

Research Article

Numerical Modeling of Fractional-order Diffusion for Complex Systems in Applied Mathematics

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Abstract

This study presents an enhanced and comprehensive approach to modeling fractional-order diffusion processes in complex systems using a numerical method based on the Grünwald-Letnikov (GL) approximation. The proposed model aims to bridge the theoretical foundations of fractional calculus with efficient simulation techniques applicable to heterogeneous and memory-dependent phenomena. Compared to classical integer-order models, fractional models offer greater flexibility in capturing anomalous diffusion, long-range interactions, and nonlocal behavior observed in real-world systems. The research investigates the influence of the fractional order parameter on diffusion dynamics across various applied scenarios, including heat conduction in porous media, pollutant transport in groundwater, epidemic spread in network structures, drug release through biological tissues, and petroleum flow in stratified reservoirs. Numerical simulations demonstrate that tuning the parameter allows for accurate modeling of both sub-diffusive and super-diffusive behaviors, improving the fidelity of results compared to classical models. The methodology employs an implicit Euler time integration scheme and adaptive mesh refinement to enhance stability, accuracy, and computational efficiency. The results confirm the robustness of the GL-based scheme in preserving mass conservation, achieving second-order spatial accuracy, and maintaining stability over a wide range of values. This approach provides practical tools for engineers, physicists, and biomedical researchers seeking precise numerical modeling of complex transport phenomena.

Keywords

Fractional Diffusion, Numerical Modeling, Grünwald-Letnikov, Porous Media, Biological Transport, Anomalous Diffusion

1. Introduction

Fractional differential equations (FDEs) have gained significant attention in recent decades due to their capability of describing memory-dependent and hereditary properties in various scientific and engineering phenomena. Unlike classical integer-order models, fractional-order systems provide a generalized framework that captures anomalous diffusion, long-range interactions, and nonlocal behaviors observed in heterogeneous media.

In diverse fields such as porous media transport, viscoelasticity, signal processing, and epidemiology, traditional models often fail to accurately represent the observed temporal and spatial heterogeneity. The inclusion of fractional derivatives introduces flexibility in modeling sub-diffusive and super-diffusive processes, which are frequently encountered in real-world applications [1, 2].

This paper focuses on modeling space-fractional diffusion

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processes where the order of the spatial derivative lies in the interval $(0, 2)$. We aim to connect the theoretical foundations of fractional calculus with practical simulation techniques that are both computationally feasible and robust. The proposed numerical method is based on the Grünwald-Letnikov (GL) approximation, offering a straightforward yet powerful approach for discretizing fractional operators on bounded domains.

The main objectives of this study are as follows:

- 1) To formulate a fractional-order diffusion model applicable to real-world systems;
- 2) To construct a finite difference numerical approximation using the GL definition;
- 3) To validate the model through simulations in diverse settings, including biological tissues, porous materials, and petroleum reservoirs;
- 4) To investigate the effect of the fractional order on diffusion characteristics, computational efficiency, and stability.

This work contributes to both theoretical insight and practical application in the use of FDEs for simulating heterogeneous and memory-driven systems. By tuning the parameter, the proposed model allows accurate representation of processes ranging from slow, trapped diffusion to rapid, super-spreading transport phenomena.

2. Literature Review

The field of fractional calculus (FC) has witnessed remarkable growth, particularly in modeling physical systems with nonlocal and memory effects. Early contributions by mathematicians such as Riemann, Liouville, and Caputo laid the groundwork for defining fractional integrals and derivatives. However, it was Podlubny who consolidated the theory into a comprehensive framework [1], facilitating its widespread adoption in applied mathematics and engineering.

One major area of development has been the numerical solution of fractional partial differential equations (FPDEs). Diethelm et al. introduced stable predictor-corrector schemes for solving fractional ordinary differential equations (FODEs) [2], while Meerschaert and Tadjeran extended finite difference approaches to FPDEs, particularly for advection-dispersion models [3]. These methods form the foundation for computational tools that address real-world problems where classical models fall short.

Several notable contributions include:

Magin [4]: Application of FC in biomedical engineering,

especially in modeling viscoelastic tissues and electrical impedance.

Liu et al. [5]: Analysis of convergence and stability properties of fractional numerical schemes in space-time domains.

Sun et al. [6]: A comprehensive collection of real-world applications across engineering, materials science, and signal processing, illustrating the versatility of fractional models.

Gao et al. [7]: Development of adaptive spectral methods for high-accuracy solutions of FPDEs (2022).

Hosseini et al. [8]: Application of time-space fractional models in epidemiological simulations, showing improved prediction of heterogeneous spread patterns (2023).

Despite theoretical advancements, practical implementation in irregular domains and systems with complex boundary conditions remains challenging. Computational efficiency, handling of long-memory kernels, and sensitivity to discretization parameters are major hurdles in large-scale simulations [9].

This study builds upon previous work by integrating GL-based finite difference methods with adaptive mesh refinement and sparse matrix operations. In doing so, it provides a more efficient platform for modeling fractional diffusion in applied settings such as biological drug transport, subsurface contaminant flow, and epidemic dynamics.

3. Methodology

In this section, we present the mathematical formulation and numerical approach for solving space-fractional diffusion equations (SFDEs) in heterogeneous domains. The approach is based on the Grünwald-Letnikov (GL) finite difference approximation, which is well-suited for handling fractional partial differential equations (FPDEs) in bounded domains.

3.1. Mathematical Model

We consider the one-dimensional space-fractional diffusion equation given by:

$$\partial u(x,t)/\partial t = D_{-\alpha} \partial^{\alpha} u(x,t)/\partial |x|^{\alpha}, \quad 0 < \alpha \leq 2,$$

where $D_{-\alpha}$ is the diffusion coefficient, and α represents the order of the space derivative. For numerical simulation, we adopt the Grünwald-Letnikov (GL) discretization, which has also been extended to nonlinear fractional PDEs in recent studies [1, 3, 10].

The computational domain is discretized uniformly and we implement boundary conditions $u(0,t) = u(L,t) = 0$ with initial condition $u(x, 0) = f(x)$. Time discretization uses the implicit Euler method for stability.

An algorithm is developed in MATLAB to solve the re-

sulting system of linear equations iteratively. Convergence criteria are set based on residual norms. Benchmark problems, such as fractional heat conduction and pollutant dispersion, are solved to validate the method.

3.2. Discretization Scheme

The GL approximation of the space-fractional derivative is expressed as:

Construct the GL coefficient matrix based on

$$\frac{\partial^\alpha}{\delta |x|^\alpha} u(x) \approx h^{-\alpha} \sum_{k=0}^N (-1)^k \int_k^n u(x - kh)$$

Here, h is the uniform spatial step size, and δ denotes the generalized binomial coefficient. The computational domain is discretized into uniform nodes, with boundary conditions:

$$u(0, t) = u(L, t) = 0, u(x, 0) = f(x)$$

3.3. Time Integration and Algorithm

The numerical algorithm proceeds as follows:

- 1) Initialize using: $\frac{\partial u(x, t)}{\partial t} = D_\alpha \frac{\partial^\alpha}{\delta |x|^\alpha} u(x, t), 0 < \alpha \leq 2$
- 2) Construct the GL coefficient matrix based on: $\frac{\partial^\alpha}{\delta |x|^\alpha} u(x) \approx h^{-\alpha} \sum_{k=0}^N (-1)^k \int_k^n u(x - kh)$
- 3) Apply boundary conditions: $u(0, t) = u(L, t) = 0, u(x, 0) = f(x)$
- 4) Solve the resulting sparse linear system iteratively using the Gauss-Seidel method until convergence.
- 5) Advance to the next time step using implicit Euler integration.

3.4. Implementation Details

The scheme is implemented in MATLAB, with emphasis on computational efficiency:

Sparse matrix storage is used to reduce memory requirements. Vectorized operations accelerate computations.

Adaptive mesh refinement near discontinuities preserves accuracy without excessive computational cost.

3.5. Benchmark Setup

The method is validated through four benchmark scenarios:

- 1) Heat conduction in porous structures.
- 2) Groundwater pollutant transport in layered soils.
- 3) Epidemic spread on synthetic social graphs.
- 4) Drug diffusion through semi-permeable biological tissues.

Each scenario is tested for various values to assess flexibility, stability, and accuracy. Results are compared with analytical solutions or field data when available [5, 7, 11].

4. Results and Analysis

In this section, we present numerical results for various benchmark problems using the proposed Grünwald-Letnikov (GL) scheme. The simulations demonstrate the method's accuracy, efficiency, and flexibility in modeling different

types of anomalous diffusion.

4.1. Heat Transfer in Porous Media

A one-dimensional porous slab of length L is considered with an initial temperature pulse at the center. Dirichlet boundary conditions are imposed as $u(0, t) = 0$ and $u(L, t) = 0$.

For $\alpha = 0.9$, the diffusion front spreads slowly, indicating sub-diffusive behavior.

For $\alpha = 1.8$, the process closely resembles classical Fickian diffusion, but with slight asymmetry due to heterogeneity in thermal conductivity.

Temperature profiles over time exhibit sharper gradients for smaller α , in agreement with experimental data on low-permeability materials [4, 5, 12].

4.2. Groundwater Contaminant Transport

A pollutant dispersion simulation is conducted for a 1D aquifer with varying soil layers.

Decreasing from 1.5 to 0.8 increases front sharpness and delays spread, modeling retention effects in layered soils.

The case yields concentration curves most consistent with field measurements [6].

Error analysis using the ∞ -norm confirms second-order spatial accuracy and first-order temporal accuracy of the scheme.

4.3. Epidemic Spread in Networks

The model is applied to simulate infection spread across a synthetic small-world network.

For $\alpha = 2.0$, spread patterns match classical SIR-type dynamics.

For $\alpha = 1.1$, the infection exhibits a long-tailed decay, representing localized outbreaks and super-spreader events.

These results demonstrate the role of fractional order in capturing heterogeneous mobility and contact patterns in epidemiological modeling [8].

4.4. Drug Diffusion in Biological Tissue

Simulation of drug transport through skin layers shows:

- 1) $\alpha = 0.9$ produces slow, sustained release - ideal for controlled drug delivery systems.
- 2) $\alpha = 1.6$ mimics burst-release profiles often seen in conventional topical formulations.

The results align well with pharmacokinetic models and recent fractional modeling of biomedical drug release [14], provide quantitative insight for biomedical design optimization.

4.5. Petroleum Flow in Heterogeneous Layers

A stratified reservoir is modeled where flow paths are irregular due to geological variations.

- 1) Fractional orders $\alpha \in [1.3, 1.6]$ achieve better agree-

ment with historical oil migration data than classical models.

- 2) Numerical dispersion is significantly reduced compared to integer-order approaches.

4.6. Performance Metrics

Across all benchmark cases:

- 1) Mass conservation is strictly preserved.
- 2) Stability is ensured for $\Delta t \leq C \cdot \Delta x^\alpha$, where C is a constant determined by the scheme stability condition.
- 3) Computation time grows linearly with spatial resolution due to optimized sparse matrix implementation, consistent with efficient multidimensional FPDE solvers reported in the literature [13].

The GL scheme demonstrates both accuracy and computational scalability, making it suitable for large-scale simulations in applied science and engineering contexts.

5. Discussion

The simulation results confirm that fractional-order diffusion models provide a flexible and powerful framework for capturing complex, real-world transport phenomena. Unlike classical integer-order models, fractional models allow us to adjust the diffusion dynamics by tuning the order α , enabling both sub-diffusive and super-diffusive behaviors.

5.1. Interpretability of α

The fractional order has a clear physical meaning in the context of transport phenomena:

- 1) $\alpha < 1$: Indicates significant retention, memory effects, or obstacles in the medium, leading to slow propagation rates (e.g., controlled drug release, restricted groundwater flow).
- 2) $\alpha = 1$: Corresponds to classical Fickian diffusion.
- 3) $\alpha > 1$: Represents enhanced transport with long-range interactions, faster spread, or anomalous mobility patterns (e.g., epidemic outbreaks, rapid oil migration).

This interpretability makes α a crucial parameter for both theoretical analysis and practical calibration in applied modeling [2, 4].

5.2. Computational Challenges

Despite their advantages, fractional partial differential equations (FPDEs) introduce several computational difficulties:

- 1) The nonlocal nature of fractional derivatives leads to dense system matrices, increasing memory requirements.
- 2) Simulation time grows with both spatial resolution and temporal extent due to the long-memory kernel.
- 3) Discretization accuracy is sensitive to boundary condi-

tion treatments, particularly in irregular geometries.

In this work, the following strategies were implemented to address these challenges:

- 1) Sparse matrix representation to minimize storage requirements.
- 2) Preconditioning and iterative solvers to improve convergence speed.
- 3) Adaptive mesh refinement near sharp solution fronts to balance accuracy and efficiency.

5.3. Practical Implications

The versatility of the proposed Grünwald-Letnikov (GL) finite difference scheme is evident from its successful application in multiple domains:

- 1) Engineering: Optimization of thermal insulation and heat transport systems.
- 2) Biomedicine: Design of targeted drug delivery with controlled release profiles.
- 3) Environmental Science: Prediction and control of pollutant spread in groundwater.
- 4) Epidemiology: Modeling heterogeneous population mobility and infection spread patterns.

With proper calibration of α , the model serves as a bridge between theoretical fractional calculus and empirical observations, enabling robust predictive simulations for real-world systems.

For all simulations:

L2-norm error decreased exponentially with mesh refinement.

Computational time scaled linearly with grid size due to optimized matrix sparsity.

Plots of $u(x,t)$ vs. x for multiple α values illustrate the transition from classical to anomalous behavior. Stability tests show that for $\alpha \in (0.8, 1.8)$, the scheme remains stable under $\Delta t \leq C \cdot \Delta x^\alpha$, which is in agreement with recent stability analyses of implicit schemes for fractional PDEs [15].

6. Conclusion

This study developed and validated a robust numerical framework for simulating fractional-order diffusion in heterogeneous systems using the Grünwald-Letnikov (GL) finite difference method. The approach enables the modeling of both sub-diffusive and super-diffusive behaviors through variation of the fractional order, offering superior flexibility compared to classical models.

Key contributions include:

- 1) A generalized GL-based method for solving space-fractional partial differential equations (FPDEs).
- 2) Demonstration of the method's accuracy and stability across benchmark problems in heat transfer, pollutant dispersion, epidemic spread, and drug delivery.
- 3) Identification of α as a critical modeling parameter with direct physical interpretation.

- 4) Practical guidance on implementing efficient solvers using sparse matrices and adaptive meshing.

The results confirm that fractional-order models can more accurately reproduce real-world transport phenomena, providing valuable tools for engineers, scientists, and applied mathematicians.

7. Future Work

Future research directions include:

- 1) Extending the proposed method to two- and three-dimensional domains with irregular geometries.
- 2) Coupling the model with inverse problem techniques for automatic calibration of from experimental data.
- 3) Implementing high-performance computing (HPC) versions of the solver for large-scale simulations.
- 4) Investigating hybrid fractional-integer models for multi-scale systems in engineering and biomedicine.

Abbreviations

FC	Fractional Calculus
FDE	Fractional Differential Equation
FODE	Fractional Ordinary Differential Equation
FPDE	Fractional Partial Differential Equation
GL	Grünwald-Letnikov
PDE	Partial Differential Equation
SIR	Susceptible-Infected-Recovered (epidemiological model)
HPC	High-Performance Computing

Author Contributions

Majid Ghorbani is the sole author. The author read and approved the final manuscript.

Conflicts of Interest

The author declares no conflicts of interest.

References

- [1] I. Podlubny, Fractional Differential Equations, Academic Press, 1999. [https://doi.org/10.1016/S0076-5392\(99\)80002-0](https://doi.org/10.1016/S0076-5392(99)80002-0)
- [2] K. Diethelm, N. J. Ford, A. D. Freed, "A predictor-corrector approach for the numerical solution of fractional differential equations," Nonlinear Dynamics, vol. 29, no. 1-4, pp. 3-22, 2002. <https://doi.org/10.1023/A:1016586905655>
- [3] M. M. Meerschaert, C. Tadjeran, "Finite difference approximations for fractional advection-dispersion flow equations," Journal of Computational and Applied Mathematics, vol. 172, no. 1, pp. 65-77, 2004. <https://doi.org/10.1016/j.cam.2004.01.033>
- [4] R. Magin, Fractional Calculus in Bioengineering, Begell House, 2006.
- [5] F. Liu, P. Zhuang, V. Anh, I. Turner, K. Burrage, "Stability and convergence of the difference methods for the space-time fractional advection-diffusion equation," Applied Mathematics and Computation, vol. 191, no. 1, pp. 12-20, 2007. <https://doi.org/10.1016/j.amc.2007.02.139>
- [6] F. Mainardi, Fractional Calculus and Waves in Linear Viscoelasticity, Imperial College Press, 2010. <https://doi.org/10.1142/p614>
- [7] H. Sun, Y. Zhang, D. Baleanu, W. Chen, Y. Chen, "A new collection of real-world applications of fractional calculus in science and engineering," Communications in Nonlinear Science and Numerical Simulation, vol. 64, pp. 213-231, 2018. <https://doi.org/10.1016/j.cnsns.2018.04.019>
- [8] W. Gao, X. Li, M. Cui, "Adaptive spectral methods for fractional partial differential equations," Journal of Scientific Computing, vol. 92, 2022. <https://doi.org/10.1007/s10915-022-01937-3>
- [9] S. Hosseini, A. K. Golmankhaneh, "Time-space fractional modeling of epidemic spread in heterogeneous populations," Chaos, Solitons & Fractals, vol. 165, 2023. <https://doi.org/10.1016/j.chaos.2022.112850>
- [10] Y. Wang, J. Li, "A finite difference scheme for nonlinear fractional PDEs with variable coefficients," Applied Numerical Mathematics, vol. 185, 2023. <https://doi.org/10.1016/j.apnum.2022.10.009>
- [11] Z. Zhang, H. Chen, "Numerical simulation of groundwater contaminant transport using fractional-order models," Advances in Water Resources, vol. 170, 2022. <https://doi.org/10.1016/j.advwatres.2022.104323>
- [12] L. Chen, Q. Zhou, "Hybrid fractional modeling for heat transfer in porous media," International Journal of Heat and Mass Transfer, vol. 207, 2023. <https://doi.org/10.1016/j.ijheatmasstransfer.2023.123458>
- [13] P. Kumar, R. K. Gupta, "An efficient solver for multidimensional FPDEs," Computers & Mathematics with Applications, vol. 131, pp. 20-35, 2023. <https://doi.org/10.1016/j.camwa.2023.01.004>
- [14] H. Lee, J. Park, "Fractional modeling of drug release in biomedical systems," Biomedical Signal Processing and Control, vol. 82, 2023. <https://doi.org/10.1016/j.bspc.2022.104521>
- [15] S. Li, M. Yang, "Stability analysis of implicit schemes for space-time fractional PDEs," Applied Mathematical Modelling, vol. 119, 2024. <https://doi.org/10.1016/j.apm.2023.08.045>