Chapter 3

High-Order Approximation of Caputo–Prabhakar Derivative With Application in Solving Linear and Nonlinear Fractional Diffusion Models

This chapter is an extension of the chapter 2. In this chapter, we propose high-order approximation of Caputo–Prabhakar derivative using an interpolating polynomial of degree r. Further, we combine the proposed scheme with central difference approximation to solve time fractional advection–diffusion equation and reaction–diffusion equation numerically. Solvability, stability and convergence of the schemes are discussed. Numerical results are presented to support the theoretical analysis.

3.1 Introduction

In this chapter, we develop a high-order numerical scheme using an r-th degree Lagrange interpolation polynomial for the approximation of Caputo-Prabhakar derivative. Further, we use this approximation to solve linear and nonlinear time fractional models namely, time fractional advection–diffusion equation and time fractional reaction–diffusion equation with Dirichlet type boundary conditions using central difference approximation in space. The nonlinear reaction term in reaction–diffusion equation is approximated using the Newton–Raphson iterative method. The order of convergence of the whole discretized scheme is $O(\tau^{r+1-\alpha}, h^2)$, where τ and h denote the temporal and spatial step sizes respectively. The stability analysis of the finite difference scheme is discussed using von Neumann stability analysis. Further, we studied the solvability and convergence analysis of the scheme. In terms of test examples, we have shown that the numerical results validate our analytical conclusions, and the scheme works well. As far as we know, no work has yet been done for the high-order approximation of Caputo–Prabhakar derivatives as discussed in this chapter.

The outline of the chapter is as follows; Section 3.2 is devoted to the study of the numerical method for approximation of the Caputo–Prabhakar derivative and discusses some properties of the discretization coefficients. Further, the error analysis of the scheme is discussed. In Section 3.3, we use the discussed numerical scheme to solve the time fractional advection–diffusion equation and study the stability analysis of the scheme using the von Neumann stability analysis method. This section further deals with the solvability and convergence analysis of the numerical method. In Section 3.4, another application of discussed numerical scheme in solving time fractional nonlinear reaction–diffusion equation is studied. Further, Stability and convergence analysis of the scheme are discussed in Subsection 3.4.1 and Subsection

3.4.2. In Subsections 3.2.2, 3.3.4, 3.4.3, some numerical illustrations are given to ensure the validity of the proposed schemes. Last Section concludes the chapter.

3.2 Numerical Scheme

In this section, we develop a high-order numerical scheme to approximate Caputo–Prabhakar derivative using time stepping Lagrange interpolation polynomials of degree r, motivated by the research work done in [100, 101]. We choose a partition, $0 = t_0 < t_1 < \cdots < t_M = T,\ M \in \mathbb{N}$, of the temporal domain $[0, T]$, with uniform step size $\tau = \frac{T}{M}$ such that $t_k = k\tau$, for $k = 0, \cdots, M$. At node $t = t_k$,

$$\begin{aligned} {}_0^{\mathrm{CP}}D^{\gamma}_{\rho,\alpha,\omega} f(t_k) &= \int_0^{t_k} (t_k - s)^{-\alpha} E^{-\gamma}_{\rho,1-\alpha}(\omega(t_k - s)^{\rho}) f'(s) ds \\ &= \sum_{j=1}^{k} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha} E^{-\gamma}_{\rho,1-\alpha}(\omega(t_k - s)^{\rho}) f'(s) ds \\ &= \sum_{j=1}^{k} I_j[f(s)], \end{aligned} \tag{3.1}$$

where

$$I_j[f(s)] = \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha} E^{-\gamma}_{\rho,1-\alpha}(\omega(t_k - s)^{\rho}) f'(s) ds. \tag{3.2}$$

Now we discuss two separate cases for the subinterval $[t_{j-1}, t_j]$.

Case (1): For $k \geq j \geq r$, $M \geq k \geq r$.

The rth-order Lagrange interpolation polynomial approximating a function f at the nodes $(t_j, f(t_j)),\ (t_{j-1}, f(t_{j-1})), \ldots, (t_{j-r}, f(t_{j-r}))$ is defined as

$$p_r(t) = \sum_{i=0}^{r} f(t_{j-i}) \prod_{\substack{l=0 \\ l \neq i}}^{r} \frac{t - t_{j-l}}{t_{j-i} - t_{j-l}}, \qquad t \in [t_{j-1}, t_j],$$

and the error involved in approximating $f(t)$ by the interpolating polynomial $p_r(t)$ is

$$f(t) - p_r(t) = \frac{f^{(r+1)}(\xi_j)}{(r+1)!}\prod_{l=0}^{r}(t - t_{j-l}), \qquad \xi_j \in (t_{j-r}, t_j). \tag{3.3}$$

Also, we obtain

$$p_r'(t) = \sum_{i=0}^{r} f(t_{j-i})\frac{(-1)^i}{i!(r-i)!\tau^r}\frac{d}{dt}\prod_{\substack{l=0\\l\neq i}}^{r}(t - t_{j-l}). \tag{3.4}$$

Approximating $f(s)$ by $p_r(s)$ in (3.2), we obtain

$$\begin{aligned}
I_j[f(s)] \approx & I_j[p_r(s)] = \int_{t_{j-1}}^{t_j}(t_k - s)^{-\alpha}E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho})p_r'(s)ds,\\
= & \int_{t_{j-1}}^{t_j}(t_k - s)^{-\alpha}E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho})\sum_{i=0}^{r} f(t_{j-i})\frac{(-1)^i}{i!(r-i)!\tau^r}\frac{d}{ds}\prod_{\substack{l=0\\l\neq i}}^{r}(s - t_{j-l})ds,\\
= & \sum_{i=0}^{r}\frac{(-1)^i}{i!(r-i)!\tau^r}f(t_{j-i})\int_{t_{j-1}}^{t_j}(t_k - s)^{-\alpha}E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho})\frac{d}{ds}\prod_{\substack{l=0\\l\neq i}}^{r}(s - t_{j-l})ds,\\
= & \tau^{-\alpha}\sum_{i=0}^{r} W_{i,k-j}^{r} f(t_{j-i}),
\end{aligned}$$

where

$$\begin{aligned}
W_{i,k-j}^{r} &= \frac{(-1)^{i+1}}{i!(r-i)!}\sum_{n=1}^{r} n!\left(\theta_{r+1,i}^{r-n}\phi_n^{k-j} - \lambda_{r+1,i}^{r-n}\psi_n^{k-j}\right), \quad 0 \le i \le r,\\
\phi_n^{k-j} &= (k-j)^{n-\alpha}E_{\rho,n+1-\alpha}^{-\gamma}\left(\omega((k-j)\tau)^{\rho}\right),\\
\psi_n^{k-j} &= (k-j+1)^{n-\alpha}E_{\rho,n+1-\alpha}^{-\gamma}\left(\omega((k-j+1)\tau)^{\rho}\right).
\end{aligned}$$

$$\theta_{j,i}^{l} = \begin{cases} a_{j,i}^{l}, & l \neq 0\\ 1, & l = 0\end{cases}, \quad \lambda_{j,i}^{l} = \begin{cases} b_{j,i}^{l}, & l \neq 0\\ 1, & l = 0\end{cases}.$$

Here, $a^l_{j,i}$ is obtained from the set $X_{j,i} = ([0, j-1] \setminus \{i\}) \cap \mathbb{Z}$, and $b^l_{j,i}$ is obtained from the set $Y_{j,i} = ([-1, j-2] \setminus \{i-1\}) \cap \mathbb{Z}$, by summing the products of different possible combinations of l elements.

Now, the values of the weight coefficients $W^r_{i,k-j}$ for different $r = 1, 2, 3, 4, 5$ can be obtained as follows.

For $r = 1$,

$$\begin{cases} W^1_{0,z} = -\left[\phi^z_1 - \psi^z_1\right], \\ W^1_{1,z} = [\phi^z_1 - \psi^z_1]. \end{cases}$$

For $r = 2$,

$$\begin{cases} W^2_{0,z} = -\frac{1}{2}\left[(3\phi^z_1 - \psi^z_1) + 2\left(\phi^z_2 - \psi^z_2\right)\right], \\ W^2_{1,z} = \left[(2\phi^z_1) + 2\left(\phi^z_2 - \psi^z_2\right)\right], \\ W^2_{2,z} = -\frac{1}{2}\left[(\phi^z_1 + \psi^z_1) + 2\left(\phi^z_2 - \psi^z_2\right)\right]. \end{cases}$$

For $r = 3$,

$$\begin{cases} W^3_{0,z} = -\frac{1}{6}\left[(11\phi^z_1 - 2\psi^z_1) + 2(6\phi^z_2 - 3\psi^z_2) + 6(\phi^z_3 - \psi^z_3)\right], \\ W^3_{1,z} = \frac{1}{2}\left[(6\phi^z_1 + \psi^z_1) + 2(5\phi^z_2 - 2\psi^z_2) + 6(\phi^z_3 - \psi^z_3)\right], \\ W^3_{2,z} = -\frac{1}{2}\left[(3\phi^z_1 + 2\psi^z_1) + 2(4\phi^z_2 - \psi^z_2) + 6(\phi^z_3 - \psi^z_3)\right], \\ W^3_{3,z} = \frac{1}{6}\left[(2\phi^z_1 + \psi^z_1) + 2(3\phi^z_2) + 6(\phi^z_3 - \psi^z_3)\right]. \end{cases}$$

For $r = 4$,

$$\begin{cases} W^4_{0,z} = -\frac{1}{24}\left[(50\phi^z_1 - 6\psi^z_1) + 2(35\phi^z_2 - 11\psi^z_2) + 6(10\phi^z_3 - 6\psi^z_3) + 24(\phi^z_4 - \psi^z_4)\right], \\ W^4_{1,z} = \frac{1}{6}\left[(24\phi^z_1 + 5\psi^z_1) + 2(26\phi^z_2 - 5\psi^z_2) + 6(9\phi^z_3 - 5\psi^z_3) + 24(\phi^z_4 - \psi^z_4)\right], \\ W^4_{2,z} = -\frac{1}{4}\left[(12\phi^z_1 + 6\psi^z_1) + 2(19\phi^z_2 - \psi^z_2) + 6(8\phi^z_3 - 4\psi^z_3) + 24(\phi^z_4 - \psi^z_4)\right], \\ W^4_{3,z} = \frac{1}{6}\left[(8\phi^z_1 + 3\psi^z_1) + 2(14\phi^z_2 + \psi^z_2) + 6(7\phi^z_3 - 3\psi^z_3) + 24(\phi^z_4 - \psi^z_4)\right], \\ W^4_{4,z} = -\frac{1}{24}\left[(6\phi^z_1 + 2\psi^z_1) + 2(11\phi^z_2 + \psi^z_2) + 6(6\phi^z_3 - 2\psi^z_3) + 24(\phi^z_4 - \psi^z_4)\right]. \end{cases}$$

For $r = 5$,

$$\begin{cases} W^5_{0,z} &= -\frac{1}{120}\left[(274\phi^z_1 - 24\psi^z_1) + 2(225\phi^z_2 - 50\psi^z_2) + 6(85\phi^z_3 - 35\psi^z_3)\right. \\ &\left. + 24(15\phi^z_4 - 10\psi^z_4) + 120(\phi^z_5 - \psi^z_5)\right], \\ W^5_{1,z} &= \frac{1}{24}\left[(120\phi^z_1 + 26\psi^z_1) + 2(154\phi^z_2 - 15\psi^z_2) + 6(71\phi^z_3 - 25\psi^z_3)\right. \\ &\left. + 24(14\phi^z_4 - 9\psi^z_4) + 120(\phi^z_5 - \psi^z_5)\right], \\ W^5_{2,z} &= -\frac{1}{12}\left[(60\phi^z_1 + 24\psi^z_1) + 2(107\phi^z_2 + 2\psi^z_2) + 6(59\phi^z_3 - 17\psi^z_3)\right. \\ &\left. + 24(13\phi^z_4 - 8\psi^z_4) + 120(\phi^z_5 - \psi^z_5)\right], \\ W^5_{3,z} &= \frac{1}{12}\left[(40\phi^z_1 + 12\psi^z_1) + 2(78\phi^z_2 + 7\psi^z_2) + 6(49\phi^z_3 - 11\psi^z_3)\right. \\ &\left. + 24(12\phi^z_4 - 7\psi^z_4) + 120(\phi^z_5 - \psi^z_5)\right], \\ W^5_{4,z} &= -\frac{1}{24}\left[(30\phi^z_1 + 8\psi^z_1) + 2(61\phi^z_2 + 6\psi^z_2) + 6(41\phi^z_3 - 7\psi^z_3)\right. \\ &\left. + 24(11\phi^z_4 - 6\psi^z_4) + 120(\phi^z_5 - \psi^z_5)\right], \\ W^5_{5,z} &= \frac{1}{120}\left[(24\phi^z_1 + 6\psi^z_1) + 2(50\phi^z_2 + 5\psi^z_2) + 6(35\phi^z_3 - 5\psi^z_3)\right. \\ &\left. + 24(10\phi^z_4 - 5\psi^z_4) + 120(\phi^z_5 - \psi^z_5)\right]. \end{cases}$$

Case (2): $1 \le j \le k$, $1 \le k \le r - 1$.

In this case, since $j < r$, we do not have sufficient points to construct the Lagrange interpolating polynomial of degree r. Hence, for each $0 < j < r$, $I_j[f(s)]$ is approximated by $I_j[P_j(s)]$, where $P_j(s)$ is a Lagrange interpolation polynomial of degree j. Now, combining case (1) and case (2), a numerical scheme approximating the Caputo–Prabhakar derivative is obtained as

$$
\begin{aligned}
{}_{0}^{\mathrm{CP}}D_{\rho,\alpha,\omega}^{\gamma} f(t_k) &= \sum_{j=1}^{k} I_j[f(s)] \\
&= \sum_{j=1}^{r-1} I_j[P_j(s)] + \sum_{j=r}^{k} I_j[P_r(s)] \\
&= \tau^{-\alpha} \sum_{j=1}^{r-1}\sum_{i=0}^{j} W_{i,k-j}^{j} f(t_{j-i}) + \tau^{-\alpha} \sum_{j=r}^{k}\sum_{i=0}^{r} W_{i,k-j}^{r} f(t_{j-i}) \\
&= \tau^{-\alpha} I_k A_{k,r} f_k = \tau^{-\alpha} P_k^r f_k \\
&= \tau^{-\alpha} \sum_{j=0}^{k} p_{k-j}^{r} f_j + E_r^k, \qquad (3.5)
\end{aligned}
$$

where

$$P_k^r = (p_k^r, p_{k-1}^r, \ldots, p_0^r) = I_k A_{k,r},$$

$$I_k = \begin{bmatrix} 1 & 1 & \ldots & 1 \end{bmatrix}_{1\times k}, \quad f_k = \begin{bmatrix} f(t_0), \ldots, f(t_k) \end{bmatrix}^T,$$

$$A_{k,r} = \begin{bmatrix} W_{k,r-1} & \mathbf{0} \\ W_{k,r}^{*} & \end{bmatrix}_{k\times(k+1)},$$

$$W_{k,s} = \begin{bmatrix} W_{1,k-1}^{1} & W_{0,k-1}^{1} & 0 & \cdots & 0 \\ W_{2,k-2}^{2} & W_{1,k-2}^{2} & W_{0,k-2}^{2} & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ W_{s,k-s}^{s} & \cdots & \cdots & \cdots & W_{0,k-s}^{s} \end{bmatrix}_{s\times(s+1)},$$

$$W^*_{k,r} = \begin{bmatrix} W^r_{r,k-r} & \cdots & \cdots & \cdots & W^r_{0,k-r} & 0 & \cdots & 0 \\ 0 & W^r_{r,k-r-1} & \cdots & \cdots & \cdots & W^r_{0,k-r-1} & \ddots & \vdots \\ \vdots & \ddots & \ddots & & & & \ddots & 0 \\ 0 & \cdots & 0 & W^r_{r,0} & \cdots & \cdots & \cdots & W^r_{0,0} \end{bmatrix}_{(k-r+1)\times(k+1)}.$$

Remark 3.2.1. If $k < r$, then we can write the derived scheme as

$$ {}^{\mathrm{CP}}_{0}D^{\gamma}_{\rho,\alpha,\omega} f(t_k) = \sum_{j=1}^{k} I_j[f(s)] + E^k_r. \tag{3.6}$$

Also when $1 \le k < r$, then $A_{k,r} = W_{k,k}$.

Next, some properties of the discretization coefficients p^r_{k-j} will be studied for $r = 4$. For other values of $4 < r \in \mathbb{N}$, it can be studied in a similar way, so those calculations are omitted.

Lemma 3.2.1. The following relations hold between the discretization coefficients:

1. if we fix $k = 1$, then $p^r_1 = -p^r_0$.
2. $\sum_{j=0}^{k} p^r_{k-j} = 0$.

Proof. 1. Fixing $k = 1$, the numerical scheme (3.5) reduces to (3.6), so we have

$$p^r_1 = W^1_{1,0} = \phi^0_1 - \psi^0_1,$$
$$p^r_0 = W^1_{0,0} = -[\phi^0_1 - \psi^0_1],$$

and hence, $p^r_1 = -p^r_0$.

2. For $k = 1$,

$$\sum_{j=0}^{k} p^r_{k-j} = W^1_{0,0} + W^1_{1,0} = 0.$$

For $k = 2$,

$$\begin{aligned}\sum_{j=0}^{k} p^r_{k-j} &= W^1_{1,1} + W^2_{2,0} + W^1_{0,1} + W^2_{1,0} + W^2_{0,0} \\ &= (W^1_{0,1} + W^1_{1,1}) + (W^2_{0,0} + W^2_{1,0} + W^2_{2,0}) \\ &= 0.\end{aligned}$$

For $k = 3$,

$$\begin{aligned}\sum_{j=0}^{k} p^r_{k-j} &= W^1_{1,2} + W^2_{2,1} + W^3_{3,0} + W^1_{0,2} + W^2_{1,1} + W^3_{2,0} + W^2_{0,1} + W^3_{1,0} + W^3_{0,0} \\ &= (W^1_{0,2} + W^1_{1,2}) + (W^2_{0,1} + W^2_{1,1} + W^2_{2,1}) + (W^3_{0,0} + W^3_{1,0} + W^3_{2,0} + W^3_{3,0}) \\ &= 0.\end{aligned}$$

For $k \geq 4$,

$$\begin{aligned}\sum_{j=0}^{k} p^r_{k-j} &= (W^1_{0,k-1} + W^1_{1,k-1}) + (W^2_{0,k-2} + W^2_{1,k-2} + W^2_{2,k-2}) \\ &\quad + (W^3_{0,k-3} + W^3_{1,k-3} + W^3_{2,k-3} + W^3_{3,k-3}) \\ &\quad + (W^4_{0,k-4} + W^4_{1,k-4} + W^4_{2,k-4} + W^4_{3,k-4} + W^4_{4,k-4}) \\ &\quad + (W^4_{0,k-5} + W^4_{1,k-5} + W^4_{2,k-5} + W^4_{3,k-5} + W^4_{4,k-5}) + \dots \\ &\quad + (W^4_{0,0} + W^4_{1,0} + W^4_{2,0} + W^4_{3,0} + W^4_{4,0}) \\ &= 0.\end{aligned}$$

This completes the proof. □

3.2.1 Error Analysis of the Scheme

Theorem 3.2.1. If $f \in C^r[0,T]$, where $3 \leq r \in \mathbb{N}$, then for $\alpha \in (0,\ 1)$, the local truncation error E_r^k satisfies the relation

1. $\left|E_r^1\right| \leq C_1 \max_{t_0 \leq t \leq t_1} \left|f''(t)\right| \tau^{2-\alpha},\ k = 1,$
2. $\left|E_r^2\right| \leq C_2 \max_{t_0 \leq t \leq t_2} \left|f'''(t)\right| \tau^{3-\alpha},\ k = 2,$
3. $\left|E_r^k\right| \leq C_3 \max_{t_0 \leq t \leq t_k} \left|f^{(k+1)}(t)\right| \tau^{k+1-\alpha},\ 2 < k < r,\ f^{(i)}(0) = 0,\ 0 < i \leq k-1,$
4. $\left|E_r^k\right| \leq C_4 \max_{t_0 \leq t \leq t_n} \left|f^{(k+1)}(t)\right| \tau^{r+1-\alpha},\ k \geq r,\ f^{(i)}(0) = 0,\ 0 < i \leq r-1,$

where C_1, C_2, C_3 and C_4 are positive constants.

Proof. 1. For $k = 1$, the scheme (3.5) is obtained by using an interpolating polynomial of degree one, and its order of convergence is $(2 - \alpha)$ [101].

2. For $k = 2$, the scheme (3.5) is obtained by using an interpolating polynomial of degree two, and its order of convergence is $(3 - \alpha)$ [101].

3. For $2 < k < r$,

$$\begin{aligned}
\left|E_r^k\right| = &\left|\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha}\ E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f - p_j)'(s) ds\right. \\
&\left. + \int_{t_{k-1}}^{t_k} (t_k - s)^{-\alpha} E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f - p_k)'(s) ds\right| \\
= &\left|\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f(s) - p_j(s)) ds\right.
\end{aligned}$$

$$+ \int_{t_{k-1}}^{t_k} (t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho})(f(s) - p_k(s))ds \Bigg| .$$

Now, we consider the first integral:

$$\begin{aligned}
&\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho})(f(s) - p_j(s))ds \\
&= \sum_{j=1}^{k-1} \frac{f^{(j+1)}(\xi_j)}{(j+1)!} \int_{t_{j-1}}^{t_j} (s - t_j)(s - t_{j-1}) \dots (s - t_0)(t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho})ds \\
&\leq \sum_{j=1}^{k-1} - \frac{f^{(j+1)}(\xi_j)}{(j+1)} \frac{\tau^{j+1}}{4} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho}) \\
&\leq \sum_{j=1}^{k-1} - \frac{f^{(j+1)}(\xi_j)}{4(j+1)} \tau^{j+1-\alpha} \left[(k-j)^{-\alpha} \, E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - t_j)^{\rho}) \right. \\
&\quad \left. - (k-j+1)^{-\alpha} E_{\rho,1-\alpha}^{-\gamma} \left(\omega(t_k - t_{j-1})^{\rho} \right) \right] .
\end{aligned} \tag{3.7}$$

Next, we consider the second interval:

$$\begin{aligned}
&\int_{t_{k-1}}^{t_k} (t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho})(f(s) - P_k(s))ds \\
&= \int_{t_{k-1}}^{t_k} \frac{f^{(k+1)}(\xi)}{(k+1)!} (s - t_0)(s - t_1) \dots (s - t_k)(t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho})ds \\
&\leq - \frac{f^{(k+1)}(\xi)}{4(k+1)} \tau^{k+1} \int_{t_{k-1}}^{t_k} (t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^{\rho})ds \\
&= - \frac{f^{(k+1)}(\xi)}{4(k+1)} \tau^{k+1-\alpha} E_{\rho,1-\alpha}^{-\gamma}(\omega\tau^{\rho}).
\end{aligned} \tag{3.8}$$

Now, combining (3.7) and (3.8), we have

$$\begin{aligned}
\left| E_r^k \right| \leq \Bigg| &\sum_{j=1}^{k-1} \frac{f^{(j+1)}(\xi_j)}{4(j+1)} \tau^{j+1-\alpha} \left[(k-j)^{-\alpha} E_{\rho,1-\alpha}^{-\gamma} \left(\omega(t_k - t_j)^{\rho} \right) \right. \\
&\left. - (k-j+1)^{-\alpha} E_{\rho,1-\alpha}^{-\gamma} \left(\omega(t_k - t_{j-1})^{\rho} \right) \right] \\
&+ \frac{f^{(k+1)}(\xi)}{4(k+1)} \tau^{k+1-\alpha} E_{\rho,1-\alpha}^{-\gamma}(\omega\tau^{\rho}) \Bigg|
\end{aligned}$$

$$\leq C_3 \max_{t_0 \leq t \leq t_k} \left| f^{(k+1)}(t) \right| \tau^{k+1-\alpha},$$

where C_3 is a positive constant.

4. For $k \geq r$,

$$\begin{aligned}
\left|E_r^k\right| =& \left| \sum_{j=1}^{r-1} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha} E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f - P_j)'(s)ds \right. \\
&+ \sum_{j=r}^{k-1} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha} E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f - P_r)'(s)ds \\
&\left. + \int_{t_{k-1}}^{t_k} (t_k - s)^{-\alpha}\ E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f - P_r)'(s)ds \right| \\
=& \left| \sum_{j=1}^{r-1} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha-1}\ E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f(s) - P_j(s))ds \right. \\
&+ \sum_{j=r}^{k-1} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f(s) - P_r(s))ds \\
&\left. + \int_{t_{k-1}}^{t_k} (t_k - s)^{-\alpha-1}\ E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f(s) - P_r(s))ds \right|.
\end{aligned}$$

We will consider the first integral:

$$\begin{aligned}
&\sum_{j=1}^{r-1} \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)(f(s) - P_j(s))ds \\
&= \sum_{j=1}^{r-1} \frac{f^{(j+1)}(\xi)}{(j+1)!} \int_{t_{j-1}}^{t_j} (s - t_j)(s - t_{j-1}) \ldots (s - t_0)(t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)ds \\
&\leq \sum_{j=1}^{r-1} -\frac{f^{(j+1)}(\xi)}{4(j+1)!} \tau^{j+1} j! \int_{t_{j-1}}^{t_j} (t_k - s)^{-\alpha-1} E_{\rho,-\alpha}^{-\gamma}(\omega(t_k - s)^\rho)ds \\
&\leq \sum_{j=1}^{r-1} -\frac{f^{(j+1)}(\xi)}{4(j+1)} \tau^{j+1-\alpha} [(k-j)^{-\alpha} E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - t_j)^\rho) \\
&\quad - (k - j + 1)^{-\alpha} E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k - t_{j-1})^\rho)].
\end{aligned} \tag{3.9}$$

Now we will consider the second integral:

$$\begin{aligned}
&\sum_{j=r}^{k-1}\int_{t_{j-1}}^{t_j}(t_k-s)^{-\alpha-1}E_{\rho,-\alpha}^{-\gamma}(\omega(t_k-s)^{\rho})(f(s)-P_r(s))'ds\\
&=\sum_{j=r}^{k-1}\int_{t_{j-1}}^{t_j}\frac{f^{(r+1)}(\xi)}{(r+1)!}(s-t_j)(s-t_{j-1})\dots(s-t_{j-r})(t_k-s)^{-\alpha-1}E_{\rho,-\alpha}^{-\gamma}(\omega(t_k-s)^{\rho})ds\\
&\leq\sum_{j=r}^{k-1}-\frac{f^{(r+1)}(\xi)}{(r+1)!}\frac{\tau^{r+1}}{4}r!\int_{t_{j-1}}^{t_j}(t_k-s)^{-\alpha-1}E_{\rho,-\alpha}^{-\gamma}(\omega(t_k-s)^{\rho})ds\\
&\leq\sum_{j=r}^{k-1}-\frac{f^{(r+1)}(\xi)}{4(r+1)}\tau^{r+1-\alpha}[(k-j)^{-\alpha}E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k-t_j)^{\rho})\\
&\quad-(k-j+1)^{-\alpha}E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k-t_{j-1})^{\rho})].
\end{aligned}\tag{3.10}$$

Next we consider the third integral:

$$\begin{aligned}
&\int_{t_{k-1}}^{t_k}(t_k-s)^{-\alpha-1}E_{\rho,-\alpha}^{-\gamma}(\omega(t_k-s)^{\rho})(f(s)-P_r(s))ds\\
&=\frac{f^{(r+1)}(\xi)}{(r+1)!}\int_{t_{k-1}}^{t_k}(s-t_k)(s-t_{k-1})\dots(s-t_{k-r})(t_k-s)^{-\alpha-1}E_{\rho,-\alpha}^{-\gamma}(\omega(t_k-s)^{\rho})\\
&\leq-\frac{f^{(r+1)}(\xi)}{(r+1)!}r!\frac{\tau^{r+1}}{4}\int_{t_{k-1}}^{t_k}(t_k-s)^{-\alpha-1}E_{\rho,-\alpha}^{-\gamma}(\omega(t_k-s)^{\rho})ds\\
&\leq-\frac{f^{(r+1)}(\xi)}{r+1}\frac{\tau^{r+1-\alpha}}{4}E_{\rho,1-\alpha}^{-\gamma}(\tau^{\rho}).
\end{aligned}\tag{3.11}$$

Now combining (3.9), (3.10) and (3.11), we get

$$\begin{aligned}
\left|E_r^k\right|\leq&\left|\sum_{j=1}^{r-1}\frac{f^{(j+1)}(\xi)}{4(j+1)}\tau^{j+1-\alpha}[(k-j)^{-\alpha}E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k-t_j)^{\rho})\right.\\
&\left.-(k-j+1)^{-\alpha}E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k-t_{j-1})^{\rho})]\right|\\
&+\left|\sum_{j=r}^{k-1}\frac{f^{(r+1)}(\xi)}{4(r+1)}\tau^{r+1-\alpha}[(k-j)^{-\alpha}E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k-t_j)^{\rho})\right.\\
&\left.-(k-j+1)^{-\alpha}E_{\rho,1-\alpha}^{-\gamma}(\omega(t_k-t_{j+1})^{\rho})]\right|+\left|\frac{f^{(r+1)}(\xi)}{r+1}\frac{\tau^{r+1-\alpha}}{4}E_{\rho,1-\alpha}^{-\gamma}(\tau^{\rho})\right|
\end{aligned}$$

$$\leq C_4 \max_{t_0 \leq t \leq t_k} \left| f^{(r+1)}(t) \right| \tau^{r+1-\alpha}.$$

This completes the proof. □

3.2.2 Numerical Experiments

Here, we discuss two test examples in order to validate the numerical algorithm established in this chapter. Numerical results for $r = 4$ and $r = 5$ are discussed.

Example 3.2.1. For the function $f(t) = t^6$, $t \in [0, T]$, calculate the αth-order Caputo–Prabhakar derivative for $0 < \alpha < 1$. The exact solution is ${}_0^{\mathrm{CP}}D^{\gamma}_{\rho,\alpha,\omega} t^6 = 720 t^{6-\alpha} E^{-\gamma}_{\rho,7-\alpha}(\omega t^{\rho})$. Since the given function $f \in \mathrm{L}^1[0, 1]$, its Caputo–Prabhakar derivative can be calculated. For $r = 4, 5$, we have calculated maximum absolute error and convergence rate at $T = 1$, for different $\alpha = 0.2, 0.4, 0.6, 0.8$, and step sizes $\tau = 1/10,\ 1/20,\ 1/40,\ 1/80,\ 1/160$ and listed the obtained results in Table 3.1. It is evident from the Table 3.1 that the computational convergence rate is $(r + 1 - \alpha)$, and this validates our analytical results.

TABLE 3.1: MAE and CO for different α with $r = 4, 5$ for Ex. 3.2.1.

α	$\frac{1}{\tau}$	$r = 4$		$r = 5$	
		MAE	CO	MAE	CO
$\alpha = 0.2$	10	2.17269E-04		5.61268E-05	
	20	9.20339E-06	4.561170047	1.00321E-06	5.806000930
	40	3.65401E-07	4.654611755	1.79348E-08	5.805708873
	80	1.40569E-08	4.700136700	3.20696E-10	5.805415154
	160	5.07831E-10	4.790780758	5.73104E-12	5.806265187
$\alpha = 0.4$	10	8.27842E-04		2.21479E-04	
	20	3.87247E-05	4.418030780	4.53034E-06	5.611402754
	40	1.70510E-06	4.505322512	9.27205E-08	5.610588178
	80	7.29072E-08	4.547654752	1.89866E-09	5.609834164
	160	3.08555E-09	4.562458941	3.85654E-11	5.621532192
$\alpha = 0.6$	10	2.33224E-03		6.38322E-04	
	20	1.22530E-04	4.250506895	1.49810E-05	5.413076890
	40	6.08656E-06	4.331364719	3.51831E-07	5.412107834
	80	2.94567E-07	4.368959695	8.26791E-09	5.411216612
	160	1.41958E-08	4.375065330	1.92069E-10	5.427826916
$\alpha = 0.8$	10	5.85829E-03		1.62573E-03	
	20	3.49316E-04	4.067876660	4.38035E-05	5.213899935
	40	1.97627E-05	4.143679974	1.18109E-06	5.212856507
	80	1.09192E-06	4.177848534	3.18672E-08	5.211898995
	160	5.96854E-08	4.193339720	8.60343E-10	5.211019274

Example 3.2.2. Calculate the α-th order Caputo–Prabhakar derivative of $f(t) =$

$t^{(7-\alpha)}$, $t \in [0, T]$ at $T = 1$, for $0 < \alpha < 1$. The analytical expression of the Caputo–Prabhakar derivative of order α for the function f is unknown. So the convergence order of f is calculated with the help of the formula (2.47) at the various step sizes $\tau = 1/10, 1/20, 1/40, 1/80, 1/160$, for $r = 4, 5$. Results obtained for various values of $\alpha = 0.2, 0.4, 0.6, 0.8$ are given in Table 3.2 and Table 3.3. From these tables, it is evident that convergence is of order $(r + 1 - \alpha)$.

Table 3.2: CO for $r = 4$ and $\alpha = 0.2, 0.4, 0.6, 0.8$ for Ex. 3.2.2.

α	t	CO		
		$\log_2\left(\frac{\Delta e_\tau}{\Delta e_{\tau/2}}\right)$	$\log_2\left(\frac{\Delta e_{\tau/2}}{\Delta e_{\tau/4}}\right)$	$\log_2\left(\frac{\Delta e_{\tau/4}}{\Delta e_{\tau/8}}\right)$
	0.2	3.297043141	3.887934476	4.361720732
	0.4	3.888133923	4.361918662	4.556786856
$\alpha = 0.2$	0.6	4.218662364	4.494017638	4.618913879
	0.8	4.362117231	4.556988293	4.650393851
	1.0	4.442533787	4.594261524	4.670392859
	0.2	3.264374227	3.822539836	4.254058831
	0.4	3.823136148	4.254638139	4.426802609
$\alpha = 0.4$	0.6	4.126252583	4.372041805	4.480815299
	0.8	4.255263575	4.427413193	4.507724918
	1.0	4.326919661	4.459925372	4.524054787
	0.2	3.235120944	3.742039586	4.124920093
	0.4	3.742828549	4.125688384	4.273196362
$\alpha = 0.6$	0.6	4.013709373	4.226914468	4.318464967
	0.8	4.126523236	4.274001342	4.340676012
	1.0	4.188499651	4.301351990	4.354152176
	0.2	3.213208179	3.650175565	3.980696208
	0.4	3.651097925	3.981586111	4.104707046
$\alpha = 0.8$	0.6	3.886572972	4.066579453	4.141783413
	0.8	3.982555474	4.105626746	4.159681977
	1.0	4.034739895	4.128097929	4.170262620

TABLE 3.3: CO for $r = 5$ and $\alpha = 0.2, 0.4, 0.6, 0.8$ for Ex. 3.2.2.

α	t	CO		
		$\log_2\left(\frac{\Delta e_\tau}{\Delta e_{\tau/2}}\right)$	$\log_2\left(\frac{\Delta e_{\tau/2}}{\Delta e_{\tau/4}}\right)$	$\log_2\left(\frac{\Delta e_{\tau/4}}{\Delta e_{\tau/8}}\right)$
	0.2	3.178154561	6.144325501	5.491391524
	0.4	6.144517302	5.491580755	5.628329508
0.2	0.6	5.382954534	5.585449054	5.666258000
	0.8	5.491771047	5.628486888	5.635934183
	1.0	5.549527543	5.652521217	5.657650319
	0.2	3.151015664	6.224331038	5.401914777
	0.4	6.224921790	5.402488712	5.503817556
0.4	0.6	5.320493092	5.472613052	5.532773242
	0.8	5.403108203	5.504393645	5.492497663
	1.0	5.446397986	5.522341012	5.509000913
	0.2	3.125306042	6.307152597	5.287134506
	0.4	6.307958643	5.287910878	5.353002477
0.6	0.6	5.233918644	5.333512549	5.372085958
	0.8	5.288754480	5.353832890	5.409466499
	1.0	5.317027438	5.365603651	5.415207771
	0.2	3.104259189	6.403641612	5.154936411
	0.4	6.404603609	5.155840054	5.186548904
0.8	0.6	5.129777704	5.177878033	5.192206296
	0.8	5.156824473	5.187506576	5.165950915
	1.0	5.170546613	5.192738576	5.169693848

3.3 Application-1

In this section, we use the high-order numerical scheme discussed in Section (3.2) for solving the time fractional advection–diffusion equation,

$$\begin{cases} {}_0^{\text{CP}}D^{\gamma}_{\rho,\alpha,\omega}u(x,t) = K\frac{\partial^2 u(x,t)}{\partial x^2} - V\frac{\partial u(x,t)}{\partial x} + F(x,t),\ 0 < x < L,\ 0 < t < T, \\ u(x,0) = u_0(x), \\ u(0,t) = \eta_1(t), \\ u(L,t) = \eta_2(t), \end{cases} \tag{3.12}$$

where $V > 0$, $K > 0$ and $F(x,t)$ are the average fluid velocity, diffusion coefficient and the source term, respectively. The spatial domain $[0,L]$ is discretized into $N \in \mathbb{N}$, sub domains by choosing a partition $0 = x_0 < x_1 < \cdots < x_N = L$ of uniform length $h = \frac{L}{N}$ such that $x_i = ih$, for $i = 0,1,\cdots,N$. Let the analytical and approximate solution of $u(x,t)$ at the node (x_i,t_k) be U_i^k and u_i^k respectively. The first and the second-order derivatives in space are approximated using the central difference scheme:

$$\frac{\partial u(x_i,t_k)}{\partial x} = \frac{u_{i+1}^k - u_{i-1}^k}{2h} + \mathcal{O}(h^2), \tag{3.13}$$

$$\frac{\partial^2 u(x_i,t_k)}{\partial x^2} = \frac{u_{i+1}^k - 2u_i^k + u_{i-1}^k}{h^2} + \mathcal{O}(h^2). \tag{3.14}$$

By using (3.5), the time fractional Caputo–Prabhakar derivative term in (3.12) is approximated as

$${}_0^{\text{CP}}D^{\gamma}_{\rho,\alpha,\omega}u(x_i,t_k) = \tau^{-\alpha}\sum_{j=0}^{k} p_{k-j}^r u_i^j + \mathcal{O}(\tau^{r+1-\alpha}). \tag{3.15}$$

By omitting the truncation error terms in (3.13), (3.14) and (3.15) and replacing the analytical solution with numerical one, we get the finite difference scheme for the numerical solution of (3.12) as

$$\tau^{-\alpha}\sum_{j=0}^{k} p^r_{k-j}U_i^j = K\frac{U^k_{i+1}-2U^k_i+U^k_{i-1}}{h^2} - V\frac{U^k_{i+1}-U^k_{i-1}}{2h} + F^k_i,$$

which again can be written as

$$\left(K-\frac{Vh}{2}\right)U^k_{i+1} + \left(-2K-h^2\tau^{-\alpha}p^r_0\right)U^k_i + \left(K+\frac{Vh}{2}\right)U^k_{i-1} + h^2F^k_i$$
$$= h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p^r_{k-j}U^j_i, \tag{3.16}$$

where $1 \le i \le N-1$ and $1 \le k \le M$. Also from (3.12),

$$U^0_i = u_0(x_i), \quad 0 \le i \le N, \tag{3.17}$$

$$\begin{cases} U^k_0 = \eta_1(t_k), \\ U^k_N = \eta_2(t_k), \quad 1 \le k \le M. \end{cases} \tag{3.18}$$

Let $h^2\tau^{-\alpha} = \mu$. Then,

$$\begin{cases} \left(-K - \frac{Vh}{2}\right) & U_{i-1}^{1} + \left(2K + \mu p_0^r\right) U_i^1 + \left(-K + \frac{Vh}{2}\right) U_{i+1}^{1} \\ & = -\mu p_1^r U_i^0 + h^2 F_i^1, \qquad k = 1, \\ \vdots & \\ \left(-K - \frac{Vh}{2}\right) & U_{i-1}^{r-1} + \left(2K + \mu p_0^r\right) U_i^{r-1} + \left(-K + \frac{Vh}{2}\right) U_{i+1}^{r-1} \\ & = -\mu \sum_{j=0}^{r-2} p_{k-j}^r U_i^j + h^2 F_i^{r-1}, \qquad k = r-1, \\ \left(-K - \frac{Vh}{2}\right) & U_{i-1}^{k} + \left(2K + \mu p_0^r\right) U_i^k + \left(-K + \frac{Vh}{2}\right) U_{i+1}^{k} \\ & = -\mu \sum_{j=0}^{k-1} p_{k-j}^r U_i^j + h^2 F_i^k, \qquad k \geq r. \end{cases} \tag{3.19}$$

Eq. (3.19) can be written in matrix form as

$$\begin{cases} AU^1 = -\mu P_1^r U^0 + h^2 F^1 + B^1, & k = 1, \\ \vdots & \\ AU^{r-1} = -\mu P_{r-1}^r U^{r-2} + h^2 F^{r-1} + B^{r-1}, & k = r-1, \\ AU^k = -\mu P_k^r U^{k-1} + h^2 F^k + B^k, & k \geq r. \end{cases} \tag{3.20}$$

The matrix and the vectors in the (3.20) are given as

$$\begin{aligned} A &= \text{tri}\left[\left(-K - \tfrac{Vh}{2}\right) \quad \left(2K + \mu p_0^r\right) \quad \left(-K + \tfrac{Vh}{2}\right)\right], \\ U^k &= \left[U_1^k, \cdots, U_{n-1}^k\right], \\ P_k^r &= \left[p_k^r, \ldots, p_1^r\right]^T, \\ F^k &= \left[F_1^k, F_2^k, \ldots, F_{N-1}^k\right], \\ B^k &= \left[\left(K + \tfrac{Vh}{2}\right) U_0^k, \ldots, \left(K - \tfrac{Vh}{2}\right) U_N^k\right], \qquad 1 \leq k \leq M. \end{aligned}$$

3.3.1 Stability Analysis

Without loss of generality, we study the stability analysis of the finite difference scheme (3.20) for $r = 4$, using von Neumann stability analysis. For other values of $4 \geq r \in \mathbb{N}$, this study follows similarly. Let us define

$$\phi_i^k = u_i^k - U_i^k, \ i = 1, 2, \ldots, N-1, \ k = 1, 2, \ldots, M,$$

with the corresponding vector

$$\phi^k = \left[\phi_1^k, \phi_2^k, \ldots, \phi_{N-1}^k\right]^T.$$

The error equations are obtained as

$$\begin{cases} \left(-K - \frac{Vh}{2}\right)\phi_{i-1}^1 + (2K + \mu p_0^r)\,\phi_i^1 + \left(-K + \frac{Vh}{2}\right)\phi_{i+1}^1 = -\mu p_1^r \phi_i^0, \ k = 1, \\ \vdots \\ \left(-K - \frac{Vh}{2}\right)\phi_{i-1}^{r-1} + (2K + \mu p_0^r)\,\phi_i^{r-1} + \left(-K + \frac{Vh}{2}\right)\phi_{i+1}^{r-1} = -\mu \sum_{j=0}^{r-2} p_{k-j}^r \phi_i^j, \ k = r-1, \\ \left(-K - \frac{Vh}{2}\right)\phi_{i-1}^k + (2K + \mu p_0^r)\,\phi_i^k + \left(-K + \frac{Vh}{2}\right)\phi_{i+1}^k = -\mu \sum_{j=0}^{k-1} p_{k-j}^r \phi_i^j, \ k \geq r. \end{cases} \tag{3.21}$$

To check the stability using von Neumann method, let us assume $\phi_i^k = d_k e^{I\sigma i h}$, where σ is the wave number and $I = \sqrt{-1}$. From Eq. (3.21) we have,

$$\begin{cases} d_1 = \frac{-\mu p_1^r d_0}{4K\sin^2\left(\frac{\sigma h}{2}\right) + IVh\sin(\sigma h) + \mu p_0^r}, \ k = 1, \\ \vdots \\ d_{r-1} = \frac{-\mu \sum_{j=0}^{r-2} p_{k-j}^r d_j}{4K\sin^2\left(\frac{\sigma h}{2}\right) + IVh\sin(\sigma h) + \mu p_0^r}, \ k = r-1, \\ d_k = \frac{-\mu \sum_{j=0}^{k-1} p_{k-j}^r d_j}{4K\sin^2\left(\frac{\sigma h}{2}\right) + IVh\sin(\sigma h) + \mu p_0^r}, \ k \geq r. \end{cases} \tag{3.22}$$

Now we use the idea of mathematical induction to prove that $|d_k| \leq |d_0|$ for all k. Observe that

$$\left|4K\sin^2\left(\frac{\sigma h}{2}\right) + IVh\sin(\sigma h) + \mu p_0^r\right| = \sqrt{\left(4K\sin^2\left(\frac{\sigma h}{2}\right) + \mu p_0^r\right)^2 + V^2h^2\sin^2(\sigma h)}, \\ \geq \sqrt{\mu^2\left(p_0^r\right)^2} = \mu p_0^r.$$

Now, for $k = 1$,

$$|d_1| = \left|\frac{-\mu p_1^r d_0}{4K\sin^2\left(\frac{\sigma h}{2}\right) + IVh\sin(\sigma h) + \mu p_0^r}\right| \leq \left|\frac{-\mu p_1^r d_0}{\mu p_0^r}\right|$$

by property 1 of Lemma 3.2.1, $|d_1| \leq |d_0|$. Let us suppose that $\left|d_j\right| \leq |d_0|$ for $2 \leq j \leq k-1$. Hence from (3.22) we have

$$\begin{aligned} |d_k| &= \left|\frac{-\mu}{4K\sin^2\left(\frac{\sigma h}{2}\right) + IVh\sin(\sigma h) + \mu p_0^r} \sum_{j=0}^{k-1} p_{k-j}^r d_j\right| \\ &\leq \left|\frac{-\mu d_0}{4K\sin^2\left(\frac{\sigma h}{2}\right) + IVh\sin(\sigma h) + \mu p_0^r} \sum_{j=1}^{k} p_j^r\right| \end{aligned}$$

by property 2 of Lemma 3.2.1,

$$|d_k| \leq \frac{\mu|d_0|}{4K\sin^2\left(\frac{\sigma h}{2}\right) + IVh\sin(\sigma h) + \mu p_0^r}\sum_{j=1}^{k}\left|p_j^r\right|,$$
$$\leq \frac{\mu p_0^r|d_0|}{4K\sin^2\left(\frac{\sigma h}{2}\right) + IVh\sin(\sigma h) + \mu p_0^r} \leq \frac{\mu p_0^r|d_0|}{\mu p_0^r} = |d_0|,$$

which establishes that the finite difference scheme (3.20) is stable.

3.3.2 Uniqueness and Existence

Here we discuss the uniqueness and existence of the solution of the finite difference scheme (3.20).

Lemma 3.3.1. The coefficient matrix A in (3.20) is invertible.

Proof. Without loss of generality, we will prove this for $r = 4$, and for other values of $4 \leq r \in \mathbb{N}$ the proof follows in a similar way. A tridiagonal matrix of the form $\text{tri}\begin{bmatrix} z & x & y \end{bmatrix}$ has eigenvalues [98, pg.154] given as,

$$\lambda_i = x + 2y\left(\frac{z}{y}\right)^{1/2}\cos\left(\frac{i\pi}{N}\right), \; i = 1, 2, \cdots, N-1. \tag{3.23}$$

The coefficient matrix A of the finite difference scheme is

$$A = \text{tri}\begin{bmatrix} -K - \frac{Vh}{2} & 2K + \mu p_0^r & -K + \frac{Vh}{2} \end{bmatrix}.$$

By (3.23) eigenvalues of A will be

$$\lambda_i = 2K + \mu p_0^r + 2\sqrt{K^2 - \frac{V^2h^2}{4}}\cos\left(\frac{i\pi}{N}\right), \quad i = 1, 2, \cdots, N-1.$$

Case(1.) If $K^2 - \frac{V^2h^2}{4} \leq 0$, then eigenvalues of A will be of the form $\lambda_i = \Upsilon_1 + I\Upsilon_2$, where, $\Upsilon_1 = 2K + \mu p_0^r$ and $I^2 = -1$. $K > 0$ and $\mu = h^2\tau^{-\alpha} > 0$ and $p_0^r = W_{0,0}^r > 0$ if $\omega > 0$, so $\Upsilon_1 > 0$ if $\omega > 0$. So $\lambda_i \neq 0$ if $\omega > 0$.

Case(2.) If $K^2 - \frac{V^2h^2}{4} > 0$,
$\lambda_i = 2K + \mu p_0^r + 2\sqrt{K^2 - \frac{V^2h^2}{4}} \cos\left(\frac{i\pi}{N}\right) \geq 2K + \mu p_0^r + 2K > 0$, if $\omega > 0$. So, $\lambda_i \neq 0$ if $\omega > 0$.

In both the cases eigenvalues of A are non zero, so A is invertible. □

Theorem 3.3.1. There exists a unique solution of the given schemes for all values of r.

Proof. To solve the finite difference scheme (3.20) at t_k we need to solve the system of linear equations with coefficient matrix A. Lemma 3.3.1 shows that the matrix A is invertible so there always exist a unique solution of corresponding system of linear equations and hence solution of (3.20) always exists and is unique. □

3.3.3 Convergence Analysis

We will study the convergence analysis of the numerical method for $r = 4$, and for other values of r the proof follows similarly. From (3.20), the numerical solution of the problem is obtained as

$$AU^k = -\mu P_k^r U^{k-1} + h^2 F^k + B^k + O(h^2, \tau^{r+1-\alpha}). \tag{3.24}$$

Let u^k be the exact solution so

$$Au^k = -\mu P_k^r u^{k-1} + h^2 F^k + B^k. \tag{3.25}$$

So error equation will be,

$$\begin{aligned} A(U^k - u^k) &= -\mu P_k^r (U^{k-1} - u^{k-1}) + O(h^2, \tau^{r+1-\alpha}) \\ A\epsilon^k &= -\mu P_k^r \epsilon^{k-1} + O(h^2, \tau^{r+1-\alpha}) \\ \epsilon^k &= -\mu A^{-1} P_k^r \epsilon^{k-1} + O(h^2, \tau^{r+1-\alpha}) A^{-1}. \end{aligned}$$

Let $O(h^2, \tau^{r+1-\alpha})A^{-1} = b$ so

$$\epsilon^k = -\mu A^{-1} P_k^r \epsilon^{k-1} + b. \tag{3.26}$$

Since $\epsilon^0 = 0$, so

$$\begin{aligned} &\epsilon^1 = b \\ &\epsilon^2 = (-\mu A^{-1}) P_2^r \epsilon^1 + b = ((-\mu A^{-1}) P_2^r + I) b \\ &\epsilon^3 = (-\mu A^{-1}) P_3^r \epsilon^2 + b = ((-\mu A^{-1})^2 P_2^r P_3^r + (-\mu A^{-1}) P_3^r + I) b \\ &\vdots \\ &\epsilon^k = ((-\mu A^{-1})^{k-1} P_k^r P_{k-1}^r \cdots P_2^r + (-\mu A^{-1})^{k-2} P_k^r \cdots P_3^r + \cdots + (-\mu A^{-1}) P_k^r + I) b. \end{aligned}$$

So,

$$\begin{aligned} \left\|\epsilon^k\right\| \leq \Big(& \left|-\mu^{k-1}\right| \left\|\left(A^{-1}\right)^{k-1}\right\| \|P_k^r\| \left\|P_{k-1}^r\right\| \cdots \|P_2^r\| \\ & + \left|-\mu^{k-2}\right| \left\|\left(A^{-1}\right)^{k-2}\right\| \|P_k^r\| \left\|P_{k-1}^r\right\| \cdots \|P_3^r\| + \cdots \\ & + |-\mu| \left\|A^{-1}\right\| \|P_k^r\| + 1 \Big) \left\|A^{-1}\right\| O(h^2, \tau^{r+1-\alpha}). \end{aligned} \tag{3.27}$$

Now, matrix A is tridiagonal matrix given by,

$$A = \text{tri}\left[\left(-K - \tfrac{Vh}{2}\right) \quad (2K + \mu p_0^r) \quad \left(-K + \tfrac{Vh}{2}\right) \right],$$

which is strictly diagonally dominant under the assumption that $(K - \frac{Vh}{2}) > 0$, so

$$\|A^{-1}\| \leq \frac{1}{\min\limits_{i \in N}\{|a_{ii}| - R_i(A)\}},$$

where $R_i(A)$ is the absolute sum of elements of the ith-row except the diagonal entry of matrix A [102]. For the matrix A, $\min\limits_{i \in N}\{|a_{ii}| - R_i(A)\} = \mu p_0^r = C'$, so

$$\|A^{-1}\| \leq \frac{1}{C'} = C. \tag{3.28}$$

Now, $P_k^r = [p_k^r \; p_{k-1}^r \; \cdots \; p_1^r \; p_o^r]$ so $\|P_k^r\| = \max\limits_i \{p_i^r\}$. Since each p_i^r is an infinite series or sum of infinite series and every such infinite series is convergent so

$$\|P_k^r\| = C_k. \tag{3.29}$$

From (3.27), (3.28) and (3.29), we have,

$$\left\|\epsilon^k\right\| \leq C\mathcal{O}(h^2, \tau^{r+1-\alpha}).$$

So the given scheme converges conditionally.

3.3.4 Numerical Experiments

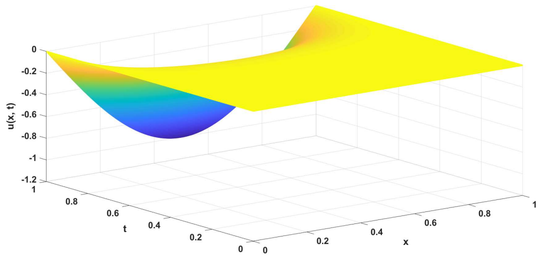
Here, we present a numerical example to validate the numerical scheme (3.20) for values of $r = 4, 5$. For numerical computations we have used formulas (2.40), (2.41) and (2.42).

Example 3.3.1. Let us consider (3.12) in the domain $[0,1] \times [0,1]$, with, $u(x,0) = 0$ and, $u(0,t) = u(1,t) = 0$. $F(x,t) = 720\cos\big(\pi x + \frac{\pi}{2}\big)t^{6-\alpha}E_{\rho,7-\alpha}^{-\gamma}(\omega t^\rho) + \pi^2 t^6 \cos\big(\pi x + \frac{\pi}{2}\big) -$

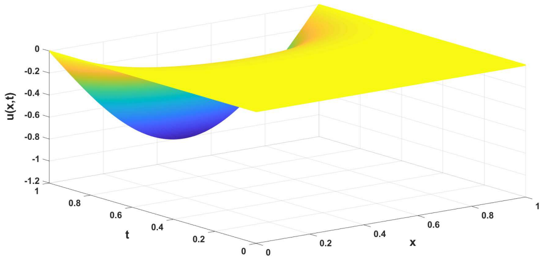
$\pi t^6 \sin\left(\pi x + \frac{\pi}{2}\right)$ is the source term and $u(x,t) = t^6 \cos\left(\pi x + \frac{\pi}{2}\right)$ is the exact solution. The convergence order is calculated for different values of α and h, in the spatial direction, with fixed temporal step size $\tau = 1/500$. The obtained results are presented through the Table 3.4 which shows that the convergence order in the spatial direction is $\mathcal{O}(h^2)$. Again we have calculated temporal convergence order for different values of τ and for fixed $h = 1/3000$. The results are shown in Table 3.5, which validates our theoretical finding of temporal convergence rate $\mathcal{O}(\tau^{r+1-\alpha})$. Fig. 3.1 gives a comparison between numerical solutions for $r = 4, 5$ and the analytical solution, for the step sizes $h = \tau = 1/500$ and $\alpha = 0.5$.

TABLE 3.4: MAE and CO for different h and α and fixed $1/\tau = 500$ for Ex. 3.3.1.

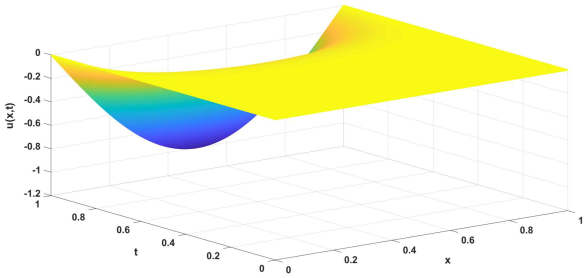
α	$\frac{1}{h}$	$r = 4$		$r = 5$	
		MAE	CO	MAE	CO
	10	7.17970E-03		7.17971E-03	
	20	1.80819E-03	1.989380393	1.80819E-03	1.989375017
$\alpha = 0.2$	40	4.51788E-04	2.000824231	4.51798E-04	2.000802433
	80	1.12935E-04	2.000156777	1.12944E-04	2.000068458
	160	2.82379E-05	1.999782727	2.82471E-05	1.999432898
	10	6.73107E-03		6.73108E-03	
	20	1.69931E-03	1.985890047	1.69932E-03	1.985881175
$\alpha = 0.4$	40	4.24623E-04	2.000692077	4.24637E-04	2.000656089
	80	1.06143E-04	2.000174473	1.06157E-04	2.000030529
	160	2.65348E-05	2.000049144	2.65489E-05	1.999473483
	10	6.18959E-03		6.18960E-03	
	20	1.56359E-03	1.984976000	1.56361E-03	1.984968852
$\alpha = 0.6$	40	3.90758E-04	2.000522538	3.90768E-04	2.000494328
	80	9.76807E-05	2.000129606	9.76909E-05	2.000016772
	160	2.44196E-05	2.000027891	2.44299E-05	1.999576680
	10	5.56161E-03		5.56160E-03	
	20	1.40059E-03	1.989462817	1.40059E-03	1.989471007
$\alpha = 0.8$	40	3.50073E-04	2.000312302	3.50063E-04	2.000344602
	80	8.75540E-05	1.999410558	8.75437E-05	1.999537879
	160	2.18883E-05	2.000009225	2.18780E-05	2.000520468



(a) Numerical solution when $r = 4$



(b) Numerical solution when $r = 5$



(c) Analytical solution

FIGURE 3.1: Numerical and analytical solutions for $\alpha = 0.5$ for Ex. 3.3.1.

TABLE 3.5: MAE and CO for $\alpha = 0.2$ and $1/h = 3000$ for Ex. 3.3.1.

$\frac{1}{\tau}$	$r = 4$		$r = 5$	
	MAE	CO	MAE	CO
10	1.91777E-05		3.31267E-03	
12	8.01857E-06	4.782686729	1.10886E-03	6.002685927
14	3.83332E-06	4.787715519	4.39555E-04	6.002746887
16	2.03015E-06	4.760094023	1.97197E-04	6.002799499
18	1.15433E-06	4.793431493	9.72386E-05	6.002845811

3.4 Application-2

In the present section, we apply the discussed high-order numerical method to solve following nonlinear time fractional reaction–diffusion equation,

$$\begin{cases} {}_0^{\mathrm{CP}}D^{\gamma}_{\rho,\alpha,\omega}u(x,t) = K\frac{\partial^2 u(x,t)}{\partial x^2} + f(u) + F(x,t), \qquad 0 < x < L,\ 0 < t < T, \\ u(x,0) = \varphi_0(x), \\ u(0,t) = 0, \\ u(L,t) = 0, \end{cases} \tag{3.30}$$

where, $K > 0$ is the diffusion coefficient and $f(u)$ is the reaction term satisfying the Lipschitz condition,

$$|f(u(x_1,t)) - f(u(x_2,t))| \leq L|u(x_1,t) - u(x_2,t)|,\ \forall x_1, x_2 \in [0, L],$$

with $L > 0$ as Lipschitz constant. $\varphi_0(x)$ and $F(x,t)$ are the sufficiently smooth known functions. Using (3.13), (3.14) and (5.26), at node point (x_i, t_k), we get the finite difference equation,

$$\tau^{-\alpha}\sum_{j=0}^{k} p^r_{k-j}u^j_i = \frac{K}{h^2}(u^k_{i+1} - 2u^k_i + u^k_{i-1}) + f(u^k_i) + F(x_i, t_k),$$

$$\begin{aligned} Ku^k_{i+1} + (-2K - h^2\tau^{-\alpha}p^r_0)u^k_i + Ku^k_{i-1} + h^2 f(u^k_i) \\ = h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p^r_{k-j}u^j_i - h^2F(x_i, t_k) + R^k_i, \end{aligned} \tag{3.31}$$

where $|R^k_i| \leq C(\tau^{r+1-\alpha}, h^2),\ 1 \leq i \leq N-1,\ r \leq k \leq N$, and $C > 0$ is a positive constant. Omitting the small terms R^n_i and replacing the analytical solution with the numerical one we get the following scheme,

$$
\begin{aligned}
KU_{i+1}^k + (-2K - h^2\tau^{-\alpha}p_0^r)U_i^k + KU_{i-1}^k + h^2 f(U_i^k) \\
= h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p_{k-j}^r u_i^j - h^2 F(x_i, t_k),
\end{aligned} \tag{3.32}
$$

which again can be written in the matrix form as,

$$
A^k U^k + h^2 I_{N-1} f(U^k) = h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p_{k-j}^r U^j - h^2 F^k, \tag{3.33}
$$

where $A^k = \text{diag}[K \ \ -2K - h^2\tau^{-\alpha}p_0^r \ \ K]$,

$U^k = [U_1^k, U_2^k, \cdots, U_{N-1}^k]^T$,

$f(U^k) = [f(U_1^k), f(U_2^k), \cdots, f(U_{N-1}^k)]^T$,

$F^k = [F_1^k, F_2^k, \cdots, F_{N-1}^k]^T$.

Now, we use the Newton–Raphson method for solving system of equation (3.33). To apply Newton–Raphson method, iterative form of (3.33) is obtained as,

$$
A^k U^{[k,s+1]} + h^2 I_{N-1} f(U^{[k,s+1]}) = h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p_{k-j}^r U^j - h^2 F^k. \tag{3.34}
$$

Using Newton's iterative method $f(U^{[k,s+1]})$ can be written as,

$$
f(U^{[k,s+1]}) = f(U^{[k,s]}) + (U^{[k,s+1]} - U^{[k,s]})f'(U^{[k,s]}). \tag{3.35}
$$

From (3.34) and (3.35) we get,

$$
\begin{aligned}
[A^k + h^2 I_{N-1} f'(U^{[k,s]})]U^{[k,s+1]} = h^2 I_{N-1}[U^{[k,s]} f'(U^{[k,s]}) \\
-f(U^{[k,s]})] + h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p_{k-j}^r U^j - h^2 F^k,
\end{aligned} \tag{3.36}
$$

where, $U^{[k,s]}$ is the value at kth time level of sth iteration.

3.4.1 Stability Analysis

Theorem 3.1. *The proposed numerical scheme* (3.32) *is stable for* $\alpha \in (0,\ 1)$.

Proof. Here, we prove that the given numerical scheme is stable using von Neumann stability analysis. Let $\hat{U}$ is the perturbed solution which is obtained by adding the perturbation term ϑ_i^k defined as $\tau_i^k = U_i^k - \hat{U}_i^k$. From Eq. (3.32) the perturbation term satisfies the following equation,

$$K\tau_{i+1}^k + (-2K - h^2\tau^{-\alpha}p_0^r)\tau_i^k + K\tau_{i-1}^k = h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p_{k-j}^r\tau_i^j - h^2(f(U_i^k) - f(\hat{U}_i^k)),$$

$$K\tau_{i+1}^k + (-2K - h^2\tau^{-\alpha}p_0^r + h^2L)\tau_i^k + K\tau_{i-1}^k \leq h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p_{k-j}^r\tau_i^j. \tag{3.37}$$

To check stability using von Neumann method let

$$\tau_i^k = \xi^k e^{I\omega ih}. \tag{3.38}$$

From (3.37) and (3.38) we have,

$$K\xi^k e^{I\omega(i+1)h} + (-2K - h^2\tau^{-\alpha}p_0^r + h^2L)\xi^k e^{I\omega ih} + K\xi^k e^{I\omega(i-1)h} \leq h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p_{k-j}^r\xi^j e^{I\omega ih},$$

$$\xi^k \leq \frac{h^2\tau^{-\alpha}}{-4K\sin^2(\frac{\omega h}{2}) - (h^2\tau^{-\alpha}p_0^r - h^2L)}\sum_{j=0}^{k-1} p_{k-j}^r\xi^j,$$

$$|\xi^k| \leq \frac{|h^2\tau^{-\alpha}|}{|4K\sin^2(\frac{\omega h}{2}) + (h^2\tau^{-\alpha}p_0^r - h^2L)|}\sum_{j=0}^{k-1} |p_{k-j}^r||\xi^j|.$$

$4K\sin^2(\frac{\omega h}{2}) - h^2L$ can be made positive by choosing appropriate values of $h,\ K,\ L$ from which we can conclude that,

$$\frac{1}{4K\sin^2(\frac{\omega h}{2}) - h^2L + h^2\tau^{-\alpha}p_0^r} \leq \frac{1}{h^2\tau^{-\alpha}p_0^r}. \tag{3.39}$$

So we have,

$$|\xi^k| \leq \frac{1}{p_0^r}\sum_{j=0}^{k-1}|p_{k-j}^r||\xi^j|. \tag{3.40}$$

Now we prove that $|\xi^k| \leq |\xi^0|$, for all k with the help of mathematical induction. For $k = 1$, $|\xi^1| \leq \frac{1}{|p_0^r|}|p_1^r||\xi^0|$. By property 1 of Lemma 3.2.1 we conclude that, $|\xi^1| \leq |\xi^0|$. Let us assume that $|\xi^j| \leq |\xi^0|$ for $j = 1, 2, \cdots, k-1$. Now consider,

$$\begin{aligned} |\xi^k| &\leq \frac{1}{p_0^r}\sum_{j=0}^{k-1}|p_{k-j}^r||\xi^j|, \\ &\leq \frac{|\xi^0|}{p_0^r}\sum_{j=0}^{k-1}|p_{k-j}^r|. \end{aligned} \tag{3.41}$$

by property 2 of Lemma 3.2.1, we see that

$$|\xi^k| \leq |\xi^0|,$$

from which we conclude that the perturbation term remains bounded by each progressing step in time direction and implies that the finite difference scheme is stable. □

Lemma 3.4.1. Eigenvalues of the matrix A^k are given as, $\lambda^i(A^k) = -4K\sin^2(\frac{i\pi}{N}) - h^2\tau^{-\alpha}p_0^r,\ i = 1, 2, \cdots, N-1$.

For the proof of Lemma 3.4.1 refer to [87].

3.4.2 Convergence Analysis

Theorem 3.2. *The finite difference scheme* (3.33) *has* $(r+1-\alpha)$ *order accuracy in temporal direction and* 2^{nd} *order accuracy in spatial direction, i.e.,*

$$\|U^k - u^k\|_2 \leq C(\tau^{r+1-\alpha}, h^2). \tag{3.42}$$

Proof. We use matrix analysis for proving the convergence of finite difference scheme (3.33) [87]. Let $E^k = U^k - u^k$, where u^k is the analytical solution and U^k is the numerical solution at kth time level. Subtracting (3.31) and (3.34) in their matrix form we obtain,

$$\begin{aligned} A^k(U^k - u^k) + h^2 I_{N-1}(f(U^k) - f(u^k)) =& h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p^r_{k-j}(U^j - u^j) + R^k, \\ (A^k + h^2 L I_{N-1})E^k \leq& h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p^r_{k-j}E^j + R^k, \end{aligned} \tag{3.43}$$

where $E^k = [E^k_1, E^k_2, \cdots, E^k_{N-1}]$, and $R^k = [R^k_1, R^k_2, \cdots, R^k_{N-1}]$. Taking inner product on both sides of (3.43) with E^k we get,

$$\langle A^k E^k, E^k\rangle + h^2 L\langle I_{N-1}E^k, E^k\rangle \leq h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p^r_{k-j}\langle E^j, E^k\rangle + \langle R^k, E^k\rangle. \tag{3.44}$$

The property of the Rayleigh–Ritz ratio is given as [103, Theorem 4.2.2],

$$\lambda_{\min}(A) \leq \frac{\langle Ax, x\rangle}{\langle x, x\rangle} \leq \lambda_{\max}(A), \tag{3.45}$$

where A is any symmetric matrix and $0 \neq x \in R^{M-1}$. $\lambda_{\min}(A)$ is the minimum eigenvalue and $\lambda_{\max}(A)$ is the maximum eigenvalue of the matrix A. So we have,

$$\langle A^k E^k, E^k\rangle \geq \lambda_{\min}(A^k)\|E^k\|^2,$$

$$\langle I_{N-1}E^k, E^k\rangle \geq \lambda_{\min}(A^k)\|E^k\|^2 \geq \|E^k\|^2,$$

$$\langle E^j, E^k\rangle \leq \|E^j\|\|E^k\|, \ \langle R^k, E^k\rangle \leq \|R^k\|\|E^k\|.$$

From Eq. (3.44) we have,

$$(\lambda_{\min}(A^k) + h^2 L)\|E^k\| \leq h^2\tau^{-\alpha}\sum_{j=0}^{k-1} p^r_{k-j}\|E^j\| + \|R^k\|.$$

Using Lemma 3.4.1 we see that, $\lambda_{\min}(A^k) = -h^2\tau^{-\alpha}p^r_0$. So we have,

$$\begin{aligned}
\|E^k\| &\leq C\frac{1}{h^2L - h^2\tau^{-\alpha}p^r_0}\sum_{j=0}^{k-1} h^2\tau^{-\alpha}p^r_{k-j}\|E^j\| + \|R^k\|,\\
&\leq C\frac{1}{h^2L - h^2\tau^{-\alpha}p^r_0}\exp\left(\frac{h^2\tau^{-\alpha}}{h^2L - h^2\tau^{-\alpha}p^r_0}\sum_{j=0}^{k-1} p^r_{k-j}\right)\|R^k\|,\\
&= C\frac{1}{h^2L - h^2\tau^{-\alpha}p^r_0}\exp\left(\frac{p^r_0}{p^r_0 - L\tau^{-\alpha}}\right)(\tau^{r+1-\alpha}, h^2),\\
&= C'(\tau^{r+1-\alpha}, h^2),
\end{aligned}$$

where, $C' = \frac{C}{h^2L - h^2\tau^{-\alpha}p^r_0}\exp\left(\frac{p^r_0}{p^r_0 - L\tau^{-\alpha}}\right)$. The proof is completed. □

3.4.3 Numerical Experiments

Here, we discuss one numerical example for $r = 4,\ 5$. Numerical experimentation is performed using the formulas (2.40), (2.41) and (2.42).

Example 3.4.1. Consider the time fractional reaction–diffusion equation

$$ {}_{0}^{\mathrm{CP}}D^{\gamma}_{\rho,\alpha,\omega}u(x,t) = u_{xx} + u(1-u^2) + F(x,t),\ 0<x<1,\ 0<t<1, $$

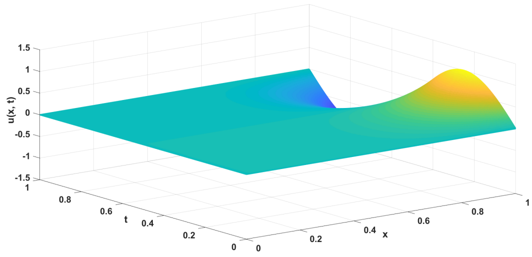
with initial and boundary conditions $u(x,0)=0$, $u(0,t)=u(1,t)=0$. The source term is $F(x,t) = 720\sin(2\pi x)t^{6-\alpha}E^{-\gamma}_{\rho,7-\alpha}(\omega t^{\rho}) + t^6\sin(2\pi x)(4\pi^2 - 1 + (t^6\sin(2\pi x))^2)$. Here, the Lipschitz constant for the reaction term is 4. The maximum absolute error and convergence order are calculated with the help of the scheme (3.36) with tolerance 10^{-8}. The spatial convergence order for $r=4,5$ is shown in Table 3.6 and Table 3.7 respectively for fixed $\tau = 1/100$, and the temporal convergence order is shown through Table 3.8 for fixed $h = 1/15000$. Fig. 3.2 gives a comparison between numerical solutions for $r=4,5$ and analytical solution. The obtained results validate the theoretically claimed convergence order.

Table 3.6: MAE and CO for different h, α and fixed $\tau = 1/100$, $r = 4$ for Ex. 3.4.1.

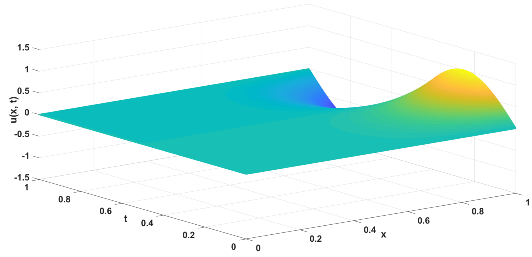
α	N	MAE	CO	TIS	CPU
	10	2.95120e-02		242	27.48
	20	7.66252E-03	1.945411810	242	40.75
0.2	40	1.91020E-03	2.004093662	242	42.79
	80	4.77212E-04	2.001025513	242	42.53
	160	1.19282E-04	2.000255526	242	40.46
	10	2.90044E-02		242	39.40
	20	7.53299E-03	1.944974253	242	42.75
0.4	40	1.87805E-03	2.003986013	242	84.96
	80	4.69188E-04	2.000997471	242	67.32
	160	1.17277E-04	2.000244102	242	76.12
	10	2.83264E-02		241	89.51
	20	7.35981E-03	1.944406392	241	93.77
0.6	40	1.83505E-03	2.003846132	241	99.32
	80	4.58459E-04	2.000957961	241	82.17
	160	1.14598E-04	2.000216307	241	61.39
	10	2.74297E-02		239	26.97
	20	7.13057E-03	1.943650436	239	27.40
0.8	40	1.77812E-03	2.003658330	239	38.51
	80	4.44257E-04	2.000893353	239	40.67
	160	1.11054E-04	2.000129927	239	43.80

TABLE 3.7: MAE and CO for different h, α and fixed $\tau = 1/100$, $r = 5$ for Ex. 3.4.1.

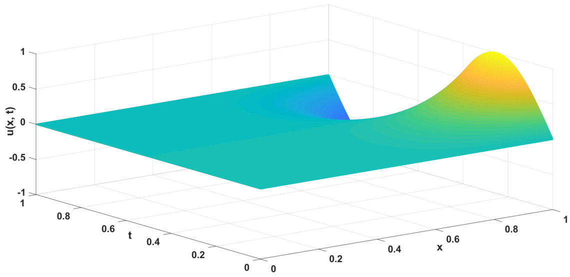
α	N	MAE	CO	TIS	CPU
	10	2.95120E-02		242	127.31
	20	7.66252E-03	1.945411827	242	135.08
0.2	40	1.91020E-03	2.004093727	242	138.27
	80	4.77211E-04	2.001025773	242	134.98
	160	1.19282E-04	2.000256568	242	136.79
	10	2.90043E-02		242	133.95
	20	7.53299E-03	1.944974342	242	115.89
0.4	40	1.87805E-03	2.003986369	242	117.93
	80	4.69188E-04	2.000998896	242	118.78
	160	1.17276E-04	2.000249802	242	115.89
	10	2.83263E-02		241	161.76
	20	7.35981E-03	1.944406780	241	130.55
0.6	40	1.83505E-03	2.003847677	240	133.28
	80	4.58456E-04	2.000964136	240	130.52
	160	1.14594E-04	2.000241007	240	130.15
	10	2.74297E-02		238	153.92
	20	7.13056E-03	1.943651993	239	133.30
0.8	40	1.77811E-03	2.003664517	238	133.69
	80	4.44247E-04	2.000918090	238	130.46
	160	1.11044E-04	2.000228867	238	135.06



(a) Numerical solution when $r = 4$



(b) Numerical solution when $r = 5$



(c) Analytical solution

FIGURE 3.2: Numerical and analytical solutions for $\alpha = 0.5$ for Ex. 3.4.1.

TABLE 3.8: MAE and CO for different $M = 1/\tau$, with $\alpha = 0.2$, $h = 1/15000$ and $r = 4,\ 5$ for Ex. 3.4.1.

α	N	MAE	CO	TIS
	10	3.35065E-03		28
	20	5.23193E-05	6.000955227	53
$r = 4$	40	8.16878E-07	6.001078697	101
	80	1.41548E-08	5.850757996	194
	160	2.39396Ee-10	5.885746445	381
	10	5.17531E-06		28
	20	2.32392E-07	4.477014592	53
$r = 5$	40	1.01248E-08	4.520598741	102
	80	4.20470E-10	4.589740319	195
	160	1.42673E-11	4.881218922	381

3.5 Conclusions

An $(r + 1 - \alpha)$th-order accurate numerical scheme for approximating the Caputo–Prabhakar derivative of order $\alpha \in (0, 1)$ is developed, using a time stepping interpolation polynomial of degree r. Later on, this developed scheme is combined with the central difference scheme for space discretization to solve a time fractional advection–diffusion equation and time fractional reaction–diffusion equation with nonlinear reaction term. The nonlinear reaction term is approximated using the Newton–Raphson iterative algorithm. Stability, solvability, and convergence analysis of the whole discretized scheme are studied rigorously. The delivered numerical results confirmed that analytically discussed convergence rates are achieved. Both the advection–diffusion equations and reaction–diffusion equations considered are assumed to have smooth solutions, however, Caputo–Prabhakar time fractional partial differential equations with nonsmooth solution will be the scope of our future study. The discussed high-order scheme can be applied to solve other linear and nonlinear fractional models involving the Caputo–Prabhakar derivative.

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