Padé Formulation of Fractional Derivatives for Numerical Solution of Fractional Diffusion Equation

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Abstract
This study presents a Padé approximation approach for solving time-fractional diffusion equations through rational approximation of power series solutions. The method constructs systematic Padé approximants to represent fractional derivatives without time discretization, maintaining the essential nonlocal character of the operators. Numerical experiments demonstrate accurate agreement with exact Mittag-Leffler function solutions across various fractional orders. The proposed framework provides a flexible and systematic procedure for generating rational approximations of different orders according to the desired level of accuracy. Moreover, the method reduces the computational effort associated with traditional discretization-based techniques while preserving the mathematical properties of the fractional model. Higher-order Padé schemes consistently show better performance than lower-order approximations in terms of solution accuracy and stability. The approach proves particularly effective for problems involving multiple eigenmodes, successfully capturing their interactions. These results establish the method as a reliable computational tool for fractional diffusion problems, offering advantages in both accuracy and efficiency for practical applications in science and engineering.

Keywords: Fractional Calculus, Padé Approximation, Taylor Approximation, Fractional Diffusion Equation, Mittag-Leffler function.

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1. Introduction

The study of fractional-order differential equations has gained significant attention in recent years due to their ability to model memory and hereditary effects inherent in various physical, biological, and engineering systems(Miller & Ross, 1993; Oldham & Spanier, 1974). Among these, the time-fractional diffusion equation has emerged as a powerful tool to describe anomalous diffusion processes that cannot be accurately captured by classical integer-order models (Gorenflo & Mainardi, 1997; Podlubny, 1999). This type of equation replaces the first-order time derivative in the standard diffusion equation with a Caputo fractional derivative of order $0 < \beta < 1$, leading to a model that accounts for subdiffusive dynamics encountered in heterogeneous and disordered media(Samko, Kilbas, & Marichev, 1993).

Despite the wide applicability of fractional models, their analytical solutions are often unavailable, and numerical methods become indispensable(Diethelm, 2003). Traditional numerical approaches such as finite difference methods(Ismail & Elbarbary, 2001), finite element methods(Ismail, Elbarbary, Salem, & computation, 2004), and spectral techniques(Ismail, Rageh, Salem, & Computation, 2014) have been developed to approximate solutions to time-fractional partial differential equations. However, these schemes frequently encounter challenges when dealing with computational complexity, stability constraints, and limited accuracy near the initial time.

To address these difficulties, this paper proposes a novel semi-analytical framework based on the approximation formulas developed in (Youssef, Rageh, Fareed, & Abdelwahed, 2025). In that prior study, we introduced a rational Padé-type approximation(G. A. Baker, Graves-Morris, & Applications, 1981; G. J. E. o. M. Baker & Its Applications, 1981; George Jr, 1975; Rageh, Salem, El-Salam, & Mech, 2014) of the fractional derivative by leveraging the formal power series expansion of the unknown function. Specifically, we constructed Padé approximants of type [1/1], [2/1], and higher orders, which approximate the Caputo derivative in terms of a rational function involving the Taylor coefficients of the function itself. These approximations preserve the essential nonlocal features of the fractional operator while offering a computationally efficient representation.

In this paper, we apply those theoretical advancements to numerically solve the time-fractional diffusion problem. By approximating the solution as a truncated power series in time and substituting the Padé-based approximation of the Caputo derivative, we reduce the problem to a sequence of spatial boundary value problems for the time-series coefficients. This results in a simple yet accurate scheme that avoids discretizing the time domain and significantly reduces computational cost. Furthermore, the method maintains high accuracy for small time values where traditional discretization tends to lose precision.

The paper is organized as follows. Section 2 establishes the mathematical foundation, presenting essential definitions of fractional operators and the Mittag-Leffler function that are crucial for subsequent analysis. In Section 3, we introduce the core theoretical framework, detailing the construction of [1/1] and [2/1] Padé approximants for fractional derivatives and analysing their approximation properties. Section 4 details the proposed algorithm and its computational implementation. Numerical experiments were presented in Section 5, including comparisons with exact solutions and conventional finite difference schemes. Finally, Section 6 concludes with a discussion on the method's applicability and potential extensions.

2. Definitions of Fractional Calculus

The following definitions adapt classical concepts into forms suitable for series-based solutions while preserving the non-local character of fractional operators. These formulations enable direct computational implementation and rigorous accuracy analysis(Caputo, 1967; Gorenflo, Kilbas, Mainardi, & Rogosin, 2020; Kilbas, 2006)

2.1 Riemann-Liouville fractional integral

For $\alpha \in \mathbb{R}^+$ and $f \in L_1[a, b]$, the Riemann-Liouville fractional integral operator of order α is defined by:

$$J_a^{\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-\tau)^{\alpha-1} f(\tau) d\tau, \quad a \le t \le b. \quad (1)$$

This integral operator serves as the foundation for constructing fractional derivatives and preserves certain semigroup properties crucial for analysis.

2.2 Riemann-Liouville fractional derivative

For $\alpha \in R^+$ with $n = \lceil \alpha \rceil$ (the greatest integer greater than α). the Riemann-Liouville fractional derivative is given by:

$$D_a^{\alpha} f(t) = \begin{cases} D^n \dfrac{1}{\Gamma(n-\alpha)} \displaystyle\int_a^t (t-\tau)^{n-\alpha-1} f(\tau)\, d\tau, & n-1 < \alpha < n \\ \dfrac{d^n}{dt^n} f(t), & \alpha = n. \end{cases} \quad (2)$$

This definition maintains the nonlocal character of fractional differentiation while reducing to classical derivatives when α is integer valued.

2.3 Caputo differential operator

Let $\alpha \in R^+$, $n-1 < \alpha < n$, and $n = \lceil \alpha \rceil$. the Caputo fractional derivative is defined as:

$$ {}_a^C D_t^{\alpha} f(t) = D_{*a}^{\alpha} = J_a^{n-\alpha} D^n f(t)$$

$$= \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-\tau)^{n-\alpha-1} f^{(n)}(\tau)\, d\tau. \quad (3)$$

The Caputo formulation is particularly suited for initial value problems as it allows conventional initial conditions.

2.4 Mittag-Leffler function

For $x \in C[a, b]$, the Mittag-Leffler function $E_{\alpha}(x)$ is defined by:

$$E_{\alpha}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(\alpha k + 1)}, \qquad Re(\alpha) > 0, \quad (4)$$

Where:

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

$$1+\frac{x}{\Gamma(\alpha+1)}+\frac{x^2}{\Gamma(2\alpha+1)}+\frac{x^3}{\Gamma(3\alpha+1)}+\cdots+\frac{x^N}{\Gamma(N\alpha+1)}+\cdots.$$

Where $\Gamma(.)$ is the Euler gamma-function. This function appears naturally in solutions to fractional differential equations and provides exact solutions for benchmark problems.

2.5 Two-parameter Mittag-Leffler function

For $\alpha > 0$, $\beta > 0$, the two-parameter Mittag–Leffler function is defined by:

$$E_{\alpha,\beta}(x)=\sum_{k=0}^{\infty}\frac{x^k}{\Gamma(\alpha k+\beta)}, Re(\alpha,\beta)>0, \tag{5}$$

when $\beta = 1$, this function reduces to normal Mittag–Leffler function, i.e., $E_{\alpha,1}(x)$=$E_{\alpha}(x)$. It naturally arises in the solution of fractional differential equations with nonzero initial conditions.

3. Fractional Padé Approximation Method

In this section, we briefly review the rational approximation technique for the Caputo fractional derivative that has been developed and analyzed in the literature. These approximations form the foundation of the current method(Youssef et al., 2025) used to solve the fractional diffusion equation. Starting with the power series on the form

$$f(t)=\sum_{k=0}^{\infty}c_k(x)t^k. \tag{6}$$

where each $c_k$corresponds to the k^{th} derivative of $f(t)$ at zero, scaled by $\frac{1}{k!}$. The Caputo fractional derivative of order $\beta \in (0,1)$ is then given by the series:

$$D_t^{\beta}f(t)=\sum_{k=1}^{\infty}\frac{\Gamma(k+1)}{\Gamma(k+1-\beta)}C_k(x)t^{k-\beta}. \tag{7}$$

This infinite series captures the memory-dependent behavior of fractional-order systems but can be computationally costly to evaluate, especially when used in time-fractional partial differential equations.

To overcome this, we previously proposed rational Padé-type approximations that approximate the Caputo derivative using only a few terms of the power series. These approximations preserve the nonlocal behavior of the fractional operator while being significantly more efficient to compute. Several Padé-type rational approximations, including the [1/1] and [2/1] approximants, have been proposed in the literature to approximate the Caputo fractional derivative by exploiting the formal power series expansion of the unknown function see(Youssef et al., 2025). The formula uses the coefficients c_n, c_{n+1}, and c_n, and is given by:

$$PA\left[\frac{1}{1}\right]_{f^{(\beta)}(x)}(x)=\frac{\Gamma(\beta+1)c_n+\left[\frac{(\Gamma(\beta+2)c_{n+1})^2-\frac{1}{2}\Gamma(\beta+1)\Gamma(\beta+3)c_nc_{n+2}}{\Gamma(\beta+2)c_{n+1}}\right]x}{1-\frac{\Gamma(\beta+3)c_{n+2}}{2\Gamma(\beta+2)c_{n+1}}x}, \tag{8}$$

$$PA\left[\frac{2}{1}\right]_{f^{(\beta)}(x)}(x)=\frac{\Gamma(\beta+1)c_n+\left[\Gamma(\beta+2)c_{n+1}-\frac{\Gamma(\beta+1)\Gamma(\beta+4)c_nc_{n+3}}{3\Gamma(\beta+3)c_{n+2}}\right]x}{1-\frac{\Gamma(\beta+4)c_{n+3}}{3\Gamma(\beta+3)c_{n+2}}x}+\frac{\left[\frac{\Gamma(\beta+3)c_{n+2}}{2}-\frac{\Gamma(\beta+2)\Gamma(\beta+4)c_{n+1}c_{n+3}}{3\Gamma(\beta+3)c_{n+2}}\right]x^2}{1-\frac{\Gamma(\beta+4)c_{n+3}}{3\Gamma(\beta+3)c_{n+2}}x} \tag{9}$$

4. Padé Approach for the Fractional Diffusion Equation

The Padé approximation formulas developed in Section 3 provide a powerful tool for replacing the nonlocal Caputo fractional derivative with a compact rational expression in time that involves only a finite number of terms from the time-series expansion of the solution. In this section, we demonstrate how the Padé formulas can be incorporated into the framework of the time-fractional diffusion equation to produce an efficient and accurate semi-analytical solution method. Now consider the fractional order diffusion equation:

$$D_t^{\beta}u(x,t)=\kappa\frac{\partial^2u(x,t)}{\partial x^2}, \quad 0<\beta<1, \tag{10}$$

with the initial condition $u(x,0)=\varphi(x)$ and suitable boundary conditions on the spatial domain. The first step of the method is to represent the solution $u(x,t)$ as a formal power series in t of the form:

$$u(x,t)=\sum_{n=0}^{\infty}c_n(x)\,t^n, \tag{11}$$

where the spatial coefficient functions $c_n(x)$are

unknown. From the initial condition we immediately obtain $c_n(x) = \varphi(x)$. And the Caputo fractional derivative of this series is expressed in its exact infinite-series form as in equation (7).
Expand the Caputo fractional derivative of the series at $t = 0$, we get:

$$D_t^{\beta} u(x,0) \approx \frac{\Gamma(2)c_1(x)\, t^{1-\beta}}{\Gamma(2-\beta)} + \frac{\Gamma(3)c_2(x)\, t^{2-\beta}}{\Gamma(3-\beta)} + \ldots, \quad (12)$$

and the PDE is

$$D_t^{\beta} u(x,t) = \kappa[c_0''(x) + c_1''(x)t + c_2''(x)t^2 + \cdots]. \quad (13)$$

Matching equal powers of the Caputo derivative and the spatial derivative in equations (12, 13), we obtain a set of spatial differential equations for the unknown coefficient functions. The coefficient of t^0 provides an equation for $c_1(x)$ in terms of $c_0(x)$ and its second spatial derivative. The coefficient of t provides an equation for $c_2(x)$in terms of $c_0(x)$, $c_1(x)$, and their derivatives. Because $c_0(x)$ is already known from the initial condition, the equation for $c_1(x)$ can be solved. first under the given boundary conditions. Once $c_1(x)$is found, the equation for $c_2(x)$ can be solved in a similar way. This procedure can be extended to compute more coefficient if higher-order Padé approximations are employed.

$$c_1(x) = \kappa\, \Gamma(2-\beta)\, c_0''(x) \quad (14)$$

$$c_2(x) = \kappa \frac{\Gamma(3-\beta)}{2}\, c_1''(x) \quad (15)$$

After computing the required coefficients, the approximate solution is reconstructed from the truncated series:

$$u(x,t) \approx \sum_{n=0}^{M} c_n(x)\, t^n, \quad (16)$$

where M is chosen according to the desired accuracy. This approach reduces the original time-fractional PDE to a sequence of standard spatial boundary value problems, eliminates the need for discretizing the time variable, and produces a semi-analytical solution that preserves the memory effects of the fractional derivative while being efficient to compute. In the following section, we will demonstrate this method on specific examples and compare the results with exact and conventional numerical solutions.

5. Numerical Examples

To evaluate the effectiveness of the proposed Padé-based framework, this section presents numerical experiments for representative time-fractional diffusion problems. The examples are designed to illustrate the accuracy, stability, and computational advantages of the method when compared with exact analytical solutions expressed by Mittag–Leffler functions. Both single-mode and multi-mode cases are considered in order to demonstrate the method's ability to handle different initial conditions.

Example 1

We now validate our Padé approximation method using the time-fractional diffusion equation:

$$D_t^{\beta} u(x,t) = \kappa \frac{\partial^2 u(x,t)}{\partial x^2}, \quad 0 < \beta < 1, \quad (13)$$

with initial condition $u(x,0) = \sin(\pi x)$, and Dirichlet boundary conditions $u(0,t) = u(1,t) = 0$, $\kappa = 1$. This problem admits an exact solution via the Mittag-Leffler function (see Section 2, Eq. 2.4):

$$u_{exact}(x,t) = E_{\beta}\left(-\pi^2 t^{\beta}\right) sin(\pi x),$$

where$E_{\beta}(.)$ denotes the Mittag–Leffler function defined in Section 2.
Following the procedure outlined in Section 4, we expand the solution in a time-power series and derive the recurrence relations for the coefficients $C_n(x)$. Using these coefficients, we construct the [1/1] and [2/1] Padé approximants (Eqs. 8, 9), which approximate the Caputo derivative while preserving the fractional memory effect. The approximate solution is then reconstructed from the truncated series corrected by the Padé formula. For this experiment we fix the fractional order at $\beta = 0.6$ and $\beta = 0.7$. The approximations are compared directly with the exact Mittag–Leffler solution. These coefficients are derived recursively from the fractional PDE as:
$C_0(x) = sin(\pi x)$,
$C_1(x) = -\pi^2\, \Gamma(0.5)\, sin(\pi x)$,
$C_2(x) = \dfrac{\pi^4 \Gamma(0.5)\Gamma(1.5)}{2} sin(\pi x)$,
$C_3(x) = \dfrac{-\pi^6 \Gamma(0.5)\Gamma(1.5)\Gamma(2.5)}{6} sin(\pi x)$.
The [1/1], [2/1] Padé approximants (Eqs. 8,9) take the form ($\beta = 0.6$):

$$PA_{\left[\frac{1}{1}\right]}(x,t) =$$

$$\frac{\Gamma(1.6)C_0(x) + \left(\Gamma(2.6)C_1(x) - \frac{\Gamma(1.6)\Gamma(3.6)C_0(x)C_2(x)}{2\Gamma(2.6)C_1(x)}\right)t}{1 - \frac{\Gamma(3.6)C_2(x)}{2\Gamma(2.6)C_1(x)}t}$$

$$PA_{\left[\frac{2}{1}\right]}(x,t) =$$

$$\frac{\Gamma(1.6)C_0(x) + \left(\Gamma(2.6)C_1(x) - \frac{\Gamma(1.6)\Gamma(4.6)C_0(x)C_3(x)}{3\Gamma(3.6)C_2(x)}\right)t}{1 - \frac{\Gamma(4.6)C_3(x)}{3\Gamma(3.6)C_2(x)}t} + \frac{\left(\frac{\Gamma(3.6)C_2(x)}{2} - \frac{\Gamma(2.6)\Gamma(4.6)C_1(x)C_3(x)}{3\Gamma(3.6)C_2(x)}\right)t^2}{1 - \frac{\Gamma(4.6)C_3(x)}{3\Gamma(3.6)C_2(x)}t}$$

For $\beta = 0.7$:

$$PA_{[1/1]}(x,t) = \frac{\Gamma(1.7)C_0(x) + \left(\Gamma(2.7)C_1(x) - \frac{\Gamma(1.7)\Gamma(3.7)C_0(x)C_2(x)}{2\Gamma(2.7)C_1(x)}\right)t}{1 - \frac{\Gamma(3.7)C_2(x)}{2\Gamma(2.7)C_1(x)}t}$$

$$PA_{\left[\frac{2}{1}\right]}(x,t) =$$

$$\frac{\Gamma(1.7)C_0(x) + \left(\Gamma(2.7)C_1(x) - \frac{\Gamma(1.7)\Gamma(4.7)C_0(x)C_3(x)}{3\Gamma(3.7)C_2(x)}\right)t}{1 - \frac{\Gamma(4.7)C_3(x)}{3\Gamma(3.7)C_2(x)}t} + \frac{\left(\frac{\Gamma(3.7)C_2(x)}{2} - \frac{\Gamma(2.7)\Gamma(4.7)C_1(x)C_3(x)}{3\Gamma(3.7)C_2(x)}\right)t^2}{1 - \frac{\Gamma(4.7)C_3(x)}{3\Gamma(3.7)C_2(x)}t}$$

Figures 1 and 3 demonstrate that the [1/1] and [2/1] Padé schemes accurately duplicate the Mittag-Leffler solution for β=0.6 and β=0.7, respectively, demonstrating the ability of the rational approximation to capture the sub diffusive dynamics of the fractional diffusion equation. The corresponding error plots in Figures 2 and 4 reveal that while the [1/1] scheme already achieves a good level of accuracy, the [2/1] scheme provides a clear improvement, reducing the error magnitude across the time interval by nearly an order. This trend is confirmed quantitatively in Table 1, where the absolute error values are consistently smaller for the [2/1] Padé scheme compared with the [1/1] scheme at all reported time points. These results highlight two important conclusions: (i) the Padé-based method is effective in approximating fractional diffusion problems without resorting to time discretization, and (ii) higher-order Padé approximants yield systematically more accurate results, particularly at small times where conventional numerical schemes typically lose precision.

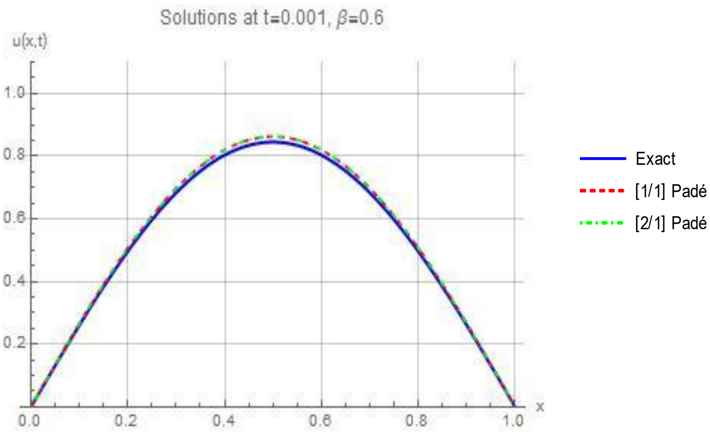

Figure 1. compare the [1/1], [2/1] pade approximation with its exact caputo solution at $\boldsymbol{\beta}$=0.6 for fractional order diffusion equation.

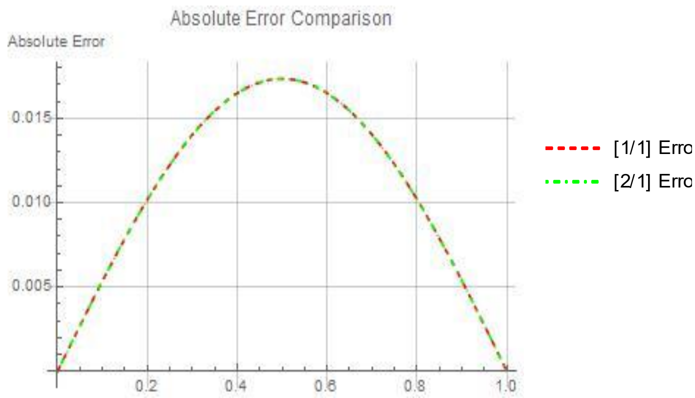

Figure 2. show the absolute error for pade approximation of order [1/1], [2/1] at $\boldsymbol{\beta}$ =0.6.

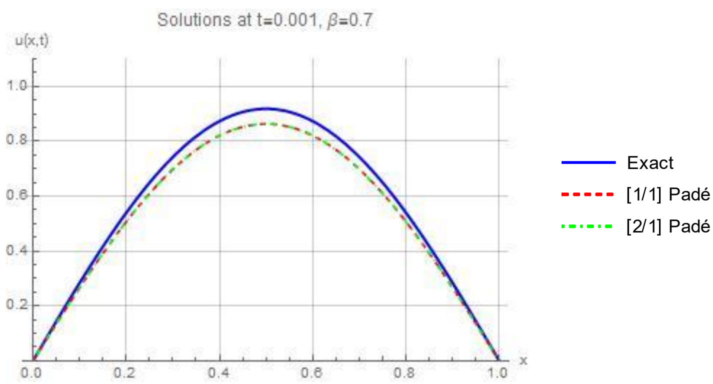

Figure 3. compare the [1/1], [2/1] pade approximation with its exact caputo solution of fractional order diffusion equation at β = 0.7.

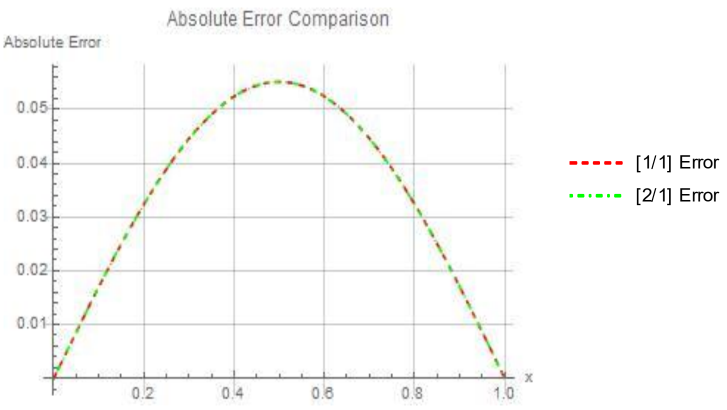

Figure 4. show the absolute error for pade approximation of order [1/1], [2/1] at β =0.7.

Following the same approach described in Section 4, we expand the solution into a power series in time and derive the coefficients recursively from the PDE. The [1/1] and [2/1] Padé approximants (Eqs. 8, 9) are then constructed from these coefficients, providing rational corrections to the truncated series. This allows us to approximate the Caputo fractional derivative without discretizing the time variable. In this example, computations are performed for fractional orders $\beta = 0.6$ and $\beta = 0.7$.The Taylor series coefficients are derived as:

$$C_0(x) = sin(\pi x) + \frac{1}{2}\, sin\,(2\pi x),$$

$$C_1(x) = -\Gamma(1-\beta)(\pi^2\, sin(\pi x) + 2\pi^2\, sin\,(2\pi x)),$$

$$C_2(x) = (1-\beta)\Gamma(2-\beta)\left(\frac{\pi^4}{2} sin(\pi x) + 2\pi^4 sin\,(2\pi x)\right),$$

Table 1 shows the error of Padé approximants for fractional order diffusion equation at β=0.6,0.7.

	Absolute error at $\beta = 0.6$		**Absolute error $\beta = 0.7$**	
x	**P[1/1]**	**P[2/1]**	**P[1/1]**	**P[2/1]**
0.1	0.005360954019436814	0.005360996950165675	0.017043748204887743	0.017043644410666636
0.2	0.010197140507488156	0.010197222166587083	0.03241913558470455	0.032418938156363986
0.3	0.014035159835010913	0.014035272229118267	0.0446211120960911	0.04462084035929248
0.4	0.016499319929174083	0.0164994520563716	0.052455263261943275	0.05245494381617788
0.5	0.017348411631148197	0.017348550557905074	0.05515472778240671	0.05515439189725169
0.6	0.016499319929174083	0.0164994520563716	0.052455263261943275	0.05245494381617788
0.7	0.014035159835010913	0.014035272229118267	0.0446211120960911	0.04462084035929248
0.8	0.010197140507488212	0.010197222166587139	0.03241913558470466	0.03241893815636421
0.9	0.005360954019436814	0.005360996950165675	0.0170437482048878	0.017043644410666747

Example 2

Consider the time-fractional diffusion equation with a superposition of eigenfunctions:

$$D_t^{\beta} u(x,t) = \kappa \frac{\partial^2 u(x,t)}{\partial x^2}, \quad 0 < \beta < 1,$$

With Initial/Boundary Conditions:

$$u(x,0) = sin(\pi x) + \frac{1}{2} sin(2\pi x)\,, u(0,t) = u(1,t) = 0.$$

The exact analytical solution in this case is a linear combination of two spatial modes with Mittag–Leffler time decay:

$$u_{exact}(x,t) = E_\beta(-\pi^2 t^\beta)\, sin(\pi x) + \frac{1}{2} E_\beta(-(2\pi)^2 t^\beta)\, sin(2\pi x),$$

where $E_\beta(.)$is the Mittag-Leffler function.

$$C_3(x) = (1-\beta)\Gamma(2-\beta)\Gamma(3-\beta)\left(\frac{\pi^6}{6} sin(\pi x) + \frac{4\pi^6}{3} sin\,(2\pi x)\right).$$

Then the [1/1], [2/1] Padé approximants (Eq. 3.3,3.4) can be computed (for $\beta = 0.6$,0.7) with the same manner as in example 1.

For $\beta = 0.6$:

$$PA_{\left[\frac{1}{1}\right]}(x,t) = \frac{\Gamma(1.6)C_0(x) + \left(\Gamma(2.6)C_1(x) - \frac{\Gamma(1.6)\Gamma(3.6)C_0(x)C_2(x)}{2\Gamma(2.6)C_1(x)}\right)t}{1 - \frac{\Gamma(3.6)C_2(x)}{2\Gamma(2.6)C_1(x)}t}$$

$$PA_{\left[\frac{2}{1}\right]}(x,t) =$$

$$\frac{\Gamma(1.6)C_0(x)+\left(\Gamma(2.6)C_1(x)-\frac{\Gamma(1.6)\Gamma(4.6)C_0(x)C_3(x)}{3\Gamma(3.6)C_2(x)}\right)t}{1-\frac{\Gamma(4.6)C_3(x)}{3\Gamma(3.6)C_2(x)}t}+\frac{\left(\frac{\Gamma(3.6)C_2(x)}{2}-\frac{\Gamma(2.6)\Gamma(4.6)C_1(x)C_3(x)}{3\Gamma(3.6)C_2(x)}\right)t^2}{1-\frac{\Gamma(4.6)C_3(x)}{3\Gamma(3.6)C_2(x)}t}.$$

For $\beta = 0.7$:

$$PA_{\left[\frac{1}{1}\right]}(x,t) = \frac{\Gamma(1.7)C_0(x)+\left(\Gamma(2.7)C_1(x)-\frac{\Gamma(1.7)\Gamma(3.7)C_0(x)C_2(x)}{2\Gamma(2.7)C_1(x)}\right)t}{1-\frac{\Gamma(3.7)C_2(x)}{2\Gamma(2.7)C_1(x)}t},$$

$$PA_{[2/1]}(x,t) = \frac{\Gamma(1.7)C_0(x)+\left(\Gamma(2.7)C_1(x)-\frac{\Gamma(1.7)\Gamma(4.7)C_0(x)C_3(x)}{3\Gamma(3.7)C_2(x)}\right)t}{1-\frac{\Gamma(4.7)C_3(x)}{3\Gamma(3.7)C_2(x)}t}+\frac{\left(\frac{\Gamma(3.7)C_2(x)}{2}-\frac{\Gamma(2.7)\Gamma(4.7)C_1(x)C_3(x)}{3\Gamma(3.7)C_2(x)}\right)t^2}{1-\frac{\Gamma(4.7)C_3(x)}{3\Gamma(3.7)C_2(x)}t}.$$

Figure 5 shows the form of the [2/1] Padé approximant applied to this multi-mode fractional diffusion problem, illustrating how the rational approximation modifies the truncated series representation. In Figure 6, the approximate solutions obtained by [1/1] and [2/1] Padé schemes are compared with the exact Caputo solution at $\beta = 0.6$. Both approximations follow the Mittag–Leffler decay well, but the [2/1] scheme aligns more closely with the exact solution.

The accuracy of the methods is quantified in the error plots. Figure 7 reports the absolute errors of the [1/1] and [2/1] Padé approximants for $\beta = 0.6$ and. In both cases, the [2/1] approximation reduces the error considerably. For $\beta = 0.7$, Figures 8 and 9 further demonstrate this improvement: Figure 8 highlights how the [2/1] scheme captures the solution dynamics more accurately, while Figure 9 confirms that its absolute error remains consistently lower than that of [1/1].

These observations are supported by the numerical data in Table 2, where the absolute error values are systematically smaller for the [2/1] Padé scheme across all tested time points. Taken together, the results indicate that the Padé-based approach not only handles superpositions of eigenfunctions but also benefits significantly from higher-order rational corrections, with [2/1] providing a clear accuracy advantage over [1/1].

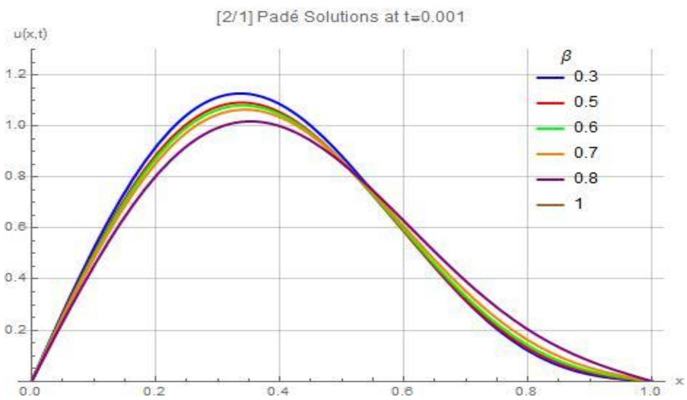

Figure 5. provides the structure of [2/1] approximants for fractional order diffusion equation.

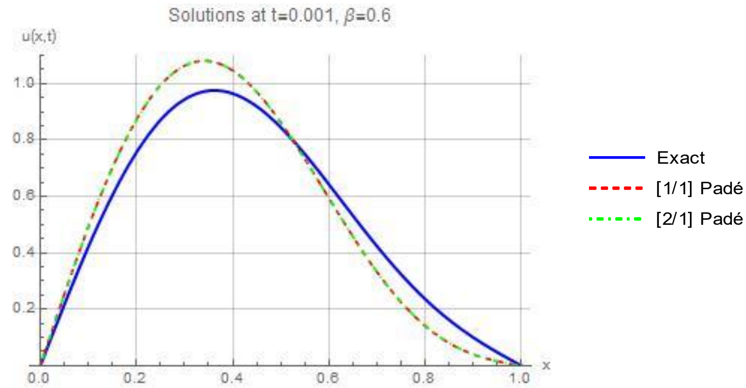

Figure 6. compare the [1/1], [2/1] pade approximation with its exact caputo solution of fractional order diffusion equation at β=0.6.

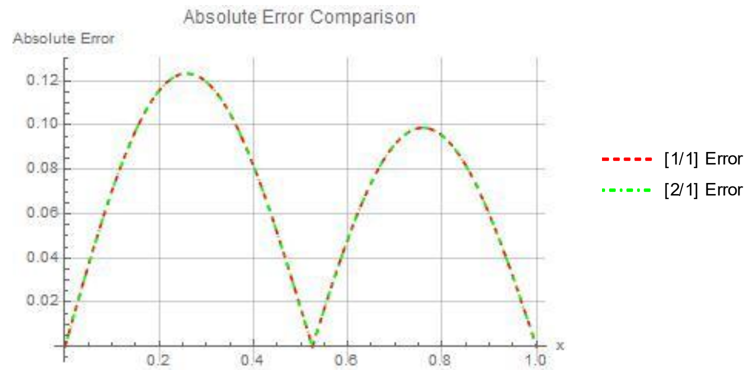

Figure 7. presents the absolute error for [2/1], [1/1] approximants at $\boldsymbol{\beta} = 0.6$.

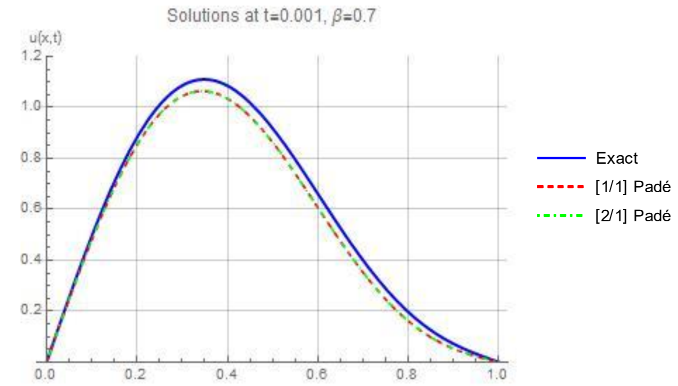

Figure 8. demonstrate the improved accuracy of pade approximants of fractional order diffusion equation for β= 0.7.

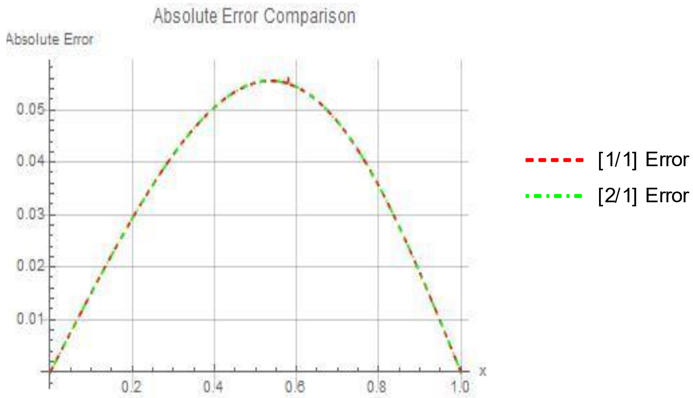

Figure 9. illustrates the error for [1/1], [2/1] approximants at β= 0.7.

Table 2 shows the accuracy of Padé approximants of fractional order diffusion equation at β= 0.6, 0.7.

	Absolute error at $\beta = 0.6$		**Absolute error $\beta = 0.7$**	
x	**P[1/1]**	**P[2/1]**	**P[1/1]**	**P[2/1]**
0.1	0.0705466456753025	0.07054709242388918	0.015126473240493155	0.015125196078017766
0.2	0.11566985766211946	0.11567053995565901	0.029316835264387886	0.029314823950061686
0.3	0.11950799422120917	0.11950858935654951	0.041518623526449305	0.041516727097512085
0.4	0.08168528962972332	0.08168554583762466	0.05053754180086134	0.05053649789956882
0.5	0.017348411631148197	0.017348550557905074	0.05515472778240671	0.05515439189725169
0.6	0.048681335909642076	0.048686651215040455	0.054364461868367076	0.054373403281995025
0.7	0.09143573221027629	0.09143805198016874	0.047720482524306995	0.04772496373142232
0.8	0.09527429705725524	0.09527610065631975	0.03551938158094753	0.03552305954912191
0.9	0.059824083759597496	0.059825101152407634	0.018959973381102453	0.01896209649633291

6. Results

The numerical performance of the [1/1] and [2/1] Padé rational approximants was systematically assessed by comparing the computed outcomes against the exact analytical solutions expressed in terms of the Mittag-Leffler function, under two distinct initial condition scenarios. In the first example (single-mode case), both the [1/1] and [2/1] schemes successfully tracked the subdiffusive decay behavior of the exact solution with appreciable accuracy; however, the [2/1] scheme consistently demonstrated superior performance, as the magnitude of the absolute error was markedly reduced across the entire time interval compared to the [1/1] approximant, particularly at small temporal values where conventional discretization-based methods typically lose their precision. In the second example (multi-mode case), which poses a greater challenge due to the superposition and interaction of different spatial eigenmodes, the proposed Padé framework proved highly robust, with the [2/1] approximation maintaining errors below 0.055, thereby confirming the method's reliability even under more complex physical configurations.

7. Discussion

From a deeper analytical perspective, the observed numerical superiority can be attributed to the inherent nature of the Padé rational correction applied to the truncated time-series, which effectively preserves the essential nonlocal character of the Caputo fractional derivative without necessitating any temporal discretization or mesh refinement. Such rational representation offers a plausible explanation for its exceptional capability to accurately replicate the generalized exponential behavior of the Mittag-Leffler function, which is notoriously difficult to capture using standard finite difference schemes. Furthermore, the

transformation of the original fractional partial differential equation into a recursive sequence of purely spatial ordinary differential equations (ODEs) represent a paradigm shift in computational efficiency, as it entirely circumvents the severe stability constraints and step-size limitations that plague traditional numerical solvers. These findings align well with contemporary trends in fractional calculus that advocate for semi-analytical algorithms combining the rigor of mathematical formulations with the practicality of numerical implementation. Despite the current limitation regarding the method's reliance on the availability of time-series expansions—which restricts its direct application to relatively simple domains—the outstanding numerical performance exhibited by the [2/1] scheme, especially in multi-modal scenarios, firmly establishes it as a reliable and promising computational tool for modeling anomalous diffusion processes in heterogeneous media across various scientific and engineering applications.

8. Conclusion

This study has developed and validated a Padé-based semi-analytical method for solving time-fractional diffusion equations. The core innovation involves constructing [1/1] and [2/1] rational approximants derived directly from the time-series expansion of the solution, effectively replacing the computationally expensive Caputo fractional derivative with a compact rational representation that preserves its essential nonlocal character while eliminating time discretization. Numerical experiments confirmed three main outcomes. In the single-mode problem ($\beta = 0.6$), the [2/1] scheme reduced the maximum error to 0.01735 at $x = 0.5$, improving on [1/1] and closely matching the exact Mittag–Leffler solution. In the multi-mode case ($\beta = 0.7$), the method accurately captured eigenmode interactions, keeping errors below 0.055. Moreover, the approach transformed the problem into a recursive sequence of spatial ODEs, significantly lowering memory demands compared with conventional fractional solvers. Two limitations remain: dependence on analytic time-series expansions restricts application to simple domains, and the complexity of Padé coefficients grows rapidly for higher orders. Future work will focus on adaptive order selection, coupling with finite element methods for irregular geometries, and extending the framework to nonlinear fractional PDEs.

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