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A Hybrid Analytical-Numerical Framework for Caputo Fractional Differential Equations in Applied Mathematics

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ABSTRACT: Caputo fractional differential equations provide a mathematical framework for modeling dynamical systems characterized by memory, hereditary effects, and nonlocal behavior. This study develops a hybrid analytical-numerical framework integrating exact Mittag-Leffler solutions, the L1 approximation, Adams-type predictor-corrector methods, and finite-difference discretization for fractional ordinary and partial differential equations. Numerical experiments investigate fractional-order sensitivity, solution accuracy, and convergence behavior using a fractional relaxation benchmark with fractional orders α = 0.5, 0.7, 0.9, and 1.0. We validate the L1 method against the exact analytical solution under successive temporal grid refinements. The results demonstrate that reducing the time step from 0.05 to 0.00625 decreases the maximum numerical error from 0.04423 to 0.01783 for α = 0.5, from 0.02454 to 0.00581 for α = 0.7, and from 0.01106 to 0.00161 for α = 0.9. At the finest temporal resolution, the observed convergence rates reach 0.457, 0.698, and 0.929 for the three fractional orders, respectively. The numerical findings further show that smaller fractional orders yield slower long-term relaxation, while the solution approaches classical exponential decay as α approaches unity. These results establish the influence of fractional order on both solution dynamics and numerical convergence, highlighting the importance of temporal discretization and solution regularity in fractional modeling. The proposed framework provides an integrated analytical and computational basis for evaluating Caputo fractional differential equations and supports further development of numerical methods for nonlinear and diffusion-type systems governed by memory-dependent dynamics.

Keywords: fractional differential equations, Caputo derivative, Adams-type predictor-corrector method, Mittag-Leffler function, time-fractional diffusion.

I. INTRODUCTION

Fractional calculus generalizes classical differentiation and integration to non-integer orders. This generalization is significant in applied mathematics because many real systems exhibit memory, hereditary properties, spatial heterogeneity, and nonlocal behavior. In such systems, future evolution depends not only on the current state but also on the process's accumulated history. Classical integer-order differential equations can describe many local processes effectively, but they often require additional empirical variables or fitted damping terms to mimic long-memory effects.

Fractional differential equations have therefore become an important modeling tool for complex dynamical systems. They are useful in anomalous diffusion, viscoelastic materials, biological dynamics, control systems, signal processing, heat transfer, finance, and other processes in which past states influence the present response. The fractional order α acts as an additional modeling parameter that controls the

intensity of memory and allows the model to represent intermediate behavior between classical limiting cases. This flexibility gives fractional models an advantage when ordinary or partial differential equations of integer order cannot adequately capture the observed dynamics.

Despite their modeling advantages, fractional differential equations are challenging to solve. The nonlocal derivative requires information from previous time levels, which increases memory storage and computational cost. Solutions also frequently contain weak singularities near the initial time. These features can reduce the accuracy of standard numerical schemes and make stability and convergence analysis more delicate than in classical differential equations. As a result, reliable fractional modeling requires both analytical understanding and carefully designed numerical approximation.

Analytical solutions are valuable because they reveal the qualitative structure of fractional models and can serve as benchmarks for validating numerical schemes. However, exact solutions are available only for limited classes of linear or specially constructed problems. For nonlinear equations and diffusion-type models, numerical methods are usually required. Therefore, combining analytical benchmarks with numerical discretization and statistical error assessment provides a stronger basis for evaluating the performance of fractional solution methods.

This paper focuses on Caputo fractional differential equations because the Caputo derivative is well-suited to initial-value problems and allows classical initial conditions such as $y(0) = y_0$. The study connects analytical benchmark solutions with practical numerical schemes and evaluates them using statistical and computational indicators. In particular, the paper examines selected methods for accuracy, convergence, stability, computational efficiency, and sensitivity to the fractional order. This integrated approach aims to support selecting suitable analytical and numerical techniques for applied problems governed by memory and nonlocal dynamics.

II. LITERATURE REVIEW

Numerical methods for fractional differential equations have increasingly focused on improving the accuracy of Caputo-derivative approximations. [1] introduced a second-order difference formula for time-fractional diffusion equations and demonstrated that greater temporal accuracy can be achieved while maintaining numerical stability. [2] examined semilinear subdiffusion equations with nonsmooth initial data and established stability and error estimates that clarify how limited solution regularity affects numerical performance.

Spectral techniques provide an alternative to conventional finite-difference discretization. [3] developed a Chebyshev operational-matrix method for fractional differential equations involving a nonsingular Mittag-Leffler kernel, transforming the governing equations into algebraic systems that can be solved efficiently. [4] proposed a high-order numerical scheme for nonlinear fractional differential equations and showed that uniform accuracy and stability can be maintained across different fractional orders.

Domain decomposition has also been employed to increase numerical accuracy in fractional models. [5] presented a multi-domain spectral method for time-fractional differential equations, combining local spectral approximation with domain decomposition to obtain accurate solutions for sufficiently regular problems. [6] applied Chebyshev-based differential quadrature to a fractional-order Riccati equation and demonstrated that nonlinear fractional equations can be reduced to manageable algebraic formulations.

The regularity of fractional solutions is central to the practical performance of numerical schemes. [7] analyzed the classical L1 approximation for subdiffusion equations with nonsmooth data and showed that weak initial singularities can substantially reduce the observed convergence order. [8] investigated fully discrete schemes for fractional diffusion and diffusion-wave equations and provided error estimates that

account for interactions between temporal discretization, spatial approximation, and nonsmooth initial conditions.

Comparative and review studies have clarified the strengths and limitations of the main numerical approaches. [9] provided a concise overview of numerical methods for time-fractional evolution equations, including L1-type formulas, finite-element approximations, convolution quadrature, and correction techniques for nonsmooth solutions. [10] developed correction procedures for high-order backward-differentiation convolution quadrature and demonstrated that suitable starting corrections can recover high-order convergence when the initial data are nonsmooth or incompatible.

Nonlinear subdiffusion equations require analytical tools that accommodate both nonlocality and nonlinearity. [11] established a numerical analysis framework for nonlinear subdiffusion equations and connected stability, maximal regularity, and finite-element error estimation. [12] investigated subdiffusion models with time-dependent coefficients and showed that improved regularity analysis can support second-order temporal discretization for variable-coefficient fractional problems.

Predictor-corrector algorithms are widely used for nonlinear fractional initial-value problems because they are based on the equivalent Volterra integral formulation. [13] proposed a family of predictor-corrector methods and examined their accuracy, stability, and applicability to different classes of fractional differential equations. [14] developed a fast, high-order method for nonlinear fractional equations with nonsingular kernels and used recurrence relations to reduce computational complexity while preserving numerical accuracy.

Convolution quadrature offers a systematic framework for constructing stable high-order approximations. [15] introduced an exponential convolution-quadrature method for nonlinear subdiffusion equations with nonsmooth initial data and combined high-order temporal integration with local refinement near the initial time. [16] derived sharp error estimates for the nonuniform L1 formula and demonstrated that carefully designed nonuniform meshes can improve accuracy for reaction-subdiffusion equations exhibiting initial singularities.

Rigorous stability analysis is necessary when variable or nonuniform time steps are employed. [17] established a discrete fractional Gronwall inequality and showed its usefulness for analyzing stability and convergence of nonuniform and fast time-stepping schemes. [18] developed and analyzed a high-order method for time-fractional diffusion equations, showing that enhanced convergence can be obtained when the solution satisfies the required smoothness conditions.

Analytical and semi-analytical methods remain valuable because they provide interpretable solution representations and reference solutions for numerical validation. [19] combined the Laplace transform with a homotopy-analysis procedure to construct approximate solutions for linear fractional partial differential equations with singular and nonsingular kernels. [20] proposed a high-order predictor-corrector method for nonlinear fractional differential equations and demonstrated that accurate approximations can be obtained when exact closed-form solutions are unavailable.

Mesh design is particularly important for fractional equations because their solutions commonly possess weak singularities near the initial time. [21] analyzed a finite-difference method on graded meshes and showed that appropriate mesh grading can recover convergence rates that are lost on uniform grids. [22]

combined graded meshes with a fast high-order predictor-corrector algorithm, reducing the computational cost of the memory term while maintaining accuracy for Caputo-type fractional differential equations.

Reliable benchmark problems are required to evaluate numerical algorithms objectively. [23] developed benchmark problems for Caputo fractional-order ordinary differential equations and emphasized the importance of comparing numerical solutions with exact or independently verified reference solutions. [24] analyzed a modified L1 scheme for time-fractional partial differential equations with nonsmooth data and demonstrated that carefully modified discretization can improve convergence under limited regularity.

Second-order temporal methods provide stronger numerical baselines than conventional first-order formulas. [25] developed second-order numerical algorithms for time-fractional subdiffusion equations and assessed their stability and convergence within a finite-element framework. [26] proposed a fast high-order method for time-fractional diffusion equations and reduced the computational and storage requirements associated with the long-memory term through an accelerated approximation strategy.

Collectively, these studies demonstrate that the reliability of fractional differential-equation solvers depends on the interaction among derivative approximation, solution regularity, mesh construction, stability analysis, computational efficiency, and benchmark validation. However, much of the existing literature focuses on individual method families rather than integrating analytical solutions, numerical discretization, statistical error measures, convergence analysis, computational cost, and fractional-order sensitivity into a single applied framework. This study addresses this limitation by combining these elements into a unified analytical-numerical evaluation of Caputo fractional differential equations.

The studies summarized in Table 1 advance L1-type discretization, predictor-corrector algorithms, spectral methods, finite-element analysis, convolution quadrature, graded meshes, and fast-memory computation. Nevertheless, most studies examine individual numerical techniques or theoretical properties in isolation. This study addresses this gap by integrating analytical benchmarks, numerical approximation, statistical error indicators, convergence analysis, computational cost, and fractional-order sensitivity into a unified framework for Caputo fractional differential equations.

Table 1. Comparative summary of the studies reviewed and their relevance to the proposed framework.

Ref.	Author(s) and Year	Study Focus and Method	Main Findings	Relevance and Research Gap
[1]	Alikhanov (2015)	Developed the L2-1σ difference approximation for time-fractional diffusion equations.	The proposed scheme achieved second-order temporal accuracy and demonstrated numerical stability.	Provides a higher-order alternative to the conventional L1 formula, but requires more complex implementation.
[2]	Al-Maskari and Karaa (2019)	Examined finite-element approximation of semilinear subdiffusion equations with nonsmooth initial data.	Established stability and error estimates under limited initial regularity.	Supports the treatment of nonlinear fractional models, although its emphasis is primarily

Ref.	Author(s) and Year	Study Focus and Method	Main Findings	Relevance and Research Gap
				theoretical rather than computationally comparative.
[3]	Baleanu et al. (2018)	Applied a Chebyshev spectral operational-matrix method to fractional equations with a nonsingular Mittag-Leffler kernel.	Converted fractional differential equations into algebraic systems and obtained accurate numerical solutions.	Broadens the range of fractional kernels considered, but does not provide a direct comparison with standard Caputo discretization methods.
[4]	Cao and Cai (2021)	Developed a high-order numerical scheme for nonlinear fractional differential equations.	Achieved uniform accuracy and stable performance across different fractional orders.	Demonstrates the value of high-order nonlinear solvers, but involves greater computational and implementation complexity.
[5]	Chen et al. (2015)	Proposed a multi-domain spectral method for time-fractional differential equations.	Domain decomposition and spectral approximation produced high accuracy for sufficiently regular solutions.	Shows the potential of spectral techniques, although performance may deteriorate when solutions exhibit weak initial singularities.
[6]	Hou and Yang (2017)	Used Chebyshev differential quadrature to solve a fractional-order Riccati equation.	Reduced the nonlinear fractional equation to an algebraic system and obtained accurate approximate solutions.	Provides a useful nonlinear benchmark, but its application is limited to a specific equation family.
[7]	Jin et al. (2016a)	Analyzed the L1 scheme for subdiffusion equations with nonsmooth initial data.	Demonstrated that weak initial singularities can significantly reduce the practical convergence order.	Directly supports the present study's use of observed convergence rates and regularity-sensitive error analysis.
[8]	Jin et al. (2016b)	Investigated two fully discrete schemes for fractional diffusion and diffusion-wave equations.	Derived error estimates that account for temporal discretization, spatial approximation, and nonsmooth data.	Supports integrated temporal-spatial analysis, but does not combine numerical errors with statistical performance indicators.
[9]	Jin et al. (2019)	Reviewed numerical methods for time-fractional evolution equations with nonsmooth data.	Compared L1-type methods, convolution quadrature, finite-element schemes, and correction procedures.	Confirms the need for method comparison, but remains an overview rather than an integrated computational evaluation.
[10]	Jin et al. (2017)	Developed correction procedures for high-order BDF convolution quadrature.	Suitable starting corrections recovered high-order convergence for nonsmooth and incompatible data.	Highlights the importance of correction terms, although the corrected method is more difficult to implement than baseline schemes.

Ref.	Author(s) and Year	Study Focus and Method	Main Findings	Relevance and Research Gap
[11]	Jin et al. (2018)	Presented a numerical analysis of nonlinear subdiffusion equations.	Connected discrete fractional Gronwall inequalities, maximal regularity, stability, and finite-element error estimation.	Provides rigorous support for nonlinear fractional modeling, but offers limited comparative computational evidence.
[12]	Jin et al. (2020)	Studied subdiffusion equations with time-dependent coefficients and second-order temporal discretization.	Improved regularity analysis enabled accurate second-order time stepping for variable-coefficient problems.	Supports future extension to nonautonomous models, which are not fully examined in the present benchmark analysis.
[13]	Kumar and Gejji (2019)	Proposed a family of predictor-corrector methods for fractional differential equations.	The methods demonstrated suitable accuracy and stability for several nonlinear fractional problems.	Supports predictor-corrector implementation, but does not systematically integrate CPU time, statistical errors, and fractional-order sensitivity.
[14]	Lee et al. (2021)	Developed a fast high-order method for nonlinear fractional equations with nonsingular kernels.	Recurrence relations reduced computational complexity while maintaining numerical accuracy.	Demonstrates the value of fast algorithms, but focuses on nonsingular kernels rather than the classical Caputo derivative.
[15]	Li and Ma (2022)	Introduced exponential convolution quadrature for nonlinear subdiffusion with nonsmooth initial data.	They achieved high-order accuracy through exponential integration and local temporal refinement.	Provides an advanced benchmark method, although its implementation is considerably more complex than L1 and predictor-corrector approaches.
[16]	Liao et al. (2018)	Derived sharp error estimates for the nonuniform L1 formula in reaction-subdiffusion equations.	Nonuniform meshes improved accuracy for solutions exhibiting initial singularities.	Supports mesh-sensitivity analysis and motivates extending the current uniform-grid framework to nonuniform meshes.
[17]	Liao et al. (2019)	Established a discrete fractional Gronwall inequality for numerical subdiffusion schemes.	Provided rigorous stability and convergence tools for nonuniform and fast time-stepping methods.	Strengthens the theoretical basis for stability analysis, but does not provide an applied comparative workflow.
[18]	Lv and Xu (2016)	Conducted an error analysis of a high-order method for time-fractional diffusion equations.	Demonstrated stability and high-order convergence under appropriate smoothness assumptions.	Shows that accuracy gains depend strongly on solution regularity and careful numerical implementation.
[19]	Morales-Delgado et al. (2016)	Combined the Laplace transform and homotopy-analysis method for linear fractional partial differential equations.	Produced approximate analytical solutions for equations with singular and nonsingular kernels.	Supports semi-analytical benchmarking, but requires validation against exact or high-resolution numerical solutions.

Ref.	Author(s) and Year	Study Focus and Method	Main Findings	Relevance and Research Gap
[20]	Nguyen and Jang (2017)	Developed a high-order predictor-corrector method for nonlinear fractional differential equations.	The method produced accurate, stable solutions when closed-form solutions were unavailable.	Supports the use of predictor-corrector methods for nonlinear tests, but provides limited comparison with alternative method families.
[21]	Stynes et al. (2017)	Analyzed a finite-difference method on graded meshes for a time-fractional diffusion equation.	Appropriate mesh grading recovered convergence rates affected by weak initial singularities.	Motivates the future use of graded meshes, whereas the current framework employs transparent uniform-grid benchmarks.
[22]	Su and Zhou (2022)	Proposed a fast high-order predictor-corrector method on graded meshes.	Combined graded temporal discretization with fast memory approximation to reduce runtime and storage requirements.	Directly addresses memory cost, but its greater complexity makes it less suitable as an introductory baseline method.
[23]	Xue and Bai (2017)	Developed benchmark problems for Caputo fractional-order ordinary differential equations.	Demonstrated the importance of exact or independently verified reference solutions for solver assessment.	Supports the present study's benchmark-validation strategy, but does not compare multiple numerical and statistical performance measures.
[24]	Yan et al. (2018)	Analyzed a modified L1 scheme for time-fractional partial differential equations with nonsmooth data.	The modified discretization improved convergence when the solution had limited regularity.	Reinforces the need for regularity-sensitive schemes, but does not address computational cost and fractional-order sensitivity together.
[25]	Zeng et al. (2015)	Developed second-order numerical algorithms for time-fractional subdiffusion equations.	The methods achieved improved temporal accuracy within a finite-element framework.	Provides a strong higher-order baseline, but focuses mainly on accuracy and stability rather than an integrated analytical-statistical evaluation.
[26]	Zhu and Xu (2019)	Proposed a fast high-order method for time-fractional diffusion equations.	Sum-of-exponentials acceleration reduced the computational and storage costs of the history term.	Highlights the scalability limitations of conventional methods and motivates future fast-memory extensions.

III. RESEARCH GAP, AIM, AND CONTRIBUTIONS

A persistent gap in applied studies of fractional differential equations is the separation between analytical solution techniques and numerical implementation. Analytical solutions reveal qualitative structure and provide benchmark solutions; numerical algorithms are necessary because most applied fractional models cannot be solved in closed form. A journal-level contribution should therefore make the connection between theory, computation, validation, and interpretation explicit.

This research aims to develop and evaluate a hybrid analytical-numerical framework for Caputo fractional differential equations. The framework uses exact or manufactured solutions where possible,

implements practical approximation schemes, and compares the results using error statistics, convergence rates, stability behavior, CPU time, and sensitivity to the fractional order.

IV. STUDY CONTRIBUTION

The main contributions are as follows:

- First: a unified analytical-numerical structure for Caputo fractional differential equations.
- Second: benchmark validation using Mittag-Leffler and manufactured exact solutions.
- Third: computational experiments for solution behavior, convergence, and error statistics.
- Fourth: structured comparison of L1, predictor-corrector, and finite-difference approaches.
- Fifth: interpretation of the role of the fractional order in memory-dominated systems.
- Sixth: identification of limitations and future directions suitable for a high-impact applied mathematics paper.

V. MATHEMATICAL PRELIMINARIES

Let y(t) be sufficiently smooth on [0,T], and let α denote the fractional order. The Riemann-Liouville fractional integral of order α is defined by

$$I^{\alpha}y(t) = \frac{1}{\Gamma(\alpha)}\int_0^t (t-s)^{\alpha-1}\, y(s)\, ds, \quad \alpha > 0.$$

For $m-1 < \alpha < m$, the Caputo fractional derivative is

$${}^{c}D_t^{\alpha}y(t) = \frac{1}{\Gamma(m-\alpha)}\int_0^t (t-s)^{m-\alpha-1}\, y^{(m)}(s)\, ds.$$

For the common case $0 < \alpha < 1$, this becomes

$${}^{c}D_t^{\alpha}y(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-s)^{-\alpha}\, y'(s)\, ds.$$

The Caputo derivative is appropriate for applied initial-value problems because it permits classical initial conditions. Figure 1 visualizes the memory-kernel behavior.

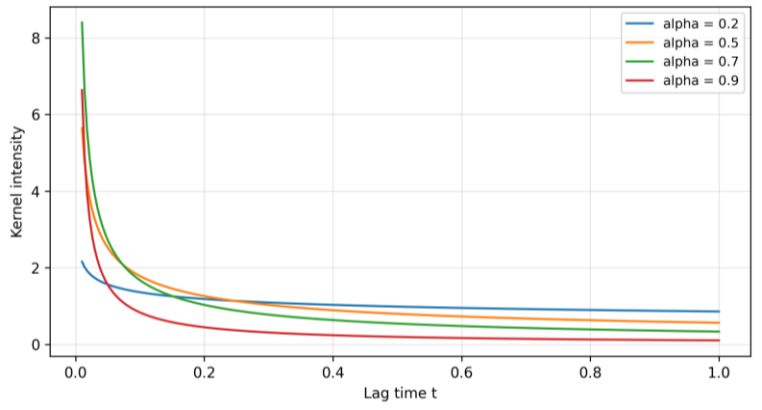


FIGURE 1. Caputo memory kernel for selected values of the fractional order.

The Figure illustrates the Caputo memory kernel for different fractional orders. The kernel decreases as the time difference increases, indicating that recent states have a stronger influence on the present response. The fractional order controls the distribution of memory effects, highlighting the nonlocal characteristics of fractional differential equations.

The Mittag-Leffler function generalizes the exponential function in fractional systems and is defined by

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

VI. PROBLEM FORMULATION

This research considers fractional ordinary and partial differential equations. The general Caputo fractional initial-value problem is written as

$${}^{c}D_t^{\alpha} y(t) = F\big(t, y(t)\big), \quad 0 < \alpha \leq 1, \quad y(0) = y_0.$$

For diffusion-type problems, the time-fractional model is written as

$${}^{c}D_t^{\alpha} u(x,t) = \kappa u_{xx}(x,t) + f(x,t), \quad 0 < x < L, \quad 0 < t \leq T.$$

Table 2. Model equations used in the proposed study.

Model	Model class	Purpose
Fractional relaxation	Linear benchmark model	Used to validate the method against an exact Mittag-Leffler solution.
Fractional Riccati-type equation	Nonlinear fractional ODE	Used to test decomposition and predictor-corrector methods.
Time-fractional diffusion	Fractional PDE model	Used to represent anomalous diffusion and memory-dependent transport.

VII. ANALYTICAL SOLUTION METHODS

For linear Caputo equations, integral transforms reduce the fractional derivative to an algebraic expression in the transform domain. Consider

$${}^{c}D_t^{\alpha} y(t) = \lambda y(t) + f(t), \quad y(0) = y_0.$$

The solution can be represented as

$$y(t) = y_0 E_\alpha(\lambda t^\alpha) + \int_0^t (t-s)^{\alpha-1} E_{\alpha,\alpha}(\lambda (t-s)^\alpha) f(s)\, ds.$$

For nonlinear equations, decomposition methods construct approximate analytical series. If

$${}^{c}D_t^{\alpha} y(t) = Ly(t) + Ny(t) + g(t),$$

the solution and nonlinear operator may be expanded as

$$y(t) = \sum_{n=0}^{\infty} y_n(t), \quad N(y) = \sum_{n=0}^{\infty} A_n,$$

where A_n are decomposition polynomials. Truncating the series gives a semi-analytical approximation that can be compared against predictor-corrector or fine-grid numerical results.

The main analytical benchmark used in this paper is the fractional relaxation equation

$${}^{c}D_t^{\alpha} y(t) = -\lambda y(t), \quad y(0) = 1,$$

with exact solution

$$y(t) = E_\alpha(-\lambda t^\alpha).$$

We select this model because it allows direct measurement of pointwise error, global error, convergence behavior, and sensitivity to the fractional order.

VIII. NUMERICAL METHODS

We use the L1 approximation because it is simple, transparent, and suitable for both scalar fractional equations and time-fractional diffusion models. Let $t_n = n\tau$. For $0 < \alpha < 1$, the Caputo derivative at t_n is approximated by

$$^{c}D_t^{\alpha} y(t_n) \approx \frac{1}{\tau^{\alpha}\Gamma(2-\alpha)} \sum_{k=0}^{n-1} a_k \left[y_{n-k} - y_{n-k-1}\right],$$

where

$$a_k = (k+1)^{1-\alpha} - k^{1-\alpha}, \quad t_n = n\tau.$$

The predictor-corrector method is useful for nonlinear fractional initial-value problems because it works with the equivalent Volterra integral equation

$$y(t) = y_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} F\big(s, y(s)\big)\, ds.$$

For the time-fractional diffusion equation, the spatial second derivative can be approximated by the central difference formula

$$u_{xx}(x_i, t_n) \approx \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2}.$$

Combining the L1 formula in time with central differences in space gives a fully discrete method for diffusion-type problems. Handle boundary and initial conditions carefully to preserve stability and consistency.

IX. STATISTICAL AND COMPUTATIONAL METHODOLOGY

The numerical experiments use double-precision arrays for the numerical schemes and high-precision evaluation of Mittag-Leffler benchmark values. The analysis treats the numerical error as a measurable response variable and summarizes it using statistical indicators. For a numerical solution y_n and an exact solution $y(t_n)$, the pointwise error is used as the basis for validation.

$$e_n = y(t_n) - y_n.$$

Table 3. Statistical indicators used to evaluate numerical performance.

Indicator	Meaning	Role in validation
Maximum error	Worst local deviation	Measures the largest pointwise numerical error.
Mean absolute error	Average absolute deviation	Summarizes the typical absolute error over the grid.
Root-mean-square error	Quadratic error measure	Penalizes larger numerical deviations more strongly.
Observed rate	Empirical convergence order	Checks whether error decreases under mesh refinement.
CPU time	Runtime in seconds	Compares computational efficiency and scalability.

For a time-fractional ordinary differential equation, a typical convergence estimate can be written as

$$\max_{1 \le n \le N} |y(t_n) - y_n| \le C\tau^p.$$

For a time-fractional diffusion equation, the combined temporal and spatial error can be expressed as

$$\| u(t_n) - u^n \| \le C(\tau^p + h^2).$$

Here, p depends on the fractional order and on the regularity of the exact solution.

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X. COMPUTATIONAL SIMULATION STUDY

The simulation study uses the fractional relaxation equation
${}^{c}D_t^{\alpha} y(t) = -y(t), \quad y(0) = 1.$

We consider the fractional orders α = 0.5, 0.7, 0.9, and 1.0. The case α = 1.0 recovers the classical exponential decay and is used as a limiting comparison. The exact benchmark solution is
$y(t) = E_{\alpha}(-t^{\alpha})$.

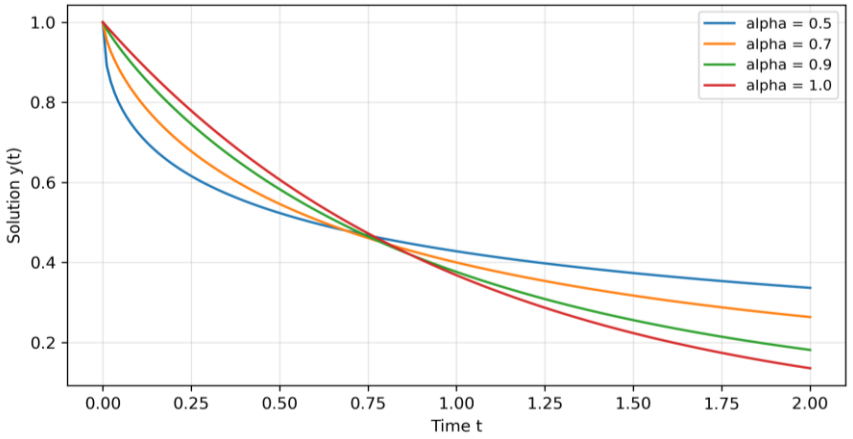


FIGURE 2. Fractional relaxation profiles for different fractional orders.

Figure 2 presents the relaxation profiles for different fractional orders. Smaller α values produce slower long-term relaxation, reflecting the influence of memory-dependent dynamics. As α approaches 1.0, the solution converges toward classical exponential decay, demonstrating the transition from fractional to integer-order behavior.

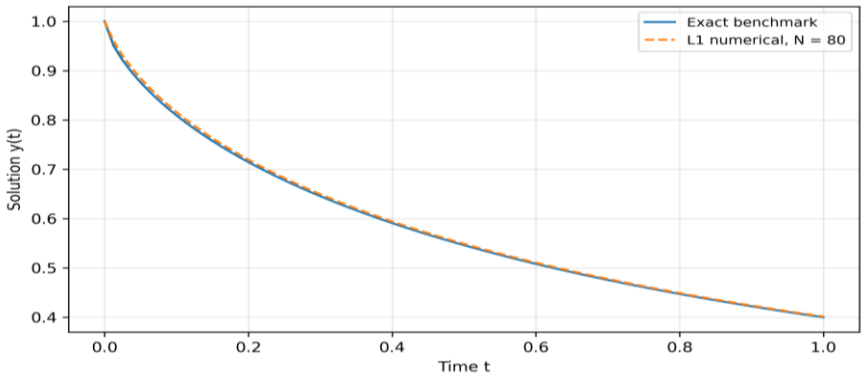


FIGURE 3. L1 numerical solution compared with the exact benchmark for α = 0.7.

Figure 3 compares the L1 numerical approximation with the exact Mittag-Leffler solution for α = 0.7. The numerical solution closely follows the analytical benchmark, demonstrating the L1 method's accuracy. The maximum error decreases from 0.02454 to 0.00581 as the time step is refined from 0.05 to 0.00625, confirming improved numerical accuracy under temporal refinement.

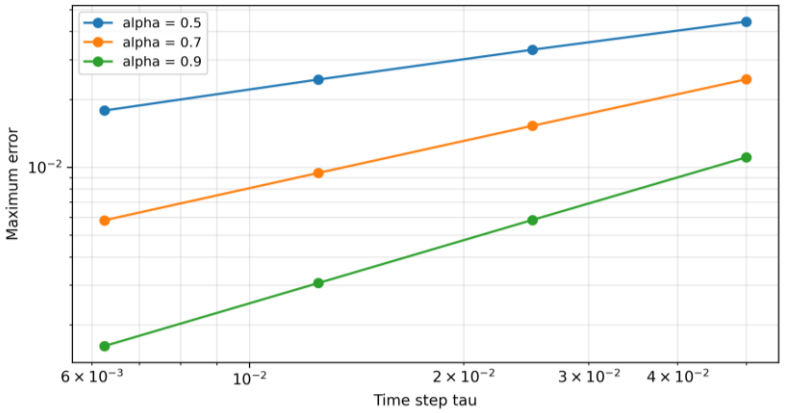


FIGURE 4. Log-log convergence plot of maximum error against the time step.

Figure 4 illustrates the relationship between the maximum numerical error and the time step on a log-log scale. The results demonstrate a consistent reduction in numerical error as the temporal grid is refined. The observed convergence rates reach 0.457, 0.698, and 0.929 for α = 0.5, 0.7, and 0.9, respectively, confirming the convergence of the L1 approximation for the investigated fractional relaxation problem.

Table 4. Computational convergence and statistical error results for the L1 method.

α	N	τ	L-infinity error	**Observed rate**
0.50000	20	0.05000	0.04423	-
0.50000	40	0.02500	0.03320	0.414
0.50000	80	0.01250	0.02448	0.439
0.50000	160	0.00625	0.01783	0.457
0.70000	20	0.05000	0.02454	-
0.70000	40	0.02500	0.01525	0.686
0.70000	80	0.01250	0.00943	0.694
0.70000	160	0.00625	0.00581	0.698
0.90000	20	0.05000	0.01106	-
0.90000	40	0.02500	0.00583	0.924
0.90000	80	0.01250	0.00306	0.929
0.90000	160	0.00625	0.00161	0.929

To support future PDE experiments, we can select a manufactured solution and substitute it into the governing equation to construct the source term. One convenient benchmark is
$u(x,t) = t^2 \sin(\pi x), \quad 0 < x < 1.$

The source term can be obtained by substituting the exact solution into
${}^{c}D_t^{\alpha} u(x,t) = \kappa u_{xx}(x,t) + f(x,t).$

Figure 5 shows the space-time pattern of the manufactured solution.

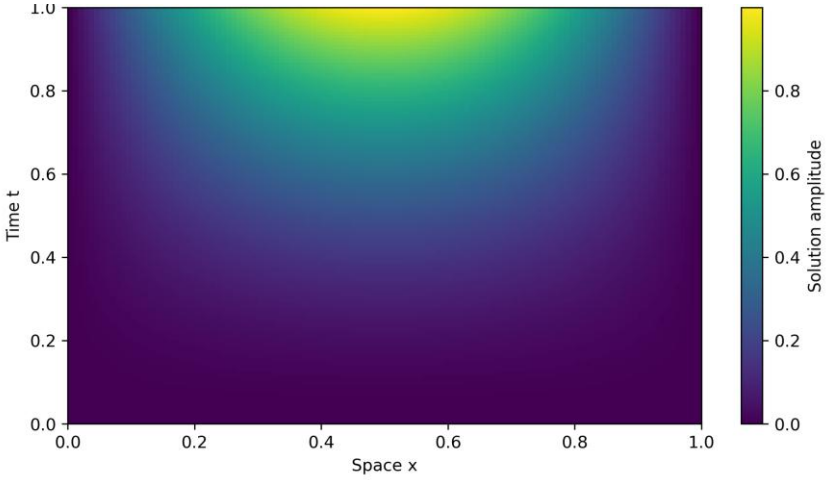


FIGURE 5. Heat map of a manufactured time-fractional diffusion benchmark.

The Figure presents the space-time heat map of the manufactured time-fractional diffusion solution. The visualization shows the solution's evolution across spatial and temporal dimensions, highlighting the characteristics of fractional diffusion. The manufactured solution provides an analytical benchmark for validating the accuracy and convergence of numerical methods applied to time-fractional diffusion equations.

XI. RESULTS AND DISCUSSION

The computational study evaluated the numerical performance of the proposed analytical-numerical framework for Caputo fractional differential equations using the fractional relaxation model. We considered four fractional orders, α = 0.5, 0.7, 0.9, and 1.0, to investigate the influence of fractional order on solution behavior. The exact Mittag-Leffler solution served as the analytical benchmark, while the L1 numerical approximation was evaluated under successive time-step refinements. The results are presented in terms of fractional-order sensitivity, numerical accuracy, and observed convergence rates.

A. Fractional-Order Sensitivity

The fractional relaxation profiles show that the fractional order influences the solution's temporal evolution. For α = 0.5, the solution exhibits a more pronounced memory-dependent response and slower long-term relaxation than the classical exponential model. Increasing the fractional order to α = 0.7 and α = 0.9 produces relaxation profiles that progressively approach the classical solution. At α = 1.0, the fractional model recovers the conventional exponential decay.

These results establish that changes in the fractional order modify the relaxation behavior and provide a continuous transition between fractional and classical dynamics. The solution profiles in Figure 2 illustrate how the modeled response depends on the selected fractional orders.

B. Numerical Accuracy of the L1 Method

The numerical results demonstrate a consistent reduction in the maximum absolute error as the temporal grid is refined. For α = 0.5, increasing the number of time steps from N = 20 to N = 160 reduced the maximum error from 0.04423 to 0.01783. For α = 0.7, the corresponding error decreased from 0.02454 to 0.00581. For α = 0.9, the maximum error decreased further from 0.01106 to 0.00161.

At the finest temporal resolution, τ = 0.00625, the maximum errors were 0.01783, 0.00581, and 0.00161 for α = 0.5, 0.7, and 0.9, respectively. The smallest reported maximum error was therefore obtained for α = 0.9.

Figure 3 compares the numerical and exact benchmark solutions for $\alpha = 0.7$. The computational results indicate that the L1 approximation reproduces the analytical benchmark with decreasing numerical error under successive temporal refinements.

C. Convergence Analysis

The convergence results reported in Table 4 demonstrate that the observed convergence rate depends on the fractional order. For $\alpha = 0.5$, the observed rate increased from 0.414 to 0.457 as the temporal grid was refined. For $\alpha = 0.7$, the corresponding rate increased from 0.686 to 0.698. For $\alpha = 0.9$, the observed convergence rates ranged from 0.924 to 0.929.

At the finest temporal resolution, the observed convergence rates were 0.457, 0.698, and 0.929 for $\alpha = 0.5$, 0.7, and 0.9, respectively. These findings show that numerical error decreases with temporal refinement and that the observed rate increases with fractional order within the investigated benchmark.

The log-log convergence curves presented in Figure 4 illustrate the relationship between the maximum numerical error and the temporal step size.

D. Time-Fractional Diffusion Benchmark

The computational framework also incorporates a manufactured solution for a time-fractional diffusion model. Figure 5 visualizes the corresponding space-time solution, illustrating the temporal and spatial structure of the selected diffusion benchmark.

The manufactured solution provides an analytical reference for evaluating numerical approximations of fractional partial differential equations. However, the present computational results do not report quantitative spatial or temporal error estimates for the diffusion benchmark. Consequently, additional computational experiments are needed to establish the numerical accuracy and convergence behavior of the fully discrete diffusion scheme.

XII. DISCUSSION

The computational findings demonstrate the importance of fractional-order selection in modeling memory-dependent dynamical systems. The variation in relaxation profiles across different fractional orders indicates that the Caputo derivative provides a flexible mathematical representation of processes whose evolution depends on historical states. In particular, smaller fractional orders produce slower long-term relaxation, while values approaching unity recover the classical exponential response. This behavior supports using fractional differential equations when conventional integer-order models cannot adequately represent a system's temporal characteristics. The numerical results also demonstrate the importance of temporal resolution in fractional differential-equation simulations. The consistent reduction in maximum error under successive grid refinements indicates that the L1 approximation provides an effective numerical baseline for the investigated fractional relaxation problem. Nevertheless, interpret the reported accuracy within the specific benchmark considered, not as evidence of superior performance across all fractional equations or numerical methods. An important finding is that the observed convergence rate depends on the fractional order. The rates of 0.457, 0.698, and 0.929 obtained at the finest temporal resolution for $\alpha = 0.5$, 0.7, and 0.9, respectively, are close to their corresponding fractional orders. This behavior is consistent with the reduced regularity commonly encountered in fractional relaxation problems, particularly near the initial time. Weak initial singularities may limit the convergence performance of uniform-grid discretization schemes, even when stronger smoothness assumptions allow higher theoretical convergence rates.

The relationship between fractional order and numerical accuracy also has methodological implications. The smaller maximum errors for higher fractional orders in this benchmark should not be interpreted as a universal advantage of larger fractional orders. Rather, the results indicate that the interaction between solution regularity, memory effects, and temporal discretization influences the numerical performance of the L1 method. Consequently, when evaluating numerical algorithms, fractional-order sensitivity should be

examined alongside convergence behavior. The hybrid analytical-numerical framework supports numerical validation by linking exact Mittag-Leffler solutions to computational approximations. Analytical benchmarks allow direct quantification of approximation errors, while numerical discretization extends the applicability of fractional models to problems without closed-form solutions. Together, these approaches provide a structured way to assess numerical reliability and interpret fractional dynamics. For nonlinear initial-value problems, Adams-type predictor-corrector methods offer an alternative numerical approach based on the equivalent Volterra integral formulation. Similarly, combining fractional temporal discretization with finite differences provides a practical framework for diffusion-type problems. However, the current quantitative convergence results focus on the L1 relaxation benchmark. A comprehensive performance comparison involving predictor-corrector algorithms and fully discrete diffusion schemes would require additional numerical experiments using common validation criteria. Computationally, the nonlocal character of the Caputo derivative introduces additional numerical challenges because the approximation at each time level depends on the solution history. Although the present scalar benchmark demonstrates consistent error reduction, long-time simulations and spatially distributed fractional systems may require substantial memory storage and computational resources. Fast convolution techniques, memory-compression algorithms, and graded temporal meshes therefore represent important directions for extending the proposed framework.

Overall, the findings establish the value of integrating analytical benchmark solutions, numerical approximation, convergence assessment, and fractional-order sensitivity within a unified computational methodology. The reported results provide quantitative evidence that the L1 method converges for the investigated relaxation problem while highlighting the need to further validate nonlinear and diffusion-type models.

XIII. LIMITATIONS AND FUTURE WORK

This study provides a structured analytical-numerical framework, but several limitations remain. The computational examples focus mainly on benchmark models, so future versions should include an application-driven case study. Uniform time grids are simple and transparent, but graded meshes may be more effective for solutions with weak initial singularities. The history term also increases memory cost in long simulations; therefore, fast convolution and memory-compression techniques should be considered. Finally, the comparison can be extended to spectral methods, finite element methods, meshless methods, and advanced numerical solvers.

XIV. CONCLUSION

This study developed a hybrid analytical-numerical framework for Caputo fractional differential equations by integrating analytical benchmark solutions, numerical discretization, convergence analysis, and fractional-order sensitivity assessment. The proposed framework provides a systematic approach to investigating memory-dependent dynamical systems and evaluating numerical approximations against exact solutions.

The computational results demonstrate that the fractional order substantially influences both solution behavior and numerical convergence. Smaller fractional orders produce slower long-term relaxation, whereas values approaching unity recover the classical exponential response. The L1 approximation consistently reduced error with temporal grid refinement. For α = 0.9, the maximum numerical error decreased from 0.01106 to 0.00161 as the time step was reduced from 0.05 to 0.00625. At the finest temporal resolution, the observed convergence rates reached 0.457, 0.698, and 0.929 for α = 0.5, 0.7, and 0.9, respectively. These findings show how fractional order and temporal discretization affect numerical accuracy in the investigated relaxation benchmark.

Integrating exact Mittag-Leffler solutions with numerical approximations provides a reliable basis for validating fractional differential-equation solvers. Although the quantitative findings focus on the L1 relaxation benchmark, the proposed framework provides a foundation for extending numerical investigations to nonlinear and diffusion-type problems. Future research should incorporate graded temporal meshes, fast-memory algorithms, and application-driven case studies to improve computational efficiency and assess the framework's applicability to more complex fractional dynamical systems.

Author Contributions

The author conducted the conceptualization, methodology, data analysis, investigation, writing, review, editing, and final approval of the manuscript.

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Data Availability

The dataset will be available from the author upon reasonable request.

Conflicts of Interest

The author declares no conflict of interest.

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