Y}_m(t)$ be the approximation obtained at step m by the extended block Arnoldi method and $R_m(t) = \mathcal{X}_m^{(\alpha)}(t) - \mathcal{A} \mathcal{X}_m(t) - \mathcal{B}L(t)$ is the residual associated to the approximation $\mathcal{X}_m(t)$. Then the residual $R_m(t)$ satisfies the relation

$$\|R_m(t)\|_F = \|H_{m+1,m} E_m^T \mathbb{Y}_m(t)\|_F, \quad (12)$$

and for the two-norm, we have

$$\|R_m(t)\|_2 = \|H_{m+1,m} E_m^T \mathbb{Y}_m(t)\|_2. \quad (13)$$

⁹⁵ **Proof 8.** The proof of theorem 4.

The following result shows that the approximation $\mathcal{X}_m(t)$ is an exact solution of a perturbed fractional differential equation.

Theorem 11. Let $\mathcal{X}_m(t) = \mathcal{V}_m \mathbb{Y}_m(t)$, we have,

$$\mathcal{X}_m^{(\alpha)}(t) = (\mathcal{A} - \mathcal{A}_m) \mathcal{X}_m(t) + \mathcal{B}L(t),$$

where $\mathcal{A}_m = V_{m+1} H_{m+1,m} V_m^T$.

Proof 9. The proof of theorem 5.

100 4.1. Grünwald-Letnikov method

In this section, we are applying the Grünwald-Letnikov method [31] for solving LSFDE (11). At each t_j , let $\mathbb{Y}_{m,j}$ of the approximation of $\mathbb{Y}_m(t_j)$, obtained at step j defined by the relation

$$\sum_{k=0}^j \omega_k^{(\alpha)} \left[\mathbb{Y}_{m,j-k} - \mathbb{Y}_{m,0} \right] = h^\alpha \left(\mathcal{H}_m \mathbb{Y}_{m,j} + \mathcal{B}_m L(t_j) \right),$$

where

$$\omega_k^{(\alpha)} = (-1)^k \frac{\Gamma(\alpha + 1)}{k! \Gamma(\alpha - k + 1)}.$$

As a $\sum_{k=0}^j \omega_k^{(\alpha)} = \omega_j^{(\alpha-1)}$, reformulation of the scheme

$$\sum_{k=0}^j \omega_k^{(\alpha)} \mathbb{Y}_{m,j-k} = \omega_j^{(\alpha-1)} \mathbb{Y}_{m,0} + h^\alpha \left(\mathcal{H}_m \mathbb{Y}_{m,j} + \mathcal{B}_m L(t_j) \right),$$

where $t_{j+1} = h + t_j$. We put

$$\mathbb{T}_m = \omega_0^{(\alpha)} I_{2ms} - h^\alpha \mathcal{H}_m \text{ and } \mathcal{E}_{m,j} = \omega_j^{(\alpha-1)} \mathbb{Y}_{m,0} + h^\alpha \mathcal{B}_m L(t_j) - \sum_{k=1}^j \omega_k^{(\alpha)} \mathbb{Y}_{m,j-k},$$

we find the following matrix equation:

$$\mathbb{T}_m \mathbb{Y}_{m,j} = \mathcal{E}_{m,j}. \quad (14)$$

4.2. FBDF method

In this section, we are applying the FBDF method [34] for solving LSFDE (11). At each t_j , let $\mathbb{Y}_{m,j}$ of the approximation of $\mathbb{Y}_m(t_j)$, 2-stage FBDF is defined as

$$\sum_{k=0}^i \varpi_k \mathbb{Y}_{m,i-k} - b_i \mathbb{Y}_{m,0} = h^\alpha \left(\mathcal{H}_m \mathbb{Y}_{m,i} + \mathcal{B}_m L(t_i) \right), i = j + 1, j + 2, \dots,$$

where

$$b_i = \frac{i^{-\alpha}}{\Gamma(1 - \alpha)},$$

$$\omega_0 = 1, \omega_1 = -\frac{4}{3}\alpha,$$

$$\omega_k = \frac{4}{3} \left(1 - \frac{\alpha + 1}{k} \right) \omega_{k-1} + \frac{1}{3} \left(\frac{2(1 + \alpha)}{k} - 1 \right) \omega_{k-2}, k = 1, 2, \dots$$

$$\varpi_k = \left(\frac{3}{2}\right)^\alpha \omega_k, k = 0, 1, \dots$$

with $h = t_{j+1} - t_j$ is the step size. We put

$$\mathbb{T}_m = \varpi_0 I_{2ms} - h^\alpha \mathcal{H}_m \text{ and } \mathcal{E}_{m,i} = b_i \mathbb{Y}_{m,0} - \sum_{k=1}^i \varpi_k \mathbb{Y}_{m,i-k} + h^\alpha \mathcal{B}_m L(t_i),$$

we find the following matrix equation:

$$\mathbb{T}_m \mathbb{Y}_{m,i} = \mathcal{E}_{m,i}, i = j + 1, j + 2, \dots, \quad (15)$$

In particular, when $\alpha = 1$, then we obtain well-known BDF method for solving linear system of differential equations (See [28]).

We summarize the steps of the second method (EBA-GLM, EBA-FBDF) in
 105 the following algorithm

Algorithm 3 The EBA-GLM or EBA-FBDF method for solving large-scale LSFDE

Inputs: \mathcal{C} an $n \times s$ matrix, \mathcal{A} an $n \times n$ matrix, \mathcal{B} an $n \times s$ matrix and t_0, T_f .

1. Choose a tolerance $tol > 0$, a maximum number of m_{max} iterations.
2. For $m = 1 : m_{max}$
3. Apply the EBA (Algorithm 1) to $(\mathcal{A}, \mathcal{B})$ to get the \mathcal{V}_m and \mathcal{H}_m .
4. Apply GLM method or FBDF method to solve (11).
5. If $\|R_m(t)\|_F < tol$, stop.
6. End For
7. Compute the approximate solution \mathcal{X}_m by $\mathcal{X}_m = \mathcal{V}_m \mathbb{Y}_m$.

Output: \mathcal{X}_m .

5. Numerical experiments

In this section, we compare the EBA-MML method (Algorithm 2), EBA-GLM and EBA-FBDF methods (Algorithm 3) presented in this paper. All the experiments were performed on a laptop with an Intel Core i3 processor

110 and 4GB of RAM. To the author's knowledge, there is no exact solution available in the literature. We compared the results obtained from the EBA-FBDF method EBA-GLM method and `fde12.m` for FDEs by Roberto Garrappa (See <https://goo.gl/XScYmi>) solver to test if our approach gives reliable results.

Example 1

Our aim in this example is for solving time-fractional diffusion equation [32, 8, 11, 3] of the form

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), \quad 0 < \alpha \leq 1, \quad (16)$$

where

$$f(x, t) = 2 \sin(2\pi x) \left(\frac{t^{2-\alpha}}{\Gamma(3-\alpha)} + 2\pi^2 t^2 \right),$$

on a finite domain $0 < x < 1$ and the parameter α refers to the fractional order of time derivative. We also assume an initial condition $u(x, 0) = 0$ and the following Dirichlet boundary conditions $u(0, t) = u(1, t) = 0$. The resulting finite difference equations are to the grid points centered at $(x_i = ih_x, i = 1, \dots, N - 1)$ defined by

$$\frac{\partial^\alpha u_i(t)}{\partial t^\alpha} = \frac{1}{h_x^2} \left(u_{i-1}(t) - 2u_i(t) + u_{i+1}(t) \right) + f(x_i, t),$$

with boundary conditions $u_0(t) = u_N(t) = 0$, we put $\mathcal{X}(t) = [u_1(t), \dots, u_{N-1}(t)]^T$, $\mathcal{A} = \frac{1}{h_x^2} \text{tridiag}(1, -2, 1)$, and $\mathcal{B} = [2 \sin(2\pi x_i)]$, we have

$$\mathcal{X}^{(\alpha)}(t) = \mathcal{A} \mathcal{X}(t) + \mathcal{B} L(t),$$

115 where $L(t) = \frac{t^{2-\alpha}}{\Gamma(3-\alpha)} + 2\pi^2 t^2$ and initial temperature distribution $u_i(0) = 0$, so $\mathcal{X}(0) = 0_{N-1 \times 1}$. The tolerance was set to 10^{-9} for the stop test on the residual, $\alpha = 0.85$ and $h = 0.01$. We chose a size of 100×100 for the matrix \mathcal{A} . In Figure 2, we plotted the solutions $u(x, t)$ for equation (16) using the new methods and `fde12` method [16] in functions of t , and the Frobenius residual norm in functions
 120 of the numbers m iterations at $\alpha = 0.85, h = 0.01, n = 100$. Computational time taken from an EBA-FBDF method is 0.82 seconds EBA-GLM method

0.85 seconds EBA-MML method 0.93 seconds versus fde12 method is 2087.76 seconds.

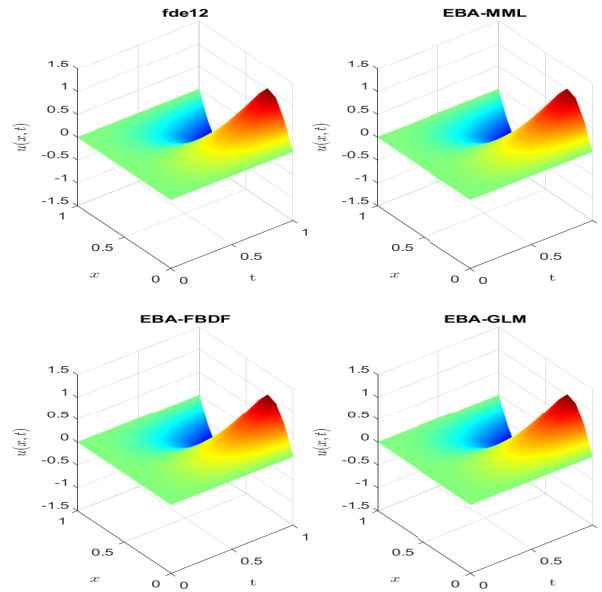


Figure 2: The numerical solution of time-fractional diffusion equation using new methods and fde12 method at $\alpha = 0.85, h = 0.01$ and $n = 100$.

In Table 1, we give the obtained runtimes in seconds, the number of iterations
 125 and the Frobenius residual norm at T_f , the tolerance was set to 10^{-9} for the
 stop test on the residual and $h = 0.1$, for the resolution of equation (1) for
 $t \in [0, 1]$.

n	Method	CPU time (seconds)	Iterations (m)	$\ R_m(T_f)\ _F$
5000	EBA-GLM	0.14	6	2.07×10^{-10}
	EBA-FBDF	0.11	6	2.08×10^{-10}
	EBA-MML	1.32	12	7.05×10^{-10}
6000	EBA-GLM	0.46	6	3.05×10^{-10}
	EBA-FBDF	0.10	6	3.32×10^{-10}
	EBA-MML	1.35	12	3.00×10^{-10}
8900	EBA-GLM	0.55	6	3.82×10^{-10}
	EBA-FBDF	0.12	6	4.12×10^{-10}
	EBA-MML	2.47	6	9.59×10^{-10}

Table 1: Runtimes in seconds, the residual norms and iterations for different new methods at $\alpha = 0.85$.

Example 2

In this example, consider the test problem in [30]

$$\begin{cases} \frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2 u(x,t)}{\partial x^2} - (1+x)u + f(x,t), \\ f(x,t) = x(\pi-x)(1+t^4), \\ u(0,t) = u(\pi,t) = 0, \\ u(x,0) = \sin(x), \end{cases} \quad \begin{matrix} t \in [0, 1], \\ x \in [0, \pi], \end{matrix} \quad (17)$$

The centered finite difference discretization of the operator $\mathcal{L}(u) = \frac{\partial^2 u}{\partial x^2} - (1+x)u$,
130 on the unit square $[0, \pi]$ to the grid points centered at $(x_i = ih_x, i = 1, \dots, N-1)$,
we obtain $\mathcal{A} = \frac{1}{h_x^2} \text{tridiag}(1, -2, 1) - \text{diag}(1+x_i)$, $\mathcal{B} = [x_i(\pi-x_i)]$, and initial
temperature distribution $u_i(0) = \sin(x_i)$, so $\mathcal{X}(0) = [\sin(x_i)]$ and where $L(t) =$
135 $1+t^4$. We chose a size of 100×100 for the matrix \mathcal{A} . In Figure 3, we plotted the
solutions $\mathcal{X}_{11}(t)$ in functions of t , and the Frobenius residual norm in functions
of the numbers m iterations. Computational time taken from an EBA-FBDF
method is 0.14 seconds EBA-GLM method 0.23 seconds EBA-MML method
4.86 seconds versus fde12 method is 9978.80 seconds.

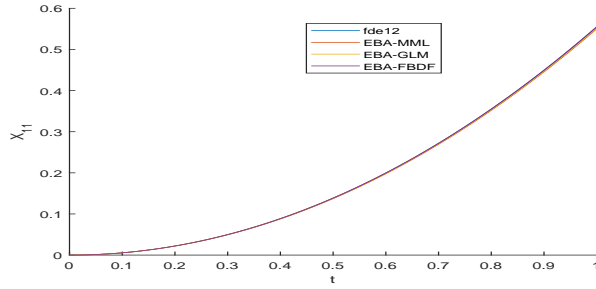


Figure 3: Comparison between the numerical solutions and fde12 solution \mathcal{X}_{11} vs t with $\alpha = 0.6$, at $h = 0.001$ and $n = 100$.

In Figure 4, we plotted the solutions $u(x, t)$ for equation (17) using the new methods and fde12 method at $\alpha = 0.6, h = 0.001$ and $n = 100$.

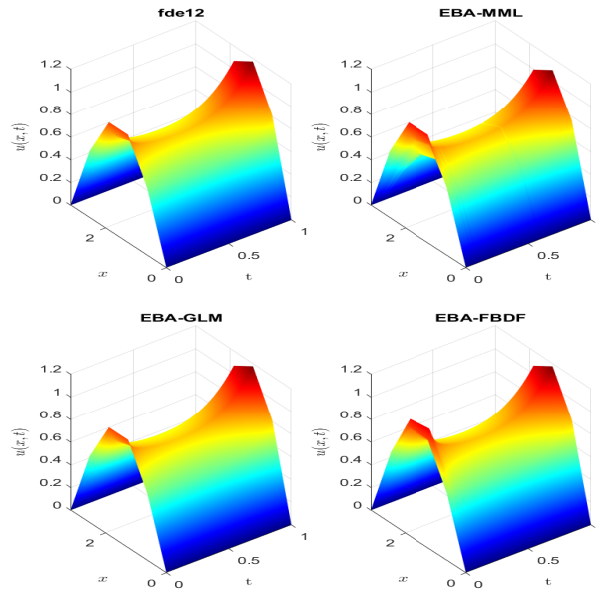


Figure 4: The numerical solution of time-fractional diffusion equation using new methods and fde12 method at $\alpha = 0.6, h = 0.001$ and $n = 100$.

140 In Figure 5, we plotted the Frobenius residual norm in functions of the numbers m iterations.

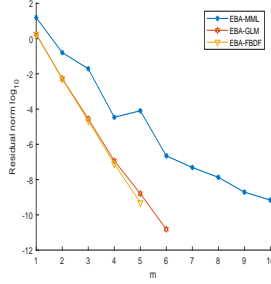


Figure 5: Residual norm vs number m of iterations at $\alpha = 0.6$, $h = 0.1$ and $n = 8499$.

In Table 2, we give the obtained runtimes in seconds, the number of iterations and the Frobenius residual norm at T_f , the tolerance was set to 10^{-9} for the stop test on the residual and $h = 0.1$.

n	Method	CPU time (seconds)	Iterations (m)	$\ R_m(T_f)\ _F$
4400	EBA-GLM	0.88	6	7.66×10^{-12}
	EBA-FBDF	0.10	5	3.45×10^{-10}
	EBA-MML	0.89	9	2.15×10^{-10}
6400	EBA-GLM	0.45	6	1.09×10^{-11}
	EBA-FBDF	1.17	5	4.63×10^{-10}
	EBA-MML	0.98	8	4.61×10^{-10}
8499	EBA-GLM	0.21	6	1.51×10^{-11}
	EBA-FBDF	0.09	5	4.92×10^{-10}
	EBA-MML	1.00	10	6.91×10^{-10}
10000	EBA-GLM	1.79	6	1.09×10^{-11}
	EBA-FBDF	0.11	5	5.35×10^{-10}
	EBA-MML	2.39	16	5.12×10^{-10}

Table 2: Runtimes in seconds, the residual norms iterations for different new methods at $\alpha = 0.6$.

145 *Example 3*

In this example, the matrix \mathcal{A} are obtained from the centered finite difference discretization of the operator $\mathcal{L}(u) = \Delta u + f_1(x, y) \frac{\partial u}{\partial x} + f_2(x, y) \frac{\partial u}{\partial y} + f_3(x, y)u$, on the unit square $[0, 1] \times [0, 1]$ with homogeneous Dirichlet boundary conditions. The number of inner grid points in each direction was n_0 for the operators \mathcal{L} . The matrix \mathcal{A} were obtained from the discretization of the operator \mathcal{L} with the dimensions $n = n_0^2$. The discretization of the operator $\mathcal{L}(u)$ yields matrix extracted from the `Lyapack` package [22] using the command `fdm_2d_matrix` and denoted as `fdm`. For this experiment, we consider $\mathcal{A} = \text{fdm}(n_0, f_1(x, y), f_2(x, y), f_3(x, y))$ with $f_1(x, y) = e^{xy}$, $f_2(x, y) = \sin(xy)$, $f_3(x, y) = \sqrt{x^2 + y^2}$, and The n -by- s matrix $\mathcal{B}L(t)$ are given by random values uniformly distributed on $[0, 1]$. We used the tolerance was set to 10^{-9} for the stop test on the residual. In Figure 6, we chose a size of 10000×10000 for the matrix \mathcal{A} , we plotted the Frobenius norms of the residuals $\|R_m(T_f)\|_F$ at T_f versus the number of iterations.

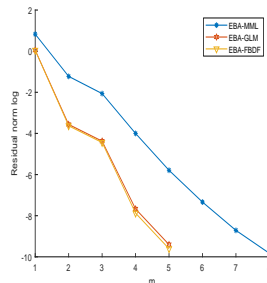


Figure 6: Residual norm vs number m of iterations we used a constant $h = 0.1$.

160 *Example 4*

For the second set of experiments, we use the matrices `add32` and `thermal` from the University of Florida Sparse Matrix Collection [9] and from the Harwell Boeing Collection <http://math.nist.gov/MatrixMarket> and The n -by- s matrix $\mathcal{B}L(t)$ are given by random values uniformly distributed on $[0, 1]$. The tolerance was set to 10^{-9} for the stop test on the residual. We used a constant $h = 0.1$. In

Figure 7, $\mathcal{A} = add32$ we plotted the Frobenius residual norm at T_f in function of the number m of iterations.

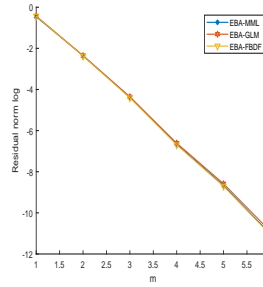


Figure 7: Residual norm vs number m of iterations

In Figure 8, $\mathcal{A} = thermal$ we plotted the Frobenius residual norm at T_f in function of the number m of iterations.

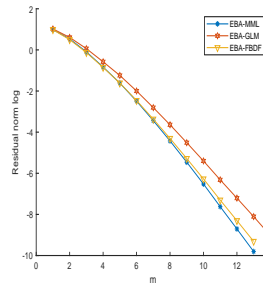


Figure 8: Residual norm vs number m of iterations.

170 In Table 3, we give the obtained runtime in seconds, the number of iterations and the Frobenius residual norm at T_f and $h = 0.1$, the tolerance was set to 10^{-9} for the stop test on the residual, for the resolution of system of fractional differential equations (1) for $t \in [0, 1]$, we use the matrices *add32*, *thermal* and *fdm*.

Test	Method	CPU time (seconds)	Iterations (m)	$\ R_m(T_f)\ _F$
$n = 3456, \mathcal{A} = thermal$	EBA-GLM	8.30	14	9.33×10^{-10}
	EBA-FBDF	7.81	13	4.88×10^{-10}
	EBA-MML	15.82	13	1.56×10^{-10}
$n = 4960, \mathcal{A} = add32$	EBA-GLM	23.12	6	1.27×10^{-11}
	EBA-FBDF	23.00	6	8.62×10^{-12}
	EBA-MML	23.78	6	9.46×10^{-12}
$n = 6400$ $\mathcal{A} = fdm$	EBA-GLM	0.42	5	2.52×10^{-10}
	EBA-FBDF	0.30	5	1.58×10^{-10}
	EBA-MML	1.20	8	5.33×10^{-11}
$n = 10000$ $\mathcal{A} = fdm$	EBA-GLM	0.60	5	3.93×10^{-10}
	EBA-FBDF	0.51	5	2.47×10^{-10}
	EBA-MML	2.33	8	5.51×10^{-11}

Table 3: Runtimes in seconds, the residual norms and iterations at $\alpha = 0.5$.

175 6. Conclusion

In this paper, we have introduced new methods to calculate the approximate solutions for large-scale LSFDEs. Numerical experiments show that the proposed extended block Krylov method is effective for large and sporadic problems. we can also use these new methods for solving other large-scale fractional
180 differential matrix equations.

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