Fractional Reaction-Diffusion Modeling and Numerical Simulation of DNA Sequence Dynamics Using a Unified FD-FEM Framework

Aytekin Enver[1] and Fatma Ayaz[2]

[1] *Gazi University, Department of Mathematics, Ankara, Türkiye*
e-mail: aytekinanwer@gmail.com

[2] *Gazi University, Department of Mathematics, Ankara, Türkiye*
e-mail: fayaz@gazi.edu.tr

Abstract

This study introduces a novel fractional reaction-diffusion framework for analyzing DNA sequence dynamics by integrating generalized Caputo time-fractional derivatives, multi-term memory effects, and constant biological delay. Building upon the concept of fractional dynamics in DNA signal processing, the proposed model describes the temporal evolution of nucleotide interactions as a delayed multi-term time-fractional diffusion equation. A high-order finite difference method is employed for the discretization of generalized fractional operators in time, while the spatial structure of DNA strands is approximated using the finite element method. A new discrete fractional sequence enables unconditional stability analysis and establishes a delay-dependent Gronwall inequality. The framework achieves temporal convergence of order $2-\alpha$ and second-order spatial accuracy. Numerical simulations demonstrate that the proposed approach successfully captures long-range memory, fractal structure, and inter-chromosomal relationships in DNA sequences. This work provides a modern and computationally efficient bridge between fractional calculus, biological modeling, and numerical simulation for genomic analysis.

Keywords: DNA dynamics, generalized Caputo fractional derivative, multi-term time-fractional diffusion.

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