# Chapter 6

# Conclusions and Future Scopes

This chapter concludes the thesis and presents some future possibilities in the direction of the research work presented in this thesis.

## 6.1 Conclusions

Numerical simulation of the physical model is necessary to get the approximated solutions when the corresponding differential equation exhibits complex behaviour such as nonlocal interaction, anomalous behaviour, involve memory of the past or future events etc. Due to the nonlocal nature of the fractional PDEs, their complexity increases, and it becomes pretty challenging to find their analytical solution. This thesis presented high-order numerical methods to approximate the Caputo–Prabhakar derivative. Further, presented numerical methods are applied for solving some linear and nonlinear time fractional diffusion models. We have also developed high-order numerical methods for solving 1D and 2D, nonlinear Caputo time fractional reaction–diffusion equations. To maintain simplicity and accuracy, the finite difference method was used. The stability, solvability, and convergence analysis of the discussed methods were studied rigorously. Theoretical findings were validated through illustrative test examples.

In Chapter 1, we introduced fractional calculus with basic definitions. The objective and motivation of the thesis, along with the present and past works of the considered model problems, were presented.

In Chapter 2, we approximated the Caputo–Prabhakar derivative using two numerical schemes. The properties of the discretization coefficients and truncation errors of the schemes were discussed. Further, we applied these schemes for solving the time fractional advection–diffusion equation numerically. We also discussed the stability analysis of the schemes. Numerical results validated our analytical findings. In the future, these schemes may be applied to solve many other physical phenomena defined in the Caputo-Prabhakar sense.

In Chapter 3, we approximated the Caputo–Prabhakar derivative of order $\alpha \in (0, 1)$ using using a time stepping interpolation polynomial of degree $r$. Further, combining the developed scheme with the central difference approximation, we solved a time fractional linear advection–diffusion equation and a nonlinear reaction–diffusion equation. To approximate the nonlinear reaction term, the Newton–Raphson iterative algorithm was used. Stability, solvability, and convergence analysis of the whole discretized scheme were studied rigorously. Numerical experimentation was performed to validate the theoretical findings.

In Chapter 4, we devised and demonstrated a time stepping cubic approximation scheme to solve a time fractional nonlinear reaction–diffusion equation. The second order diffusion term was approximated with a 4th order compact difference scheme. To approximate the nonlinear reaction term, we used Newton's approach which improved the convergence order in the temporal direction compared to the existing works in the literature. The stability of the finite difference method was established using von Neumann analysis, and convergence analysis was studied with the help of matrix analysis. The sharpness of the achieved convergence rates was validated from the test examples.

In Chapter 5, a two-dimensional nonlinear time fractional reaction–diffusion equation was solved using $L2-1_\sigma$ scheme over graded meshes along with the central difference approximation. The nonlinear reaction term was approximated using the Newton linearization algorithm, and an alternating direction implicit scheme was applied to reduce the computational cost. The discussed finite difference scheme was proved to have a unique solution, further stability and convergence analysis of the scheme were studied rigorously. Two test examples having smooth and nonsmooth solutions were discussed to validate the theoretical claims.

## 6.2 Scope for Future Work

A brief outline describing the possible extensions of the current work to be carried out in the future is presented below:

1. In this thesis, we have studied the numerical method for the time fractional diffusion problem with a constant diffusion parameter. However, considering this coefficient as a function of space and time variables is of great practical importance and interest. Hence, we plan to address this aspect in our future work.

2. In this thesis, we have proposed numerical schemes that converge with an order of two and four for the space variable(s). It would be interesting to develop higher-order numerical schemes for the spatial variables. To achieve this, we intend to use high-order compact finite difference schemes in conjunction with the operator splitting technique to solve two-dimensional time fractional diffusion equations. These schemes offer the advantage of a higher order of accuracy.

3. Many authors have overlooked the possibility of weak singularity at $t = 0$ for fractional-diffusion equations. They have presented convergence analyses under the unrealistic assumption that the solution is in $C^2[0, T]$. Consequently, their theoretical analysis which relies on the assumption of a sufficiently smooth solution is not appropriate. To address this weak singularity, we plan to employ a graded mesh. This involves concentrating more mesh points around the (weak) singular points to capture the rapid variation of the solution while using a larger step size when the solution changes slowly. This will be one of our future work.

4. For many problems in time fractional diffusion equations, researchers use the finite difference method for the time domain and the finite element method for the spatial domain. This approach yields an improved order of convergence in the spatial variable but not in the time variable. By applying the discontinuous Galerkin (DG) method, we anticipate achieving an improved order of convergence in both variables. This forms the basis of future research direction.

5. Super-convergence is a property of numerical schemes that results in a higher order of convergence. We aim to establish and prove the super-convergence

properties of the discontinuous Galerkin method for fractional diffusion equations.

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