Preface

In the realm of differentiation, classical derivatives act as local operators, in contrast to fractional derivatives, which possess a non-local nature. This distinctive feature equips fractional derivatives with the capacity to incorporate the hereditary properties observed in a wide range of physical phenomena. The application of fractional derivatives in partial differential equations leads to the creation of fractional partial differential equations (FPDEs). These equations play a pivotal role in various scientific fields, including mathematical biology, fluid mechanics, plasma physics, viscoelasticity, and optical fibers, etc. Due to the inclusion of non-integer order derivatives, FPDEs become too intricate for analytical solutions, thus emphasizing the importance of numerical methods for investigating such problems.

The primary emphasis of this thesis lies in developing numerical approximation of FPDEs arising from time-fractional derivatives, including the Caputo fractional derivative, the Caputo-Prabhakar fractional derivative, and generalized fractional derivatives. The focus of this thesis extends beyond numerical methods formulation to include a comprehensive theoretical analysis. This analysis encompasses discussions of stability and convergence properties concerning the developed methods. Beyond this, one more key aspect of this thesis is the presentation of numerical outcomes that reinforce the theoretical findings.

Initially, we investigate a generalized variable coefficient fractional reaction-diffusion equation. Generalized fractional operators use scale and weight functions, enhancing model flexibility by adjusting the domain and extending operator kernels. Therefore, we have introduced two high-order schemes that combine generalized Alikhanov's formula for time-fractional derivatives, and compact operator and parametric quintic spline for spatial derivatives. The error analysis including stability and convergence is developed for the proposed schemes.

Moving forward, we investigate the time-fractional reaction–diffusion equation with variable coefficients defined in the Caputo–Prabhakar sense. Notably, unlike other fractional derivatives, such as Caputo, Grünwald-Letnikov, Hadamard, Riemann-Liouville, Riesz, etc., the numerical approximations of the Caputo-Prabhakar fractional derivative have received limited attention due to its complex structure. Therefore, two novel numerical approximations for the Caputo-Prabhakar fractional derivative are developed and applied to devise high-order schemes for the considered problem. A general error analysis framework is also introduced.

Subsequently, we shift our focus to study the non-smooth behavior of the solution of the Caputo time-fractional linear reaction-diffusion equation. Therefore, we have employed the L1 scheme on non-uniform graded meshes to capture the solution's singular behavior at $t = 0$. Additionally, for spatial discretization, we have utilized a cubic spline difference scheme. Furthermore, the utilization of a cubic spline difference scheme introduces a need for innovative approaches in analyzing the error analysis of a fully discrete scheme, different from the traditional error analysis techniques used with graded meshes.

Next, we proceed to develop a high-order convergent numerical scheme for a non-linear Caputo time-fractional reaction-diffusion equation with a non-smooth solution. The problem is discretized using the L2-1_σ scheme on a graded mesh to approximate the Caputo fractional derivative, in conjunction with parametric quintic splines for the spatial derivative. The demonstration of the solvability, stability, and convergence of the scheme is done.

In the end, we extend our focus to higher-dimensional FPDEs. We have considered the two-dimensional time-fractional convection-diffusion equation, where the solution of the problem exhibits non-smooth behavior. We propose a high-order numerical method that combines Alikhanov's high-order scheme (L2-1_σ) for Caputo time-fractional derivatives on a non-uniform fitted mesh with a high-order two-dimensional compact difference operator on a uniform mesh for spatial derivatives. Theoretical analysis for the proposed discrete scheme is carried out.

We conduct comprehensive numerical experiments to validate the theoretical error estimates obtained.