Chapter 3

Numerical approximations of Caputo-Prabhakar fractional derivative and their application [2]

In 1973, Prabhakar [88] provided a generalization of the Mittag-Leffler function to three parameters known as the generalized Mittag-Leffler function. Moreover, following his name, it is recognized as the “Prabhakar function”. The fractional Caputo (or Riemann-Liouville) derivative and Riemann-Liouville integral to the Prabhakar fractional derivatives and integrals were generalized by Kilbas et al. [55], Garra et al. [31], and Prabhakar [88] using the Prabhakar function as a kernel. The theoretical aspects of these operators have been studied in many articles. However, due to the presence of more parameters in the Prabhakar operator, existing numerical schemes may not be useful to solve fractional differential equations defined in the Prabhakar sense.

Therefore, the objective of this chapter is threefold: firstly, to develop two new numerical formulas for approximating Caputo-Prabhakar derivatives; secondly, to apply these formulas in solving reaction-diffusion problems with variable coefficients in the Caputo-Prabhakar sense, employing compact difference operators for spatial discretization; and lastly, to establish detailed theoretical analyses for the developed schemes.

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Organization of the chapter: In Section 3.1, CPL2-1_σ and CPL-2 formulas are developed, and their basic features are discussed. In Section 3.2, two high-order fully discrete numerical schemes, CFD_1 and CFD_2, have been developed to solve the fractional reaction-diffusion problem defined in the Caputo-Prabhakar sense. Stability and convergence analysis of both schemes have been established separately in Section 3.3. Further, the numerical results of the developed numerical methods are discussed in Section 3.4 with the help of three test problems. Finally, Section 3.5 concludes the chapter.

3.1 New numerical discretizations of the Caputo-Prabhakar derivative

In what follows we consider $\alpha \in (0,1)$. Therefore, Definition 1.2.1.2.3 simplifies to

$$ {}^{CP}_{t_0}D^{\eta}_{\beta,\alpha,\kappa} f(t) = \int_0^t (t-s)^{-\alpha} E^{-\eta}_{\beta,1-\alpha}\{\kappa(t-s)^{\beta}\} f'(s)ds. \tag{3.1} $$

We shall present two novel approximations of orders $(2-\alpha)$ and $(3-\alpha)$ of the Caputo-Prabhakar fractional derivative given in (3.1), where $0 < \alpha < 1$ denotes the order of fractional derivative. Let N_t be an positive integer. We divide the interval $[0,T]$ into N_t subintervals with uniform partition $\Omega_t : 0 = t_0 < t_1 < \cdots < t_{N_t} = T$, where $t_n = n\Delta t$, for $0 \le n \le N_t$ with $\Delta t = \frac{T}{N_t}$.

3.1.1 CPL2-1_σ formula

Let $\sigma = 1 - \frac{\alpha}{2}$. We approximate the Caputo-Prabhakar derivative of the function $f(t) \in C^3[0,T]$ at the points $t_{n+\sigma}$ given in equation (3.1). Here, $t_{n+\sigma} = (n+\sigma)\Delta t$

for $0 \leq n \leq N_t - 1$. Now, CPL2-1_σ formula can be obtained in the following manner

$$\begin{aligned}{}_{0}^{CP}D^{\eta}_{\beta,\alpha,\kappa}f(t_{n+\sigma}) &= \int_0^{t_{n+\sigma}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^\beta\}}{(t_{n+\sigma}-s)^\alpha} f'(s)ds \\ &= \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^\beta\}}{(t_{n+\sigma}-s)^\alpha} f'(s)ds \\ &\quad + \int_{t_n}^{t_{n+\sigma}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^\beta\}}{(t_{n+\sigma}-s)^\alpha} f'(s)ds. \end{aligned} \tag{3.2}$$

For each $t \in [t_j, t_{j+1}]$, $(0 \leq j \leq n-1)$, we approximate the function $f(t)$ using its quadratic interpolation $P_{2,j}f(t)$ over three points $(t_j, f(t_j))$, $(t_{j+1}, f(t_{j+1}))$, and $(t_{j+2}, f(t_{j+2}))$ given by

$$f(t) \approx P_{2,j}f(t) = \sum_{i=0}^{2} \prod_{\substack{l=0 \\ l\neq i}}^{2} \frac{t - t_{j+l}}{(i-l)\Delta t^2} f(t_{j+i}). \tag{3.3}$$

Also, we have

$$f(t) - P_{2,j}f(t) = \frac{f'''(\xi_j)}{6}(t-t_j)(t-t_{j+1})(t-t_{j+2}), \tag{3.4}$$

where $\xi_j \in (t_j, t_{j+2})$. Moving forward, within the interval $[t_n, t_{n+\sigma}]$, we adopt the linear interpolation $P_{1,n}f(t)$ to provide an approximation for the function $f(t)$ based on the data points $(t_n, f(t_n))$ and $(t_{n+1}, f(t_{n+1}))$, yielding the subsequent representation

$$f(t) \approx P_{1,n}f(t) = \frac{t-t_n}{t_{n+1}-t_n} f(t_{n+1}) + \frac{t-t_{n+1}}{t_n - t_{n+1}} f(t_n) = \frac{t-t_n}{\Delta t} f(t_{n+1}) - \frac{t-t_{n+1}}{\Delta t} f(t_n). \tag{3.5}$$

The interpolating polynomials $P_{1,n}f(t)$ and $P_{2,j}f(t)$, defined in equations (3.5) and (3.3), respectively, yield the following expressions for their respective first-order derivatives

$$(P_{1,n}f(t))' = \delta t f\left(t_{n+1/2}\right), \tag{3.6}$$

$$(P_{2,j}f(t))' = \left(\frac{2t-2t_j-\Delta t}{2}\right)\delta t^2 f(t_{j+1}) + \delta t f\left(t_{j+1/2}\right), \tag{3.7}$$

where

$$\delta t f\left(t_{n+1/2}\right) = \frac{f(t_{n+1})-f(t_n)}{\Delta t}, \tag{3.8}$$

$$\delta t^2 f\left(t_j\right) = \frac{\delta t f\left(t_{j+1/2}\right)-\delta t f\left(t_{j-1/2}\right)}{\Delta t} = \frac{f(t_{j+1})-2f(t_j)+f(t_{j-1})}{\Delta t^2}. \tag{3.9}$$

In equation (3.2), we approximate $f'(s)$ by utilizing the derivatives of $P_{2,j}f(t)$ and $P_{1,n}f(t)$ within their respective intervals to get

$$\begin{aligned}
{}^{CP}_{\ 0}D^{\eta}_{\beta,\alpha,\kappa}f(t_{n+\sigma}) \approx & \sum_{j=0}^{n-1}\int_{t_j}^{t_{j+1}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^{\beta}\}}{(t_{n+\sigma}-s)^{\alpha}}\,(P_{2,j}f(s))'\,ds \\
& + \int_{t_n}^{t_{n+\sigma}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^{\beta}\}}{(t_{n+\sigma}-s)^{\alpha}}\,(P_{1,n}f(s))'\,ds \\
= & \sum_{j=0}^{n-1}\int_{t_j}^{t_{j+1}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^{\beta}\}}{(t_{n+\sigma}-s)^{\alpha}}\left[\frac{(2s-2t_j-\Delta t)}{2}\delta t^2 f(t_{j+1})\right. \\
& \left. + \delta t f\left(t_{j+1/2}\right)\right]ds + \int_{t_n}^{t_{n+\sigma}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^{\beta}\}}{(t_{n+\sigma}-s)^{\alpha}}\delta t f\left(t_{n+1/2}\right)ds.
\end{aligned}$$

Moreover, by simplifying further, we get

$$\begin{aligned}
{}^{CP}_{\ 0}D^{\eta}_{\beta,\alpha,\kappa}f(t_{n+\sigma}) \approx & \sum_{j=0}^{n-1}\left[\delta t^2 f(t_{j+1})\int_{t_j}^{t_{j+1}} \frac{(2s-2t_j-\Delta t)E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^{\beta}\}}{2(t_{n+\sigma}-s)^{\alpha}}ds\right. \\
& \left. + \delta t f\left(t_{j+1/2}\right)\int_{t_j}^{t_{j+1}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^{\beta}\}}{(t_{n+\sigma}-s)^{\alpha}}ds\right] \\
& + \delta t f\left(t_{n+1/2}\right)\int_{t_n}^{t_{n+\sigma}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^{\beta}\}}{(t_{n+\sigma}-s)^{\alpha}}ds \\
= & \Delta t^{2-\alpha}\sum_{j=0}^{n-1} r_{n-j}\delta t^2 f(t_{j+1}) + \Delta t^{1-\alpha}\sum_{j=0}^{n-1} d_{n-j}\delta t f\left(t_{j+1/2}\right) \\
& + (\sigma\Delta t)^{1-\alpha}{}_2E_{\sigma}\delta t f\left(t_{n+1/2}\right),
\end{aligned}$$

where

$$r_j = \left\{(j+\sigma)^{2-\alpha}{}_3E_{j+\sigma} - (j-1+\sigma)^{2-\alpha}{}_3E_{j-1+\sigma}\right\} \\ - \frac{1}{2}\left\{(j+\sigma)^{1-\alpha}{}_2E_{j+\sigma} + (j-1+\sigma)^{1-\alpha}{}_2E_{j-1+\sigma}\right\}, \;\; j \geq 1, \tag{3.10}$$

$$d_j = \left\{(j+\sigma)^{1-\alpha}{}_2E_{j+\sigma} - (j-1+\sigma)^{1-\alpha}{}_2E_{j-1+\sigma}\right\}, \;\; j \geq 1, \tag{3.11}$$

where

$${}_2E_j = E^{-\eta}_{\beta,2-\alpha}\left(\kappa(j\Delta t)^{\beta}\right), \;\text{ and }\; {}_3E_j = E^{-\eta}_{\beta,3-\alpha}\left(\kappa(j\Delta t)^{\beta}\right). \tag{3.12}$$

Thus, we have

$$\begin{aligned} {}^{CP}_{\;\;0}D^{\eta}_{\beta,\alpha,\kappa}f(t_{n+\sigma}) \approx & \Delta t^{1-\alpha}\sum_{j=0}^{n} w_{n-j}\delta t f\left(t_{j+1/2}\right) \\ =&\Delta t^{-\alpha}\left[w_0 f(t_{n+1}) - \sum_{j=1}^{n}(w_{n-j} - w_{n-j+1})f(t_j) - w_n f(t_0)\right], \end{aligned} \tag{3.13}$$

where

$$w_0 = d_0 = \sigma^{1-\alpha}{}_2E_{\sigma}, \;\text{ for }\; n=0, \;\text{ and}$$

$$\text{for } n \;\; \geq 1, \;\; w_j = \begin{cases} d_0 + r_1, & j=0, \\ d_j + r_{j+1} - r_j, & 1 \leq j \leq n-1, \\ d_n - r_n, & j = n. \end{cases} \tag{3.14}$$

The approximation (3.13) is the CPL2-1_σ formula for the Caputo-Prabhakar derivative. The following result shows that the accuracy of the CPL2-1_σ formula is of order $2-\alpha$.

Theorem 3.1. *If $f(t) \in C^3[0,T]$, then for any fractional order $\alpha \in (0,1)$ and $\sigma = 1 - \frac{\alpha}{2}$, we have*

$$ {}^{CP}_{0}D^{\eta}_{\beta,\alpha,\kappa} f(t_{n+\sigma}) = \Delta t^{-\alpha} \left[w_0 f(t_{n+1}) - \sum_{j=1}^{n} (w_{n-j} - w_{n-j+1}) f(t_j) - w_n f(t_0) \right] + \mathcal{O}\left(\Delta t^{2-\alpha}\right). $$

Proof. Recall that in deriving the CPL2-1_σ formula (3.13), we have approximated $f'(s)$ by $(P_{2,j}f(s))'$ and $(P_{1,n}f(s))'$ in their respective intervals. So, here it is evident that

$$ {}^{CP}_{0}D^{\eta}_{\beta,\alpha,\kappa} f(t_{n+\sigma}) - \Delta t^{-\alpha} \left[w_0 f(t_{n+1}) - \sum_{j=1}^{n} (w_{n-j} - w_{n-j+1}) f(t_j) - w_n f(t_0) \right] = R_1 + R_2, $$

where

$$ R_1 = \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma} - s)^\beta\}}{(t_{n+\sigma} - s)^\alpha} \left[f'(s) - (P_{2,j} f(s))' \right] ds $$

and

$$ R_2 = \int_{t_n}^{t_{n+\sigma}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma} - s)^\beta\}}{(t_{n+\sigma} - s)^\alpha} \left[f'(s) - (P_{1,n} f(s))' \right] ds. $$

First, we will prove that $R_1 = \mathcal{O}(\Delta t^{3-\alpha})$. Integration by parts of R_1 provides

$$ \begin{aligned} R_1 = \sum_{j=0}^{n-1} \Bigg[& \left\{ (t_{n+\sigma} - s)^{-\alpha} E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma} - s)^\beta\} \left(f(s) - P_{2,j} f(s) \right) \right\}_{t_j}^{t_{j+1}} + \\ & \int_{t_j}^{t_{j+1}} (t_{n+\sigma} - s)^{-\alpha-1} E^{-\eta}_{\beta,-\alpha}\{\kappa(t_{n+\sigma} - s)^\beta\} \left(f(s) - P_{2,j} f(s) \right) ds \Bigg] \\ = \sum_{j=0}^{n-1} & \left[\int_{t_j}^{t_{j+1}} (t_{n+\sigma} - s)^{-\alpha-1} E^{-\eta}_{\beta,-\alpha}\{\kappa(t_{n+\sigma} - s)^\beta\} \left(f(s) - P_{2,j} f(s) \right) ds \right]. \end{aligned} $$

Further, using the relation (3.4) in above expression we get

$$\begin{aligned}|R_1| =&\left|\sum_{j=0}^{n-1}\int_{t_j}^{t_{j+1}}(t_{n+\sigma}-s)^{-\alpha-1}E_{\beta,-\alpha}^{-\eta}\{\kappa(t_{n+\sigma}-s)^{\beta}\}\frac{f'''(\xi_j)}{6}(s-t_j)(s-t_{j+1})\right.\\ &\left.(s-t_{j+2})ds\right|\\ =&\left|\frac{1}{6}\sum_{j=0}^{n-1}f'''(\xi_j)\int_{t_j}^{t_{j+1}}(s-t_j)(s-t_{j+1})(s-t_{j+2})(t_{n+\sigma}-s)^{-\alpha-1}\right.\\ &\left.E_{\beta,-\alpha}^{-\eta}\{\kappa(t_{n+\sigma}-s)^{\beta}\}ds\right|\\ \leq&\left|\frac{\Delta t^3}{3}\sum_{j=0}^{n-1}f'''(\xi_j)\int_{t_j}^{t_{j+1}}(t_{n+\sigma}-s)^{-\alpha-1}E_{\beta,-\alpha}^{-\eta}\{\kappa(t_{n+\sigma}-s)^{\beta}\}ds\right|.\end{aligned}$$

Equivalently,

$$\begin{aligned}|R_1| \leq&\left|\frac{\Delta t^{3-\alpha}}{3}\sum_{j=0}^{n-1}f'''(\xi_j)\Big[(n+\sigma-j)^{-\alpha}E_{\beta,1-\alpha}^{-\eta}\{\kappa(t_{n+\sigma}-t_j)^{\beta}\}\right.\\ &\left.-(n+\sigma-j+1)^{-\alpha}E_{\beta,1-\alpha}^{-\eta}\{\kappa(t_{n+\sigma}-t_{j+1})^{\beta}\}\Big]\right|\\ \leq&\, c\max_{\xi\in[t_0,t_n]}|f'''(\xi)|\Delta t^{3-\alpha},\end{aligned}$$

where c is a constant. Thus, we have $R_1 = \mathcal{O}(\Delta t^{3-\alpha})$. Further, we will show that $R_2 = \mathcal{O}(\Delta t^{2-\alpha})$. Clearly,

$$R_2 = \int_{t_n}^{t_{n+\sigma}}\frac{E_{\beta,1-\alpha}^{-\eta}\{\kappa(t_{n+\sigma}-s)^{\beta}\}}{(t_{n+\sigma}-s)^{\alpha}}\left[f'(s)-(P_{1,n}f(s))'\right]ds.$$

Moreover, the Taylor expansion of $f'(s)$ at $s = t_{n+1/2}$ is expressed as follows

$$f'(s) = f'(t_{n+1/2}) + \frac{(s-t_{n+1/2})}{2}f''(t_{n+1/2}) + \mathcal{O}(\Delta t^2). \tag{3.15}$$

After inserting equation (3.15) into the expression for R_2, we obtain

$$
\begin{aligned}
|R_2| = &\Bigg| \int_{t_n}^{t_{n+\sigma}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^\beta\}}{(t_{n+\sigma}-s)^\alpha} \left[f'(t_{n+1/2}) - (P_{1,n}f(s))'\right] ds \\
&+ f''(t_{n+1/2}) \int_{t_n}^{t_{n+\sigma}} \frac{(s-t_{n+1/2})E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^\beta\}}{(t_{n+\sigma}-s)^\alpha} ds + \mathcal{O}(\Delta t^{3-\alpha}) \Bigg| \\
|R_2| \leq &\left| f''(t_{n+1/2}) \int_{t_n}^{t_{n+\sigma}} \frac{(s-t_{n+1/2})E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+\sigma}-s)^\beta\}}{(t_{n+\sigma}-s)^\alpha} ds \right| + \mathcal{O}(\Delta t^{3-\alpha}),
\end{aligned}
$$

On simplifying further we get

$$
\begin{aligned}
|R_2| \leq &\frac{\sigma^{1-\alpha}\Delta t^{2-\alpha}}{2} |f''(t_{n+1/2})| \left| 2\sigma E^{-\eta}_{\beta,3-\alpha}\{\kappa(t_{n+\sigma}-t_n)^\beta\} - E^{-\eta}_{\beta,2-\alpha}\{\kappa(t_{n+\sigma}-t_n)^\beta\} \right| \\
\leq &\, c|f''(t_{n+1/2})|\Delta t^{2-\alpha},
\end{aligned}
$$

where c is a constant. Thus, $R_2 = \mathcal{O}(\Delta t^{2-\alpha})$. Therefore, we get $R_1+R_2 = \mathcal{O}(\Delta t^{2-\alpha})$. Hence, we have the proof. □

3.1.1.1 Basic features of the new CPL2-1_σ formula

Lemma 3.1. *For $0 < \alpha < 1$ and $j = 1, 2, 3, \ldots$, the following inequalities hold*

$$
\frac{1}{2} < \chi_j < \frac{1}{2-\alpha},
$$

where

$$
\chi_j = \frac{(j+\sigma)^{2-\alpha}{}_3E_{j+\sigma} - (j-1+\sigma)^{2-\alpha}{}_3E_{j-1+\sigma} - (j-1+\sigma)^{1-\alpha}{}_2E_{j-1+\sigma}}{(j+\sigma)^{1-\alpha}{}_2E_{j+\sigma} - (j-1+\sigma)^{1-\alpha}{}_2E_{j-1+\sigma}}.
$$

Proof. One can have the proof following [7, Lemma 3]. □

Lemma 3.2. *The coefficients w_j $(0 \leq j \leq n, n \geq 1)$, for $0 < \alpha < 1$, given in equation (3.14) satisfy the following inequality*

$$w_n > \frac{(n+\sigma)^{-\alpha}}{4\Gamma(1-\alpha)},$$

where $\sigma = 1 - \frac{\alpha}{2}$.

Proof. For $n \geq 1$, we get

$$w_n = r_n - d_n = \left[(n+\sigma)^{1-\alpha}{}_2E_{n+\sigma} - (n-1+\sigma)^{1-\alpha}{}_2E_{n-1+\sigma}\right]\left(\frac{3}{2} - \chi_n\right).$$

Using Lemma 3.1 in above equation we get

$$\begin{aligned} w_n &> \left((n+\sigma)^{1-\alpha}{}_2E_{n+\sigma} - (n-1+\sigma)^{1-\alpha}{}_2E_{n-1+\sigma}\right)\left(\frac{3}{2} - \frac{1}{2-\alpha}\right) \\ &= \frac{4-3\alpha}{2(2-\alpha)}\int_0^1 \frac{{}_1E_{n+\sigma-s}}{(n+\sigma-s)^{\alpha}} ds \\ &> \frac{(n+\sigma)^{-\alpha}}{2(2-\alpha)}{}_1E_{n+\sigma-1}. \end{aligned}$$

We can choose the parameters η, β, and κ such that ${}_1E_{n+\sigma-1} = E^{-\eta}_{\beta,1-\alpha}\{\kappa((n+\sigma-1)\Delta t)^{\beta}\} > 0$. Thus, we get

$$w_n > \frac{(n+\sigma)^{-\alpha}}{4\Gamma(1-\alpha)}.$$

Hence, the lemma is proved. □

Lemma 3.3. *For $\alpha \in (0,1)$ and coefficients w_j $(0 \leq j \leq n, n \geq 1)$, the following inequality holds*

$$w_0 > w_1 > w_2 > \cdots > w_n.$$

Proof. The proof can be done following [7, Lemma 4]. □

3.1.2 CPL-2 formula

We approximate the Caputo-Prabhakar derivative of the function $f(t) \in C^3[0,T]$ at the points t_{n+1}, $1 \leq n \leq N_t - 1$, given in equation (3.1). The CPL-2 formula can be obtained in the following manner

$$\begin{aligned}
{}^{CP}_{\ 0}D^{\eta}_{\beta,\alpha,\kappa} f(t_{n+1}) &= \int_0^{t_{n+1}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{\alpha}} f'(s)ds \\
&= \int_0^{t_2} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{\alpha}} f'(s)ds + \\
&\qquad \sum_{j=2}^{n} \int_{t_j}^{t_{j+1}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{\alpha}} f'(s)ds. \qquad (3.16)
\end{aligned}$$

Now, for each $t \in [t_j, t_{j+1}]$ $(1 \leq j \leq n)$, making use of the quadratic interpolation $P_{2,j}f(t)$ of $f(t)$ over three points $(t_{j-1}, f(t_{j-1}))$, $(t_j, f(t_j))$, and $(t_{j+1}, f(t_{j+1}))$, we arrive at

$$\begin{aligned}
f(t) \approx P_{2,j}f(t) &= \sum_{i=-1}^{1} \prod_{\substack{l=-1 \\ l\neq i}}^{1} \frac{t - t_{j+l}}{(i-l)\Delta t^2} f(t_{j+i}), \\
(P_{2,j}f(t))' &= \left(\frac{2t - 2t_j - \Delta t}{2}\right) \delta t^2 f(t_j) + \delta t f\left(t_{j+1/2}\right), \qquad (3.17)
\end{aligned}$$

and

$$f(t) - P_{2,j}f(t) = \frac{f'''(\bar{\xi}_j)}{6}(t - t_{j-1})(t - t_j)(t - t_{j+1}), \qquad (3.18)$$

where $\bar{\xi}_j \in (t_{j-1}, t_{j+1})$. In order to obtain the CPL-2 formula we use equation (3.17) in equation (3.16) and get

$$\begin{aligned}
{}^{CP}_{\ 0}D^{v}_{\beta,\alpha,\kappa} f(t_{n+1}) \approx &\int_0^{t_2} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{\alpha}} (P_{2,1}f(s))'ds \\
&+ \sum_{j=2}^{n} \int_{t_j}^{t_{j+1}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{\alpha}} (P_{2,j}f(s))'ds
\end{aligned}$$

$$= \int_0^{t_2} \frac{E_{\beta,1-\alpha}^{-\eta}\{\kappa(t_{n+1}-s)^\beta\}}{(t_{n+1}-s)^\alpha} \left[\frac{(2s-2t_1-\Delta t)}{2}\delta t^2 f(t_1) + \delta t f\left(t_{3/2}\right)\right] ds$$
$$+ \sum_{j=2}^{n} \int_{t_j}^{t_{j+1}} \frac{E_{\beta,1-\alpha}^{-\eta}\{\kappa(t_{n+1}-s)^\beta\}}{(t_{n+1}-s)^\alpha} \left[\frac{(2s-2t_j-\Delta t)}{2}\delta t^2 f(t_j) + \delta t f\left(t_{j+1/2}\right)\right] ds, \tag{3.19}$$

which on solving gives

$${}_0^{CP}D_{\beta,\alpha,\kappa}^{\eta} f(t_{n+1}) \approx \Delta t^{1-\alpha}\Big[(a_n - b_n - b_{n-1})\,\delta t f\left(t_{1/2}\right) + (a_{n-1}+b_{n-1}+b_n)\,\delta t f\left(t_{3/2}\right)\Big]$$
$$+ \Delta t^{1-\alpha}\sum_{j=2}^{n}\Big[-b_{n-j}\delta t f\left(t_{j-1/2}\right) + (a_{n-j}+b_{n-j})\,\delta t f\left(t_{j+1/2}\right)\Big],$$

where

$$a_l = \Big\{(l+1)^{1-\alpha}{}_2E_{l+1} - l^{1-\alpha}{}_2E_l\Big\}, \ \ l \geq 0, \tag{3.20}$$
$$b_l = \Big\{(l+1)^{2-\alpha}{}_3E_{l+1} - l^{2-\alpha}{}_3E_l\Big\} - \frac{1}{2}\Big\{(l+1)^{1-\alpha}{}_2E_{l+1} + l^{1-\alpha}{}_2E_l\Big\}, \ \ l \geq 0, \tag{3.21}$$

with

$${}_2E_l = E_{\beta,2-\alpha}^{-\eta}\left(\kappa(l\Delta t)^\beta\right), \ \text{ and } \ {}_3E_l = E_{\beta,3-\alpha}^{-\eta}\left(\kappa(l\Delta t)^\beta\right). \tag{3.22}$$

After arranging the terms, we get

$${}_0^{CP}D_{\beta,\alpha,\kappa}^{\eta} f(t_{n+1}) \approx \Delta t^{1-\alpha}\Big[(a_n - b_n - b_{n-1})\,\delta t f\left(t_{1/2}\right) + (a_{n-1}+b_{n-1}+b_n-b_{n-2})$$
$$\delta t f\left(t_{3/2}\right)\Big] + \Delta t^{1-\alpha}\sum_{j=2}^{n-1}\Big[(-b_{n-j-1}+a_{n-j}+b_{n-j})\,\delta t f\left(t_{j+1/2}\right)$$
$$+ (a_0+b_0)\,\delta t f\left(t_{n+1/2}\right)\Big]. \tag{3.23}$$

Hence, we have

$${}_0^{CP}D_{\beta,\alpha,\kappa}^{\eta} f(t_{n+1}) \approx \sum_{j=0}^{n} c_{n-j}\delta t f\left(t_{j+1/2}\right), \tag{3.24}$$

where:

for $n = 1$,

$$c_n = \begin{cases} a_0 + b_0 + b_1, & j = 0, \\ a_1 - b_1 - b_0, & j = 1, \end{cases} \tag{3.25}$$

for $n = 2$,

$$c_j = \begin{cases} a_0 + b_0, & j = 0, \\ a_1 + b_1 + b_2 - b_0, & j = 1, \\ a_2 - b_2 - b_1, & j = 2, \end{cases} \tag{3.26}$$

and for $n \geq 3$,

$$c_j = \begin{cases} a_0 + b_0, & j = 0, \\ a_j - b_j - b_{j-1,} & 1 \leq j \leq n-2, \\ a_{n-1} + b_{n-1} + b_n - b_{n-2} & j = n-1, \\ a_n - b_n - b_{n-1,} & j = n. \end{cases} \tag{3.27}$$

The approximation (3.24) is the CPL-2 formula for the Caputo-Prabhakar fractional derivative. The following result shows that the accuracy of the CPL-2 formula is of order $3 - \alpha$.

Theorem 3.2. *For any fractional order* $\alpha \in (0, 1)$*,* $n = 1, 2, \cdots, N_t - 1$*, and* $f(t) \in C^3[0, t_{n+1}]$*, we have*

$$ {}^{CP}_{\;\;0}D^{\eta}_{\beta,\alpha,\kappa} f(t_{n+1}) = \sum_{j=0}^{n} c_{n-j} \delta t f\left(t_{j+1/2}\right) + \mathcal{O}\left(\Delta t^{3-\alpha}\right). $$

Proof. Recall that in deriving the CPL-2 formula (3.24), we have approximated $f'(s)$ by $(P_{2,1}f(s))'$ and $(P_{2,j}f(s))'$ in their respective intervals. So, it is evident that

$$ {}_{0}^{CP}D^{\eta}_{\beta,\alpha,\kappa}f(t_{n+1}) - \sum_{j=0}^{n} c_{n-j}\delta t f\left(t_{j+1/2}\right) = \hat{R}_1 + \hat{R}_2, $$

where

$$ \hat{R}_1 = \int_{t_0}^{t_2} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{\alpha}} \left[f(s) - P_{2,1}f(s)\right]' ds $$

and

$$ \hat{R}_2 = \sum_{j=2}^{n} \int_{t_j}^{t_{j+1}} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{\alpha}} \left[f(s) - P_{2,j}f(s)\right]' ds. $$

First, we will show that $\hat{R}_1 = \mathcal{O}(\Delta t^{3-\alpha})$. We have

$$ \begin{aligned} \hat{R}_1 &= \int_{t_0}^{t_2} \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{\alpha}} \left[f(s) - P_{2,1}f(s)\right]' ds \\ &= \int_{t_0}^{t_2} \frac{E^{-\eta}_{\beta,-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{1+\alpha}} \left[f(s) - P_{2,1}f(s)\right] ds \\ &= \frac{1}{6}\int_{t_0}^{t_2} f'''(\bar{\xi}_1)s(s-t_1)(s-t_2)(t_{n+1}-s)^{-1-\alpha}E^{-\eta}_{\beta,-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}ds, \end{aligned} $$

where $\bar{\xi}_1 \in (t_0, t_2)$. Further, for $n = 1$, we have

$$ \begin{aligned} |\hat{R}_1| &= \left|\frac{1}{6}\int_{t_0}^{t_2} f'''(\bar{\xi}_1)s(s-t_1)(s-t_2)(t_2-s)^{-1-\alpha}E^{-\eta}_{\beta,-\alpha}\{\kappa(t_2-s)^{\beta}\}ds\right| \\ &\leq \left|\frac{\Delta t^2 f'''(\bar{\xi}_1)}{3}\int_{t_0}^{t_2} (t_2-s)^{-\alpha}E^{-\eta}_{\beta,-\alpha}\{\kappa(t_2-s)^{\beta}\}ds\right| \\ &= \frac{\Delta t^2|f'''(\bar{\xi}_1)|}{3}\left|t_2^{1-\alpha}\left[E^{-\eta}_{\beta,1-\alpha}\{\kappa t_2^{\beta}\} - E^{-\eta}_{\beta,2-\alpha}\{\kappa t_2^{\beta}\}\right]\right| \\ &= c|f'''(\bar{\xi}_1)|\Delta t^{3-\alpha}, \end{aligned} $$

where c is a constant.

Next, for $n \geq 2$, we have

$$
\begin{aligned}
|\hat{R}_1| &= \left| \frac{1}{6} \int_{t_0}^{t_2} f'''(\bar{\xi_1}) s(s-t_1)(s-t_2)(t_{n+1}-s)^{-1-\alpha} E_{\beta,-\alpha}^{-\eta}\{\kappa(t_{n+1}-s)^{\beta}\} ds \right| \\
&\leq \left| \frac{2\sqrt{3}\Delta t^3 f'''(\bar{\xi_1})}{54} \int_{t_0}^{t_2} (t_{n+1}-s)^{-1-\alpha} E_{\beta,-\alpha}^{-\eta}\{\kappa(t_{n+1}-s)^{\beta}\} ds \right|.
\end{aligned}
$$

Thus, we get

$$
\begin{aligned}
|\hat{R}_1| \leq & \frac{\sqrt{3}\Delta t^3 |f'''(\bar{\xi_1})|}{27} \Bigg| \Delta t^{-\alpha} \Big[(n+1)^{-\alpha} E_{\beta,2-\alpha}^{-\eta}\{\kappa t_{n+1}^{\beta}\} - (n-1)^{-\alpha} \\
& \qquad E_{\beta,2-\alpha}^{-\eta}\{\kappa(t_{n+1}-t_2)^{\beta}\} \Big] \Bigg| \\
& \leq c |f'''(\bar{\xi_1})| \Delta t^{3-\alpha},
\end{aligned}
$$

where c is a constant. Hence, we have $\hat{R}_1 = \mathcal{O}(\Delta t^{3-\alpha})$. Further, we will show that $\hat{R}_2 = \mathcal{O}(\Delta t^{3-\alpha})$. Clearly,

$$
\begin{aligned}
\hat{R}_2 &= \sum_{j=2}^{n} \int_{t_j}^{t_{j+1}} \frac{E_{\beta,1-\alpha}^{-\eta}\{\kappa(t_{n+1}-s)^{\beta}\}}{(t_{n+1}-s)^{\alpha}} \left[f(s) - P_{2,j} f(s) \right]' ds \\
&= \sum_{j=2}^{n} \left[\int_{t_j}^{t_{j+1}} (t_{n+1}-s)^{-\alpha-1} E_{\beta,-\alpha}^{-\eta}\{\kappa(t_{n+1}-s)^{\beta}\} \left[f(s) - P_{2,j} f(s) \right] ds \right] \\
&= \frac{1}{6} \sum_{j=2}^{n} \int_{t_j}^{t_{j+1}} f'''(\bar{\xi_j})(s-t_{j-1})(s-t_j)(s-t_{j+1})(t_{n+1}-s)^{-\alpha-1} \\
& \qquad E_{\beta,-\alpha}^{-\eta}\{\kappa(t_{n+1}-s)^{\beta}\} ds,
\end{aligned}
$$

where $\bar{\xi_j} \in (t_{j-1}, t_{j+1})$.

Now, for $n \geq 2$, we have

$$
\begin{aligned}
|\hat{R}_2| \leq & \Bigg| \frac{1}{6} \sum_{j=2}^{n-1} \int_{t_j}^{t_{j+1}} f'''(\bar{\xi_j})(s-t_{j-1})(s-t_j)(s-t_{j+1})(t_{n+1}-s)^{-\alpha-1} \\
& E_{\beta,-\alpha}^{-\eta}\{\kappa(t_{n+1}-s)^{\beta}\} ds + \frac{1}{6} \int_{t_n}^{t_{n+1}} f'''(\bar{\xi_n})(s-t_{n-1})(s-t_n)
\end{aligned}
$$

$$
\begin{aligned}
&(s-t_{n+1})(t_{n+1}-s)^{-\alpha-1}E^{-\eta}_{\beta,-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}ds\Bigg| \\
&\leq \left|\frac{2\sqrt{3}\Delta t^3}{54}\sum_{j=2}^{n-1} f'''(\bar{\xi}_j)\int_{t_j}^{t_{j+1}}(t_{n+1}-s)^{-\alpha-1}E^{-\eta}_{\beta,-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}ds\right| \\
&\quad+\left|\frac{\Delta t^2 f'''(\bar{\xi}_n)}{3}\int_{t_n}^{t_{n+1}}(t_{n+1}-s)^{-\alpha}E^{-\eta}_{\beta,-\alpha}\{\kappa(t_{n+1}-s)^{\beta}\}ds\right| \\
&=\Bigg|\frac{\sqrt{3}\Delta t^3}{27}\sum_{j=2}^{n-1} f'''(\bar{\xi}_j)\Delta t^{-\alpha}\Big[(n+1-j)^{-\alpha}E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-t_j)^{\beta}\}-(n-j)^{-\alpha} \\
&\quad\times E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-t_{j+1})^{\beta}\}\Big]\Bigg|+\Bigg|\frac{\Delta t^2 f'''(\bar{\xi}_n)}{3}\Delta t^{1-\alpha}\Big[E^{-\eta}_{\beta,1-\alpha}\{\kappa(t_{n+1}-t_n)^{\beta}\} \\
&\quad-E^{-\eta}_{\beta,2-\alpha}\{\kappa(t_{n+1}-t_n)^{\beta}\}\Big]\Bigg| \\
&\leq c\max_{s\in[t_2,t_n]}|f'''(s)|\Delta t^{3-\alpha},
\end{aligned}
$$

where c is a constant. Thus, $\hat{R}_2=\mathcal{O}(\Delta t^{3-\alpha})$. So, we get $\hat{R}_1+\hat{R}_2=\mathcal{O}(\Delta t^{3-\alpha})$. Hence, we have the proof. □

3.1.2.1 Basic features of the new CPL-2 formula

Lemma 3.4. *For $0<\alpha<1$ and $j=1,2,3,\ldots$*

(a). $\dfrac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(j\Delta t)^{\beta}\}}{(j+1)^{\alpha}}<a_j<\dfrac{E^{-\eta}_{\beta,1-\alpha}\{\kappa((j+1)\Delta t)^{\beta}\}}{j^{\alpha}}$.

(b). $b_j<(j+1)^{1-\alpha}E^{-\eta}_{\beta,2-\alpha}\{\kappa((j+1)\Delta t)^{\beta}\}$.

Proof. (a). The coefficients a_j, for $j=1,2,3,\ldots$ and $0<\alpha<1$, can be written as

$$a_j=\int_0^1\frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa((j+s)\Delta t)^{\beta}\}}{(j+s)^{\alpha}}ds. \tag{3.28}$$

We can choose the parameters η, β, and κ such that $E^{-\eta}_{\beta,1-\alpha}\{\kappa((j+s)\Delta t)^{\beta}\} > 0$. Thus, from equation (3.28), the following inequalities hold

$$\frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa(j\Delta t)^{\beta}\}}{(j+1)^{\alpha}} < a_j < \frac{E^{-\eta}_{\beta,1-\alpha}\{\kappa((j+1)\Delta t)^{\beta}\}}{j^{\alpha}}.$$

(b). The coefficients b_j are given as

$$b_j = \Big\{(j+1)^{2-\alpha}{}_3E_{j+1} - j^{2-\alpha}{}_3E_j\Big\} - \frac{1}{2}\Big\{(j+1)^{1-\alpha}{}_2E_{j+1} + j^{1-\alpha}{}_2E_j\Big\}. \tag{3.29}$$

Again, we can choose the parameters η, β, and κ such that ${}_2E_j$ and ${}_2E_{j+1}$ are positive. Therefore, from equation (3.29), we have

$$b_j < (j+1)^{2-\alpha}{}_3E_{j+1} - j^{2-\alpha}{}_3E_j,$$

which can also be written as

$$b_j < \int_0^1 (j+s)^{1-\alpha}E^{-\eta}_{\beta,2-\alpha}\{\kappa((j+s)\Delta t)^{\beta}\}ds. \tag{3.30}$$

Thus, we can have the desired inequality from (3.30). □

Lemma 3.5. *The coefficients* c_j $(0 \le j \le n, n \ge 2)$, *for* $0 < \alpha < 1$ *satisfy the following inequality*

$$c_j > \frac{(j+1)^{-\alpha}}{\Gamma(1-\alpha)}.$$

Proof. For $n \ge 2$, we get

$$c_j = a_j - b_j - b_{j-1}.$$

Using Lemma 3.4, we have

$$c_j > (j+1)^{-\alpha}E^{-\eta}_{\beta,1-\alpha}\{\kappa(j\Delta t)^{\beta}\} - (j+1)^{1-\alpha}E^{-\eta}_{\beta,2-\alpha}\{\kappa((j+1)\Delta t)^{\beta}\} - j^{1-\alpha}$$

$$\times E^{-\eta}_{\beta,2-\alpha}\{\kappa(j\Delta t)^{\beta}\}.$$

Further, we can choose the parameters η, β, and κ such that ${}_2E_j$, ${}_2E_{j+1}$ and $E^{-\eta}_{\beta,1-\alpha}\{\kappa(j\Delta t)^{\beta}\}$ are positive. Therefore, we get

$$\begin{aligned} c_j >&(j+1)^{-\alpha}E^{-\eta}_{\beta,1-\alpha}\{\kappa(j\Delta t)^{\beta}\} - (j+1)^{1-\alpha}E^{-\eta}_{\beta,2-\alpha}\{\kappa((j+1)\Delta t)^{\beta}\} - (j+1)^{1-\alpha} \\ &\times E^{-\eta}_{\beta,2-\alpha}\{\kappa((j+1)\Delta t)^{\beta}\} \\ =&(j+1)^{-\alpha}E^{-\eta}_{\beta,1-\alpha}\{\kappa(j\Delta t)^{\beta}\} > \frac{(j+1)^{-\alpha}}{\Gamma(1-\alpha)}. \end{aligned}$$

Thus, we have the lemma. □

3.2 Application

The profound impact of reaction-diffusion equations in practical scenarios has established them as a prominent and engaging research topic. Understanding the dynamics of reaction-diffusion equations is paramount in environmental science, particularly when examining the entry of pollution into the atmosphere from industrial waste materials or emissions from manufacturing sources. This knowledge is fundamental for devising efficient pollution control measures [54]. The investigation of reaction and diffusion processes within porous catalysts has been a subject of enduring research aimed at understanding the intricate mechanisms governing these systems in [22, 25]. The utility of reaction-diffusion equations extends to a plethora of real-world problems, including logistic population growth, chemical reactions, nuclear reactor theory, branching Brownian motion processes, and numerous others. These equations serve as valuable models for understanding and analyzing diverse phenomena.

Therefore, we study the application of the above-derived approximations in solving the following time fractional reaction-diffusion problem with variable coefficients defined in the Caputo-Prabhakar sense

$$ {}^{CP}_{\;\,0}D^{\eta}_{\beta,\alpha,\kappa}u(x,t)+q(t)u(x,t) = p(t)\frac{\partial^2 u(x,t)}{\partial x^2}+F(x,t), \quad (x,t)\in(a,b)\times(0,T], \tag{3.31} $$

with initial condition

$$ u(x,0) = g(x), \quad x\in[a,b], \tag{3.32} $$

and boundary conditions

$$ \begin{cases} u(0,t) = \phi_1(t), & t\in(0,T], \\ u(b,t) = \phi_2(t), & t\in(0,T], \end{cases} \tag{3.33} $$

where $0<\alpha<1$ is the fractional order, $q\geq 0$, $p>p_0\geq 0$, g, ϕ_1, ϕ_2 and F are known sufficiently smooth functions.

We will also introduce a high order compact scheme for the spatial discretization of (3.31)-(3.33). The compact finite difference method is a firmly established numerical approach widely used for solving partial differential equations (PDEs). Its applicability extends across various fields of science and engineering, with a rich history of research and practical use. Many research papers have showcased the prowess and benefits of the high-order compact finite difference technique [57, 71, 100, 104].

For this end, let N_x be a positive integer and divide the interval $[a,b]$ into N_x subintervals with $\Omega_x : a = x_0 < x_1 < \cdots < x_{N_x} = b$. Suppose $x_i = a+ih$, with the mesh width $h = \frac{b-a}{N_x}$. Let u denote the exact solution of problem (3.31)-(3.33). For $0\leq i\leq N_x$ and $0\leq j\leq N_t$, we shall use the notation $u_i^j = u(x_i,t_j)$ and

$F_i^j = F(x_i, t_j)$. Further, let U_i^j denote the approximation of u_i^j. Now, let $\mathcal{D}_h = \{\vartheta|(\vartheta_0, \vartheta_1, \cdots, \vartheta_{N_x}), 0 \le i \le N_x\}$ and $\mathcal{D}_h^* = \{\vartheta|(\vartheta_0, \vartheta_1, \cdots, \vartheta_{N_x}), \vartheta_0 = \vartheta_{N_x} = 0\}$. For any grid function $y \in \mathcal{D}_h$, let us denote

$$\delta_x \vartheta_{i+\frac{1}{2}} = \frac{1}{h}(\vartheta_{i+1} - \vartheta_i), \quad \delta_x^2 \vartheta_i = \frac{1}{h}\left(\delta_x \vartheta_{i+\frac{1}{2}} - \delta_x \vartheta_{i-\frac{1}{2}}\right).$$

Further, for any grid function $y \in \mathcal{D}_h$, the compact differential operator $(\mathcal{H}_c)$ is defined as

$$\mathcal{H}_c \vartheta_i = \begin{cases} \frac{1}{12}\vartheta_{i-1} + \frac{10}{12}\vartheta_i + \frac{1}{12}\vartheta_{i+1}, & 1 \le i \le N_x - 1, \\ \vartheta_i, & i = 0 \text{ or } N_x. \end{cases} \tag{3.34}$$

Also, it is evident that

$$\mathcal{H}_c \vartheta_i = \left(I + \frac{h^2}{12}\delta_x^2\right)\vartheta_i, \quad 1 \le i \le N_x - 1. \tag{3.35}$$

Lemma 3.6. *[71] Suppose $\psi(x) \in C^6[x_{i-1}, x_{i+1}]$ and $\tilde{\phi}(s) = -3(1-s)^5 + 5(1-s)^3$. Then*

$$\frac{1}{12}\psi''(x_{i-1}) + \frac{10}{12}\psi''(x_i) + \frac{1}{12}\psi''(x_{i+1}) = \frac{\psi(x_{i-1}) - 2\psi(x_i) + \psi(x_{i+1})}{h^2} + \frac{h^4}{360}\int_0^1 \left(\psi^{(6)}(x_i - sh) + \psi^{(6)}(x_i + sh)\right)\tilde{\phi}(s)ds.$$

3.2.1 Compact finite difference scheme with CPL2-1$_\sigma$ formula (CFD$_1$)

Consider problem (3.31) at $(x_i, t_{n+\sigma})$, $0 \le i \le N_x, 0 \le n \le N_t - 1$. We have

$${}_0^{CP}D^{\eta}_{\beta,\alpha,\kappa}u(x_i, t_{n+\sigma}) + q(t_{n+\sigma})u(x_i, t_{n+\sigma}) = p(t_{n+\sigma})\frac{\partial^2 u(x_i, t_{n+\sigma})}{\partial x^2} + F(x_i, t_{n+\sigma}). \tag{3.36}$$

Lemma 3.7. *[7] If $W(t) \in C^2[0,T]$, then on the mesh Ω_t we have*

$$W(t_{n+\sigma}) = \sigma W(t_{n+1}) + (1-\sigma)W(t_n) + \mathcal{O}(\Delta t^2),$$

where $\sigma = 1 - \frac{\alpha}{2}$.

Now in order to derive the CFD$_1$ scheme, we use the CPL2-1$_\sigma$ formula for approximation of the Caputo-Prabhakar fractional derivative given in equation (3.13) and apply the compact operator $\mathcal{H}_c$ defined in equation (3.34) to both sides of equation (3.36). Further, we approximate $u_i^{n+\sigma}$ (and similarly $u_{i-1}^{n+\sigma}$, $u_{i+1}^{n+\sigma}$) by Lemma 3.7. We obtain

$$\nu\mathcal{H}_c\left[w_0 u_i^{n+1} - \sum_{k=1}^{n}(w_{n-k} - w_{n-k+1})u_i^k - w_n u_i^0\right] + q^{n+\sigma}\mathcal{H}_c u_i^{n+\sigma} = p^{n+\sigma}\delta_x^2 u_i^{n+\sigma} + \mathcal{H}_c F_i^{n+\sigma} + {}_1\mathcal{R}_i^{n+\sigma}, \quad 1 \le i \le N_x - 1, \tag{3.37}$$

$$u_i^0 = g(x_i), \quad 0 \le i \le N_x, \tag{3.38}$$

$$u_0^n = \phi_1(t_n), \quad u_{N_x}^n = \phi_2(t_n), \quad 1 \le n \le N_t, \tag{3.39}$$

where $\nu = \Delta t^{-\alpha}$, $q^{n+\sigma} = q(t_{n+\sigma})$ and $p^{n+\sigma} = p(t_{n+\sigma})$. Further, removing the truncation error term ${}_1\mathcal{R}_i^{n+\sigma} = \mathcal{O}(\Delta t^{2-\alpha}, \Delta t^2, h^4)$ from equation (3.37), we have

$$\nu\mathcal{H}_c\left[w_0 U_i^{n+1} - \sum_{k=1}^{n}(w_{n-k} - w_{n-k+1})U_i^k - w_n U_i^0\right] + q^{n+\sigma}\mathcal{H}_c U_i^{n+\sigma} = p^{n+\sigma}\delta_x^2 U_i^{n+\sigma} + \mathcal{H}_c F_i^{n+\sigma}, 1 \le i \le N_x - 1, \tag{3.40}$$

$$U_i^0 = g(x_i), \quad 0 \le i \le N_x, \tag{3.41}$$

$$U_0^n = \phi_1(t_n), \quad U_{N_x}^n = \phi_2(t_n), \quad 1 \le n \le N_t. \tag{3.42}$$

Thus, we can recursively solve the discrete scheme (3.40)-(3.42) for U_i^n, $1 \le i \le N_x - 1$, $1 \le n \le N_t$, and obtain the numerical solution of problem (3.31)-(3.33).

3.2.2 Compact finite difference scheme with CPL-2 formula ($\mathbf{CFD_2}$)

Consider problem (3.31) at (x_i, t_{n+1}), $0 \le i \le N_x, 1 \le n \le N_t - 1$. We have

$$ {}^{CP}_{0}D^{\eta}_{\beta,\alpha,\kappa} u(x_i, t_{n+1}) + q(t_{n+1})u(x_i, t_{n+1}) = p(t_{n+1}) \frac{\partial^2 u(x_i, t_{n+1})}{\partial x^2} + F(x_i, t_{n+1}). \quad (3.43) $$

Now in order to derive the CFD_2 scheme, we use the CPL-2 formula for approximation of Caputo-Prabhakar fractional derivative given in equation (3.24) and apply the compact operator $\mathcal{H}_c$ defined in equation (3.34) to both sides of equation (3.43). We obtain

$$ \nu \mathcal{H}_c \left[c_0 u_i^{n+1} - \sum_{j=1}^{n} (c_{n-j} - c_{n-j+1}) u_i^j - c_n u_i^0 \right] + q^{n+1} \mathcal{H}_c u_i^{n+1} = p^{n+1} \delta_x^2 u_i^{n+1} + \mathcal{H}_c F_i^{n+1} $$
$$ + {}_2\mathcal{R}_i^{n+1}, \quad 1 \le i \le N_x - 1, \quad (3.44) $$
$$ u_i^0 = g(x_i), \quad 0 \le i \le N_x, \quad (3.45) $$
$$ u_0^n = \phi_1(t_n), \quad u_{N_x}^n = \phi_2(t_n), \quad 1 \le n \le N_t, \quad (3.46) $$

where $\nu = \Delta t^{-\alpha}$, $q^{n+1} = q(t_{n+1})$ and $p^{n+1} = p(t_{n+1})$. Further, removing the truncation error term ${}_2\mathcal{R}_i^{n+1} = \mathcal{O}(\Delta t^{3-\alpha}, h^4)$ from equation (3.44), we have

$$ \nu \mathcal{H}_c \left[c_0 U_i^{n+1} - \sum_{j=1}^{n} (c_{n-j} - c_{n-j+1}) U_i^j - c_n U_i^0 \right] + q^{n+1} \mathcal{H}_c U_i^{n+1} = p^{n+1} \delta_x^2 U_i^{n+1} $$
$$ + \mathcal{H}_c F_i^{n+1}, 1 \le i \le N_x - 1, \quad (3.47) $$
$$ U_i^0 = g(x_i), \quad 0 \le i \le N_x, \quad (3.48) $$
$$ U_0^n = \phi_1(t_n), \quad U_{N_x}^n = \phi_2(t_n), \quad 1 \le n \le N_t. \quad (3.49) $$

Remark 3.3. We assume that the solution U_i^1 is found with the order of accuracy

$\mathcal{O}(\Delta t^{3-\alpha}, h^4)$. For example, we can use *NS1*[101] formula and solve problem (3.31)-(3.33) on the time interval $[0, \Delta t]$ with step size $\widetilde{\Delta} t = \mathcal{O}\left(\Delta t^{\frac{3-\alpha}{2-\alpha}}\right)$.

Note that we can recursively solve the discrete scheme (3.47)-(3.49) for U_i^n, $1 \leq i \leq N_x - 1$, $2 \leq n \leq N_t - 1$, and obtain the numerical solution of problem (3.31)-(3.33).

3.3 Stability and convergence analysis

In this section we provide stability and convergence analysis of both schemes: CFD_1 and CFD_2. We now introduce notation for the analysis of both schemes. For any v, $\vartheta \in \mathcal{D}_h^*$, we define the discrete inner product and norms as follows

$$\langle v, \vartheta \rangle_h = h \sum_{i=1}^{N_x - 1} v_i \cdot \vartheta_i, \qquad \|v\|_h = \sqrt{\langle v, v \rangle_h},$$

$$|v|_1 = \sqrt{h \sum_{i=1}^{N_x} \left(\delta_x v_{i-\frac{1}{2}}\right)^2}, \qquad \|v\|_\infty = \max_{1 \leq i \leq N_x - 1} |v_i|,$$

$$\|\delta_x^2 v\| = \sqrt{h \sum_{i=1}^{N_x - 1} (\delta_x^2 v_i)^2}.$$

Similarly, we can define $\|\mathcal{H}_c v\|$.

3.3.1 Stability and convergence analysis of CFD_1 scheme

In this subsection we provide stability and convergence analysis of CFD_1 scheme (3.40)-(3.42).

Lemma 3.8. *For the numbers $\tilde{r}_m$, $0 \leq m \leq j+1$, the following inequalities hold*

$$\tilde{r}_{j+1} \sum_{k=0}^{j} (\tilde{r}_{k+1} - \tilde{r}_k) w_{j-k} \geq \frac{1}{2} \sum_{k=0}^{j} \left((\tilde{r}_{k+1})^2 - (\tilde{r}_k)^2\right) w_{j-k} + \frac{1}{2w_0} \left(\sum_{k=0}^{j} (\tilde{r}_{k+1} - \tilde{r}_k) w_{j-k}\right)^2,$$

$$\tilde{r}_j \sum_{k=0}^{j} (\tilde{r}_{k+1} - \tilde{r}_k) w_{j-k} \geq \frac{1}{2} \sum_{k=0}^{j} \left((\tilde{r}_{k+1})^2 - (\tilde{r}_k)^2 \right) w_{j-k} - \frac{1}{2(w_0 - w_1)} \left(\sum_{k=0}^{j} (\tilde{r}_{k+1} - \tilde{r}_k) w_{j-k} \right)^2.$$

Proof. Using Lemma 1 of [7], we immediately get the proof. □

Using Lemma 3.8, we obtain the following inequality that is needed in getting the a priori estimate.

Lemma 3.9. *For the numbers $\tilde{r}_m$, $0 \leq m \leq n+1$, the following inequality holds*

$$\{\sigma \tilde{r}_{n+1} + (1-\sigma)\tilde{r}_n\} \sum_{k=0}^{n} (\tilde{r}_{k+1} - \tilde{r}_k) w_{n-k} \geq \frac{1}{2} \sum_{k=0}^{n} \left((\tilde{r}_{k+1})^2 - (\tilde{r}_k)^2 \right) w_{n-k},$$

where $\sigma = 1 - \frac{\alpha}{2}$.

Let $\tilde{u}_i^n$ solve the following problem

$$\nu \mathcal{H}_c \left[w_0 \tilde{u}_i^{n+1} - \sum_{k=1}^{n} (w_{n-k} - w_{n-k+1}) \tilde{u}_i^k - w_n \tilde{u}_i^0 \right] + q^{n+\sigma} \mathcal{H}_c \tilde{u}_i^{n+\sigma} = p^{n+\sigma} \delta_x^2 \tilde{u}_i^{n+\sigma} + \mathcal{H}_c \tilde{F}_i^{n+\sigma}, \; 1 \leq i \leq N_x - 1, \tag{3.50}$$

$$\tilde{u}_i^0 = g_0(x_i), \quad 0 \leq i \leq N_x, \tag{3.51}$$

$$\tilde{u}_0^n = \phi_1(t_n), \quad \tilde{u}_{N_x}^n = \phi_2(t_n), \quad 1 \leq n \leq N_t, \tag{3.52}$$

Suppose $\varrho_i^j = \tilde{u}_i^j - U_i^j$. Then, from equations (3.50)-(3.52) and (3.40)-(3.42), it is evident that $\varrho_i^j \in \mathcal{D}_h^*$ and solves the following linear system

$$\nu \mathcal{H}_c \left[w_0 \varrho_i^{n+1} - \sum_{k=1}^{n} (w_{n-k} - w_{n-k+1}) \varrho_i^k - w_n \varrho_i^0 \right] + q^{n+\sigma} \mathcal{H}_c \varrho_i^{n+\sigma} = p^{n+\sigma} \delta_x^2 \varrho_i^{n+\sigma} + \mathcal{H}_c \bar{F}_i^{n+\sigma}, \; 1 \leq i \leq N_x - 1, \tag{3.53}$$

$$\varrho_i^0 = g_0(x_i) - g(x_i), \quad 0 \leq i \leq N_x, \tag{3.54}$$

$$\varrho_0^n = 0, \quad \varrho_{N_x}^n = 0, \quad 1 \leq n \leq N_t, \tag{3.55}$$

where $\bar{F}_i^{n+\sigma} = \tilde{F}_i^{n+\sigma} - F_i^{n+\sigma}$. Now, we will prove a result that will directly show that the CFD$_1$ scheme (3.40)-(3.42) is stable.

Theorem 3.4. *The solution to the discrete problem (3.53)-(3.55) satisfies*

$$\|\varrho^{n+1}\|_h^2 \leq \left(\frac{12}{5}\right)^2 \left[\|\mathcal{H}_c\varrho^0\|_h^2 + c \max_{0\leq l\leq N_t-1} \|\mathcal{H}_c\bar{F}^{l+\sigma}\|_h^2\right]. \tag{3.56}$$

Proof. On multiplying equation (3.53) with $h\mathcal{H}_c\varrho_i^{n+\sigma}$ and then summing from $i = 1$ to $N_x - 1$, we get

$$\begin{aligned}\nu\Bigg[w_0\langle\mathcal{H}_c\varrho^{n+\sigma}, \mathcal{H}_c\varrho^{n+1}\rangle_h - \sum_{k=1}^{n}(w_{n-k} - w_{n-k+1})\langle\mathcal{H}_c\varrho^{n+\sigma}, \mathcal{H}_c\varrho^{k}\rangle_h - w_n\langle\mathcal{H}_c\varrho^{n+\sigma}, \mathcal{H}_c\varrho^{0}\rangle_h\Bigg] \\ = p^{n+\sigma}\langle\mathcal{H}_c\varrho^{n+\sigma}, \delta_x^2\varrho^{n+\sigma}\rangle_h - q^{n+\sigma}\langle\mathcal{H}_c\varrho^{n+\sigma}, \mathcal{H}_c\varrho^{n+\sigma}\rangle_h + \langle\mathcal{H}_c\varrho^{n+\sigma}, \mathcal{H}_c\bar{F}^{n+\sigma}\rangle_h.\end{aligned} \tag{3.57}$$

Now, applying Lemma 3.9 to the left side of the equation (3.57) gives

$$\begin{aligned}&w_0\langle\mathcal{H}_c\varrho^{n+\sigma}, \mathcal{H}_c\varrho^{n+1}\rangle_h - \sum_{k=1}^{n}(w_{n-k} - w_{n-k+1})_h\langle\mathcal{H}_c\varrho^{n+\sigma}, \mathcal{H}_c\varrho^{k}\rangle_h - w_n\langle\mathcal{H}_c\varrho^{n+\sigma}, \mathcal{H}_c\varrho^{0}\rangle_h \\ &\geq \frac{1}{2}\left[w_0\|\mathcal{H}_c\varrho^{n+1}\|_h^2 - \sum_{k=1}^{n}(w_{n-k} - w_{n-k+1})\|\mathcal{H}_c\varrho^{k}\|_h^2 - w_n\|\mathcal{H}_c\varrho^{0}\|_h^2\right].\end{aligned} \tag{3.58}$$

Next,

$$\begin{aligned}\langle\mathcal{H}_c\varrho^{n+\sigma}, \delta_x^2\varrho^{n+\sigma}\rangle_h &= \langle\varrho^{n+\sigma}, \delta_x^2\varrho^{n+\sigma}\rangle_h + \frac{h^2}{12}\langle\delta_x^2\varrho^{n+\sigma}, \delta_x^2\varrho^{n+\sigma}\rangle_h \\ &\leq -h\sum_{i=0}^{N_x-1}\left(\delta_x\varrho_{i+\frac{1}{2}}^{n+\sigma}\right)^2 + \frac{h}{6}\left[\sum_{i=1}^{N_x-1}\left(\delta_x\varrho_{i+\frac{1}{2}}^{n+\sigma}\right)^2 + \sum_{i=1}^{N_x-1}\left(\delta_x\varrho_{i-\frac{1}{2}}^{n+\sigma}\right)^2\right], \\ &\qquad \left(\text{since } h^2\left(\delta_x^2\varrho_i^{n+\sigma}\right)^2 \leq 2\left(\delta_x\varrho_{i+\frac{1}{2}}^{n+\sigma}\right)^2 + 2\left(\delta_x\varrho_{i-\frac{1}{2}}^{n+\sigma}\right)^2\right) \\ &\leq -\frac{2}{3}\sum_{i=0}^{N_x-1}h\left(\delta_x\varrho_{i+\frac{1}{2}}^{n+\sigma}\right)^2, \quad (\text{using discrete Poincare inequality }) \\ &\leq -\frac{8}{3(b-a)}\|\varrho^{n+\sigma}\|_h^2.\end{aligned} \tag{3.59}$$

Moreover, for $\epsilon = \frac{8p^{n+\sigma}}{3(b-a)} > 0$, the Young's inequality yields

$$\begin{aligned}\langle \mathcal{H}_c\varrho^{n+\sigma}, \mathcal{H}_c\bar{F}^{n+\sigma}\rangle_h &\leq \epsilon\|\mathcal{H}_c\varrho^{n+\sigma}\|_h^2 + \frac{1}{4\epsilon}\|\mathcal{H}_c\bar{F}^{n+\sigma}\|_h^2 \\ &= h\epsilon\sum_{i=1}^{N_x-1}\left(\frac{\varrho_{i-1}^{n+\sigma}+10\varrho_i^{n+\sigma}+\varrho_{i+1}^{n+\sigma}}{12}\right)^2 + \frac{1}{4\epsilon}\|\mathcal{H}_c\bar{F}^{n+\sigma}\|_h^2 \\ &= \frac{8p^{n+\sigma}}{3(b-a)}\|\varrho^{n+\sigma}\|_h^2 + \frac{3(b-a)}{32p^{n+\sigma}}\|\mathcal{H}_c\bar{F}^{n+\sigma}\|_h^2. \end{aligned} \tag{3.60}$$

Now, the use of inequalities (3.58), (3.59) and (3.60) in equation (3.57) yields

$$\begin{aligned} w_0\|\mathcal{H}_c\varrho^{n+1}\|_h^2 - \sum_{k=1}^{n}(w_{n-k}-w_{n-k+1})\|\mathcal{H}_c\varrho^k\|_h^2 - w_n\|\mathcal{H}_c\varrho^0\|_h^2 \\ \leq \frac{3(b-a)}{16\nu p^{n+\sigma}}\|\mathcal{H}_c\bar{F}^{n+\sigma}\|_h^2, \end{aligned}$$

which gives

$$\begin{aligned} w_0\|\mathcal{H}_c\varrho^{n+1}\|_h^2 - \sum_{k=1}^{n}(w_{n-k}-w_{n-k+1})\|\mathcal{H}_c\varrho^k\|_h^2 \\ \leq w_n\left[\|\mathcal{H}_c\varrho^0\|_h^2 + \frac{3(b-a)}{16\nu p^{n+\sigma}w_n}\|\mathcal{H}_c\bar{F}^{n+\sigma}\|_h^2\right]. \end{aligned}$$

Thus, using Lemma 3.2 and noting that $n\Delta t \leq T$, we get

$$w_0\|\mathcal{H}_c\varrho^{n+1}\|_h^2 - \sum_{k=1}^{n}(w_{n-k}-w_{n-k+1})\|\mathcal{H}_c\varrho^k\|_h^2 \leq w_n\bar{\chi}, \tag{3.61}$$

where

$$\bar{\chi} = \|\mathcal{H}_c\varrho^0\|_h^2 + c\max_{0\leq l\leq N_t-1}\|\mathcal{H}_c\bar{F}^{l+\sigma}\|_h^2$$

and $c = \frac{3(b-a)\Gamma(1-\alpha)T^{\alpha}}{4p^{n+\sigma}}$.

Next, we prove by induction that

$$\|\mathcal{H}_c\varrho^{n+1}\|_h^2 \leq \bar{\chi}, \quad 0\leq n\leq N_t-1. \tag{3.62}$$

Putting $n = 0$ in equation (3.61) we get

$$\|\mathcal{H}_c\varrho^1\|_h^2 \leq \bar{\chi},$$

which is identical to (3.62) for $n = 0$. Now let us assume that (3.62) holds for $n = 0, 1, \ldots, j-1$, that is,

$$\|\mathcal{H}_c\varrho^{n+1}\|_h^2 \leq \bar{\chi}, \quad 0 \leq n \leq j-1. \tag{3.63}$$

Using $n = j$ in inequality (3.61) and Lemma 3.3 together with assumption (3.63) we get

$$w_0\|\mathcal{H}_c\varrho^{j+1}\|_h^2 \leq \sum_{k=1}^{j}(w_{j-k} - w_{j-k+1})\|\mathcal{H}_c\varrho^k\|_h^2 + w_j\bar{\chi} \leq \left[\sum_{k=1}^{j}(w_{j-k} - w_{j-k+1}) + w_j\right]\bar{\chi}$$
$$= w_0\bar{\chi}.$$

Thus, (3.62) holds for all n. The norms $\|\mathcal{H}_c\varrho\|_h$ and $\|\varrho\|_h$ are equivalent, since

$$\frac{5}{12}\|\varrho\|_h \leq \|\mathcal{H}_c\varrho\|_h \leq \|\varrho\|_h. \tag{3.64}$$

Thus, (3.56) follows from (3.62) and the first inequality in (3.64). □

Now we will prove the main convergence theorem.

Theorem 3.5. *Let $u \in C^{6,3}([a,b] \times [0,T])$ be the solution of problem (3.31)-(3.33) and $\{U_i^n, 0 \leq i \leq N_x, 1 \leq n \leq N_t\}$ be the solution of the discrete problem (3.40)-(3.42). Then, the following result holds*

$$\|u_i^{n+1} - U_i^{n+1}\|_h \leq c(\Delta t^{2-\alpha}, \Delta t^2, h^4).$$

Proof. Let $\varphi_i^{n+1} = u_i^{n+1} - U_i^{n+1}$. Now subtracting the linear system (3.40)-(3.42) from (3.37)-(3.39) we get

$$\nu \mathcal{H}_c \left[w_0 \varphi_i^{n+1} - \sum_{k=1}^{n} (w_{n-k} - w_{n-k+1}) \varphi_i^k - w_n \varphi_i^0 \right] + q^{n+\sigma} \mathcal{H}_c \varphi_i^{n+\sigma} = p^{n+\sigma} \delta_x^2 \varphi_i^{n+\sigma} + {}_1\mathcal{R}_i^{n+\sigma}, \ 1 \le i \le N_x - 1, \tag{3.65}$$

$$\varphi_i^0 = 0, \quad 0 \le i \le N_x, \tag{3.66}$$

$$\varphi_0^n = 0, \quad \varphi_{N_x}^n = 0, \quad 1 \le n \le N_t. \tag{3.67}$$

Since $\varphi_i^{n+1} \in \mathcal{D}_h^*$, therefore applying Theorem 3.4 for the error equation (3.65)-(3.67) we have

$$\|\varphi^{n+1}\|_h^2 \le c \max_{0 \le l \le N_t - 1} \|{}_1\mathcal{R}^{l+\sigma}\|_h^2, \qquad 0 \le n \le N_t - 1. \tag{3.68}$$

Since we have the following truncation error bound

$$\max_{0 \le l \le N_t - 1} \|{}_1\mathcal{R}^{l+\sigma}\|_h = \mathcal{O}(\Delta t^{2-\alpha}, \Delta t^2, h^4),$$

therefore, using it in equation (3.68) yields the result. □

3.3.2 Stability and convergence analysis of CFD$_2$ scheme

Here, we first define the inner product $\langle .,. \rangle$ for any grid functions v, $\vartheta \in \mathcal{D}_h^*$ as follows

$$\langle v, \vartheta \rangle = h \sum_{i=0}^{N_x - 1} \delta_x v_{i+\frac{1}{2}} \cdot \delta_x \vartheta_{i+\frac{1}{2}} - \frac{h^2}{12} h \sum_{i=1}^{N_x - 1} \delta_x^2 v_i \cdot \delta_x^2 \vartheta_i. \tag{3.69}$$

Lemma 3.10. *[95] For any grid function $\vartheta \in \mathcal{D}_h^*$, the following inequality holds*

$$\|\vartheta\|_\infty \le \frac{\sqrt{b-a}}{2} |\vartheta|_1.$$

Lemma 3.11. *For any grid function $\vartheta \in \mathcal{D}_h^*$, the following inequalities hold*

$$\frac{2}{3}|\vartheta|_1^2 \leq \langle \vartheta, \vartheta \rangle \leq |\vartheta|_1^2.$$

Proof. From equation (3.69) we have

$$\begin{aligned}
\langle \vartheta, \vartheta \rangle &= h \sum_{i=0}^{N_x-1} \left(\delta_x \vartheta_{i+\frac{1}{2}} \right)^2 - \frac{h^2}{12} h \sum_{i=1}^{N_x-1} \left(\delta_x^2 \vartheta_i \right)^2, \\
&\leq h \sum_{i=0}^{N_x-1} \left(\delta_x \vartheta_{i+\frac{1}{2}} \right)^2, \\
&= |\vartheta|_1^2.
\end{aligned}$$

Now

$$\begin{aligned}
\langle \vartheta, \vartheta \rangle &= h \sum_{i=0}^{N_x-1} \left(\delta_x \vartheta_{i+\frac{1}{2}} \right)^2 - \frac{h^2}{12} h \sum_{i=1}^{N_x-1} \left(\delta_x^2 \vartheta_i \right)^2, \\
&= |\vartheta|_1^2 - \frac{h^2}{12} \|\delta_x^2 \vartheta\|^2, \\
&\geq \frac{2}{3}|\vartheta|_1^2, \ \left(\text{using the inverse estimate} \|\delta_x^2 \vartheta\| \leq \frac{2}{h}|\vartheta|_1 \right).
\end{aligned}$$

Thus, we have the proof. □

Let $\hat{u}_i^j$ solve the following problem

$$\nu \mathcal{H}_c \left[c_0 \hat{u}_i^{n+1} - \sum_{j=1}^{n} (c_{n-j} - c_{n-j+1}) \hat{u}_i^j - c_n \hat{u}_i^0 \right] + q^{n+1} \mathcal{H}_c \hat{u}_i^{n+1} = p^{n+1} \delta_x^2 \hat{u}_i^{n+1}$$
$$+ \mathcal{H}_c F_i^{n+1}, \ 1 \leq i \leq N_x - 1, \tag{3.70}$$

$$\hat{u}_i^0 = g(x_i) + \gamma_i, \quad 0 \leq i \leq N_x, \tag{3.71}$$

$$\hat{u}_0^n = \phi_1(t_n), \quad \hat{u}_{N_x}^n = \phi_2(t_n), \quad 1 \leq n \leq N_t. \tag{3.72}$$

Suppose $e_i^j = \hat{u}_i^j - U_i^j$. Then, from equations (3.70)-(3.72) and (3.47)-(3.49), it is evident that $e_i^j \in \mathcal{D}_h^*$ and solves the following linear system

$$\nu \mathcal{H}_c \left[c_0 e_i^{n+1} - \sum_{j=1}^{n} (c_{n-j} - c_{n-j+1}) e_i^j - c_n e_i^0 \right] + q^{n+1} \mathcal{H}_c e_i^{n+1} = p^{n+1} \delta_x^2 e_i^{n+1},$$

$$1 \leq i \leq N_x - 1, \tag{3.73}$$

$$e_i^0 = \gamma_i, \quad 0 \leq i \leq N_x, \tag{3.74}$$

$$e_0^n = 0, \quad e_{N_x}^n = 0, \quad 1 \leq n \leq N_t. \tag{3.75}$$

Theorem 3.6. *The solution to the discrete problem (3.73)-(3.75) satisfies*

$$\|e^{n+1}\|_\infty \leq \sqrt{\frac{3(b-a)}{8}} |e^0|_1, \tag{3.76}$$

Proof. On multiplying equation (3.73) by $h(-\delta_x^2 e_i^{n+1})$, summing over i for $i = 1, 2, \ldots, N_x - 1$, we have

$$h \sum_{i=1}^{N_x-1} (-\delta_x^2 e_i^{n+1}) \left[\left(1 + \frac{h^2}{12}\delta_x^2\right) \left(c_0 e_i^{n+1} - \sum_{j=1}^{n} (c_{n-j} - c_{n-j+1}) e_i^j - c_n e_i^0 \right) \right]$$
$$+ \frac{q^{n+1}}{\nu} h \sum_{i=1}^{N_x-1} (-\delta_x^2 e_i^{n+1}) \left(1 + \frac{h^2}{12}\delta_x^2\right) e_i^{n+1} = -\frac{p^{n+1}}{\nu} h \sum_{i=1}^{N_x-1} (\delta_x^2 e_i^{n+1})^2.$$

Applying the summation formula by parts and using equation (3.75), we get

$$h \sum_{i=0}^{N_x-1} (\delta_x e_{i+1/2}^{n+1}) \left[c_0 \delta_x e_{i+1/2}^{n+1} - \sum_{j=1}^{n} (c_{n-j} - c_{n-j+1}) \delta_x e_{i+1/2}^j - c_n \delta_x e_{i+1/2}^0 \right]$$
$$- \frac{h^2}{12} h \sum_{i=1}^{N_x-1} \delta_x^2 e_i^{n+1} \left[c_0 \delta_x^2 e_i^{n+1} - \sum_{j=1}^{n} (c_{n-j} - c_{n-j+1}) \delta_x^2 e_i^j - c_n \delta_x^2 e_i^0 \right] + \frac{q^{n+1}}{\nu}$$
$$\times \left[h \sum_{i=0}^{N_x-1} (\delta_x e_{i+1/2}^{n+1})^2 - \frac{h^2}{12} h \sum_{i=1}^{N_x-1} (\delta_x^2 e_i^{n+1})^2 \right] = -\frac{p^{n+1}}{\nu} h \sum_{i=1}^{N_x-1} (\delta_x^2 e_i^{n+1})^2.$$

Arranging the terms of the above equation we get

$$
\begin{aligned}
c_0 &\left(h\sum_{i=0}^{N_x-1}(\delta_x e_{i+1/2}^{n+1})^2 - \frac{h^2}{12}h\sum_{i=1}^{N_x-1}(\delta_x^2 e_i^{n+1})^2 \right) - \sum_{j=1}^{n}(c_{n-j}-c_{n-j+1}) \\
&\qquad \times \left(h\sum_{i=0}^{N_x-1}(\delta_x e_{i+1/2}^{j})(\delta_x e_{i+1/2}^{n+1}) - \frac{h^2}{12}h\sum_{i=1}^{N_x-1}(\delta_x^2 e_i^{j})(\delta_x^2 e_i^{n+1}) \right) \\
&- c_n\left(h\sum_{i=0}^{N_x-1}(\delta_x e_{i+1/2}^{0})(\delta_x e_{i+1/2}^{n+1}) - \frac{h^2}{12}h\sum_{i=1}^{N_x-1}(\delta_x^2 e_i^{0})(\delta_x^2 e_i^{n+1}) \right) + \frac{q^{n+1}}{\nu} \\
&\times \left[h\sum_{i=0}^{N_x-1}(\delta_x e_{i+1/2}^{n+1})^2 - \frac{h^2}{12}h\sum_{i=1}^{N_x-1}(\delta_x^2 e_i^{n+1})^2 \right] = -\frac{p^{n+1}}{\nu}h\sum_{i=1}^{N_x-1}(\delta_x^2 e_i^{n+1})^2.
\end{aligned}
$$

Thus, using the definition (3.69), we have

$$
\begin{aligned}
\left(c_0 + \frac{q^{n+1}}{\nu}\right)\langle e^{n+1}, e^{n+1}\rangle = \sum_{j=1}^{n}(c_{n-j}-c_{n-j+1})\langle e^{j}, e^{n+1}\rangle + c_n\langle e^{0}, e^{n+1}\rangle \\
- \frac{p^{n+1}}{\nu}\|\delta_x^2 e^{n+1}\|^2,
\end{aligned}
$$

which can also be written as

$$
c_0\langle e^{n+1}, e^{n+1}\rangle \leq \sum_{j=1}^{n}(c_{n-j}-c_{n-j+1})\langle e^{j}, e^{n+1}\rangle + c_n\langle e^{0}, e^{n+1}\rangle.
$$

Here, we make an assumption that we have verified numerically to hold. Assume that for $\alpha \in (0, \bar{\alpha})$, the coefficients c_j $(0 \leq j \leq n, n \geq 2)$ satisfy

$$
c_0 > c_1 > c_2 > \cdots > c_n. \tag{3.77}
$$

Now, using the Cauchy-Schwarz inequality, we get

$$
\begin{aligned}
c_0\langle e^{n+1}, e^{n+1}\rangle \leq \frac{1}{2}\sum_{j=1}^{n}(c_{n-j}-c_{n-j+1})(\langle e^{j}, e^{j}\rangle + \langle e^{n+1}, e^{n+1}\rangle) + \frac{1}{2}c_n(\langle e^{0}, e^{0}\rangle \\
+ \langle e^{n+1}, e^{n+1}\rangle).
\end{aligned}
$$

Equivalently,

$$\begin{aligned} c_0\langle e^{n+1}, e^{n+1}\rangle \leq & \frac{1}{2}(c_0 - c_n)\langle e^{n+1}, e^{n+1}\rangle + \frac{1}{2}\sum_{j=1}^{n}(c_{n-j} - c_{n-j+1})\langle e^j, e^j\rangle + \frac{1}{2}c_n\langle e^0, e^0\rangle \\ & + \frac{1}{2}c_n\langle e^{n+1}, e^{n+1}\rangle. \end{aligned}$$

Thus, we have

$$c_0\langle e^{n+1}, e^{n+1}\rangle \leq \sum_{j=1}^{n}(c_{n-j} - c_{n-j+1})\langle e^j, e^j\rangle + c_n\langle e^0, e^0\rangle. \tag{3.78}$$

Now, we prove by induction that

$$\langle e^{n+1}, e^{n+1}\rangle \leq \langle e^0, e^0\rangle, \quad n = 0, 1, \ldots, N_t - 1. \tag{3.79}$$

Put $n = 0$ in equation (3.78) to get

$$\langle e^1, e^1\rangle \leq \langle e^0, e^0\rangle$$

which is identical to (3.79) for $n = 0$. Further, let us assume that (3.79) holds for $k = 0, 1, \ldots, n$, that is,

$$\langle e^k, e^k\rangle \leq \langle e^0, e^0\rangle, \quad k = 1, 2, \ldots, n. \tag{3.80}$$

The inequality (3.78) together with the assumption (3.80) yield

$$\begin{aligned} c_0\langle e^{n+1}, e^{n+1}\rangle &\leq \sum_{j=1}^{n}(c_{n-j} - c_{n-j+1})\langle e^j, e^j\rangle + c_n\langle e^0, e^0\rangle \\ &\leq \left[\sum_{j=1}^{n}(c_{n-j} - c_{n-j+1}) + c_n\right]\langle e^0, e^0\rangle = c_0\langle e^0, e^0\rangle. \end{aligned}$$

Thus, (3.79) holds for all n. Finally, combining inequality (3.79) with Lemmas 3.10 and 3.11, we have

$$\|e^{n+1}\|_\infty^2 \leq \frac{(b-a)}{4}|e^{n+1}|_1^2 \leq \frac{3(b-a)}{8}\langle e^{n+1}, e^{n+1}\rangle \leq \frac{3(b-a)}{8}\langle e^0, e^0\rangle \leq \frac{3(b-a)}{8}|e^0|_1^2,$$

which completes the proof. □

Now we will prove the main convergence theorem.

Theorem 3.7. *Let $u \in C^{6,3}([a,b]\times[0,T])$ be the solution of problem (3.31)-(3.33) and $\{U_i^n, 0 \leq i \leq N_x, 1 \leq n \leq N_t\}$ be the solution of the discrete problem (3.47)-(3.49). Then, the following result holds*

$$\|u_i^{n+1} - U_i^{n+1}\|_\infty \leq c(\Delta t^{3-\alpha}, h^4). \tag{3.81}$$

Proof. Let $\rho_i^{n+1} = u_i^{n+1} - U_i^{n+1}$. Now subtracting the linear system (3.47)-(3.49) from (3.44)-(3.46) we get

$$\nu\mathcal{H}_c\left[c_0\rho_i^{n+1} - \sum_{j=1}^{n}(c_{n-j} - c_{n-j+1})\rho_i^j\right] + q^{n+1}\mathcal{H}_c\rho_i^{n+1} = p^{n+1}\delta_x^2\rho_i^{n+1} + {}_2\mathcal{R}_i^{n+1},$$

$$1 \leq i \leq N_x - 1, \tag{3.82}$$

$$\rho_i^0 = 0, \quad 0 \leq i \leq N_x, \tag{3.83}$$

$$\rho_0^n = 0, \quad \rho_{N_x}^n = 0, \quad 1 \leq n \leq N_t. \tag{3.84}$$

On multiplying equation (3.82) by $h(-\delta_x^2\rho_i^{n+1})$ and summing over i for $i = 1, 2, \ldots, N_x - 1$, we have

$$\left(c_0 + \frac{q^{n+1}}{\nu}\right)\langle\rho^{n+1}, \rho^{n+1}\rangle = \sum_{j=1}^{n}(c_{n-j} - c_{n-j+1})\langle\rho^j, \rho^{n+1}\rangle - \frac{p^{n+1}}{\nu}\|\delta_x^2\rho^{n+1}\|^2$$

$$-\frac{h}{\nu}\sum_{i=1}^{N_x-1}(\delta_x^2\rho_i^{n+1})({}_2\mathcal{R}_i^{n+1}) = \mathcal{D}_1 + \mathcal{D}_2 + \mathcal{D}_3, \qquad (3.85)$$

where

$$\mathcal{D}_1 = \sum_{j=1}^{n}(c_{n-j} - c_{n-j+1})\langle\rho^j, \rho^{n+1}\rangle \leq \frac{1}{2}(c_0 - c_n)\langle\rho^{n+1}, \rho^{n+1}\rangle + \frac{1}{2}\sum_{j=1}^{n}(c_{n-j} - c_{n-j+1}) \times \langle\rho^j, \rho^j\rangle,$$

$$\mathcal{D}_2 = -\frac{p^{n+1}}{\nu}\|\delta_x^2\rho^{n+1}\|^2,$$

and

$$\begin{aligned}\mathcal{D}_3 = &-\frac{1}{\nu}h\sum_{i=1}^{N_x-1}(\delta_x^2\rho_i^{n+1})({}_2\mathcal{R}_i^{n+1}) \leq \frac{1}{\nu}\left[p^{n+1}\|\delta_x^2\rho^{n+1}\|^2 + \frac{1}{4p^{n+1}}\|{}_2R^{n+1}\|^2\right] \\ \leq &\frac{p^{n+1}}{\nu}\|\delta_x^2\rho^{n+1}\|^2 + \frac{\Delta t^\alpha}{4p^{n+1}}\|{}_2\mathcal{R}^{n+1}\|^2 \leq \frac{p^{n+1}}{\nu}\|\delta_x^2\rho^{n+1}\|^2 + c^*\Delta t^\alpha(\Delta t^{3-\alpha}, h^4)^2,\end{aligned}$$

with c^* a positive constant.

Now substituting the values of $\mathcal{D}_1$, $\mathcal{D}_2$, and $\mathcal{D}_3$ in equation (3.85) and noticing $c_n > 0$, $\frac{q^{n+1}}{\nu} > 0$, yields

$$c_0\langle\rho^{n+1}, \rho^{n+1}\rangle \leq \sum_{j=1}^{n}(c_{n-j} - c_{n-j+1})\langle\rho^j, \rho^j\rangle + \tilde{\gamma}\Delta t^\alpha(\Delta t^{3-\alpha}, h^4)^2, \qquad (3.86)$$

where $\tilde{\gamma} = 2c^*$.

Now we prove by induction that

$$\langle\rho^{n+1}, \rho^{n+1}\rangle \leq \tilde{\gamma}c_n^{-1}\Delta t^\alpha(\Delta t^{3-\alpha}, h^4)^2, \quad n = 0, 1, \ldots, N_t - 1. \qquad (3.87)$$

Put $n = 0$ in equation (3.86) to get

$$\langle \rho^1, \rho^1 \rangle \leq \tilde{\gamma} c_0^{-1} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2,$$

which is identical to (3.87) for $n = 0$. Now let us assume that (3.87) holds for $k = 0, 1, \ldots, n$, that is

$$\langle \rho^k, \rho^k \rangle \leq \tilde{\gamma} c_{k-1}^{-1} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2, \quad k = 1, 2, \ldots, n. \tag{3.88}$$

The inequality (3.86) together with (3.77) and assumption (3.88) yield

$$\begin{aligned} c_0 \langle \rho^{n+1}, \rho^{n+1} \rangle &\leq \sum_{j=1}^{n} (c_{n-j} - c_{n-j+1}) \tilde{\gamma} c_{j-1}^{-1} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2 + \tilde{\gamma} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2 \\ &\leq \sum_{j=1}^{n} (c_{n-j} - c_{n-j+1}) \tilde{\gamma} c_{n}^{-1} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2 + \tilde{\gamma} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2. \end{aligned}$$

Equivalently,

$$c_0 \langle \rho^{n+1}, \rho^{n+1} \rangle \leq (c_0 - c_n) \tilde{\gamma} c_n^{-1} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2 + \tilde{\gamma} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2,$$

which gives

$$\langle \rho^{n+1}, \rho^{n+1} \rangle \leq \tilde{\gamma} c_n^{-1} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2.$$

Thus, (3.87) holds for all n. Now, combining inequality (3.87) with Lemmas 3.10 and 3.11, we have

$$\|\rho^{n+1}\|_{\infty}^2 \leq \frac{(b-a)}{4} |\rho^{n+1}|_1^2 \leq \frac{3(b-a)}{8} \langle \rho^{n+1}, \rho^{n+1} \rangle \leq \frac{3(b-a)}{8} \tilde{\gamma} c_n^{-1} \Delta t^{\alpha} (\Delta t^{3-\alpha}, h^4)^2.$$

Finally, using Lemma 3.5 with $n\Delta t \leq T$ yields (3.81). Thus, we have the proof. $\square$

3.4 Numerical results

In this segment, we present numerical results for three test problems to assess the practical performance of the proposed numerical scheme. If $u(x_i, t_n)$ and $U(x_i, t_n)$ are the exact and approximate solutions of problem (3.31)-(3.33) respectively at the grid point (x_i, t_n), then the accuracy of the numerical solution is measured as follows

$$\mathcal{L}_\infty(h, \Delta t) = \|u - U\|_\infty = \max_{1\leq n\leq N_t} \max_{1\leq i\leq N_x} |u(x_i, t_n) - U(x_i, t_n)|, \tag{3.89}$$

$$\mathcal{L}_2(h, \Delta t) = \|u - U\|_2 = \max_{1\leq n\leq N_t} \sqrt{h \sum_{i=1}^{N_x-1} (u(x_i, t_n) - U(x_i, t_n))^2}. \tag{3.90}$$

The following formula is used to evaluate the order of convergence

$$cov.order = \begin{cases} log_2\left(\frac{\mathcal{L}_l(h,\Delta t_1)}{\mathcal{L}_l(h,\Delta t_2)}\right), & \text{in time}, \\ log_2\left(\frac{\mathcal{L}_l(h_1,\Delta t)}{\mathcal{L}_l(h_2,\Delta t)}\right), & \text{in space}, \end{cases} \tag{3.91}$$

where $l = 2$ or ∞.

Example 3.1. [101] Let us consider the function $f(t) = t^4$.

We numerically compute the Caputo-Prabhakar derivative of order $0 < \alpha < 1$ of this function using CPL2-1_σ and CPL-2 type formulas. The Caputo-Prabhakar derivative of $f(t)$ is given by

$${}^{CP}_{\ 0}D^{\eta}_{\beta,\alpha,\kappa} f(t) = 24t^{4-\alpha} E^{-\eta}_{\beta,5-\alpha}(\kappa t^{\beta}). \tag{3.92}$$

First, we take a positive integer N_t and let $\Delta t = 1/(N_t - 1 + \sigma)$. We evaluate the α-order Caputo-Prabhakar derivative of $f(t)$ at $t = t_{N_t-1+\sigma} = 1$ numerically using

CPL2-1_σ formula. Further, we use CPL-2 formula at $t = t_{N_t} = 1$, taking $\Delta t = 1/N_t$ for the approximation of the Caputo-Prabhakar derivative.

TABLE 3.1: (Example 3.1) Comparison with method in [101] taking different Δt and α using CPL2-1_σ formula.

		$NS1$ scheme[101]		CPL2-1_σ formula	
α	N_t	$\mathcal{L}_\infty$-error	cov.order$_t$	$\mathcal{L}_\infty$-error	cov.order$_t$
0.2	100	2.92662e-04	-	2.21262e-05	-
	200	8.86059e-05	1.723757659	5.61906e-06	1.977358603
	400	2.65645e-05	1.737904658	1.44343e-06	1.960819923
	800	7.90371e-06	1.748897714	3.73923e-07	1.948694524
0.4	100	1.47581e-03	-	6.35471e-05	-
	200	4.96921e-04	1.570416172	1.82866e-05	1.797036120
	400	4.96921e-04	1.580328503	5.35648e-06	1.771431898
	800	5.53033e-05	1.587249740	1.58794e-06	1.754128065
0.6	100	5.71319e-03	-	1.81328e-04	-
	200	2.17575e-03	1.392781457	5.98205e-05	1.599896952
	400	8.25247e-04	1.398617328	2.01229e-05	1.571798676
	800	3.12264e-04	1.402056679	6.85475e-06	1.553663984

Table 3.1 provides a comparative analysis between our findings and those of a prior study [101], showcasing both the maximum absolute error and the order of convergence. This table shows that the convergence order, when employing the CPL2-1_σ formula for various fractional orders, is at least $2-\alpha$ at $t = t_{N_t-1+\sigma} = 1$. This result aligns with the findings in [101], although the proposed methodology showcases improved error accuracy. Likewise, Table 3.2 exhibits the maximum absolute error and convergence order attained by utilising the CPL-2 formula. This table further demonstrates that the convergence order across various fractional orders achieved by applying the CPL-2 formula is approximately $3-\alpha$. This result mirrors the findings in [101], while our work showcases an enhanced order of accuracy.

TABLE 3.2: (Example 3.1) Comparison with method in [101] taking different Δt and α using CPL-2 formula.

		$NS2$ scheme[101]		CPL-2 formula	
α	N_t	$\mathcal{L}_\infty$-error	cov.order$_t$	$\mathcal{L}_\infty$-error	cov.order$_t$
0.2	100	3.32797e-06	-	5.11628e-07	-
	200	4.99005e-07	2.737515094	7.60127e-08	2.750783006
	400	7.41959e-08	2.749644469	1.12215e-08	2.759972443
	800	7.41959e-08	2.758787851	1.64838e-09	2.767144093
0.4	100	1.71402e-05	-	3.00994e-06	-
	200	2.86770e-06	2.579412678	4.99298e-07	2.591762886
	400	4.77128e-07	2.587447205	8.25311e-08	2.596891139
	800	7.90924e-08	2.587447205	1.36097e-08	2.600294373
0.6	100	6.88032e-05	-	1.37821e-05	-
	200	1.30627e-05	2.397022839	2.59835e-06	2.407125862
	400	2.47207e-06	2.401662957	4.89143e-07	2.409269094
	800	4.67021e-07	2.404159009	9.20220e-08	2.410206949

TABLE 3.3: (Example 3.2) Comparison with method in [101] taking $\alpha = 0.85$ and $N_x = 512$.

	$NS1$ scheme[101]		CFD$_1$ scheme	
N_t	$\mathcal{L}_\infty$-error	cov.order$_t$	$\mathcal{L}_\infty$-error	cov.order$_t$
20	7.50178e-04	-	1.68162e-04	-
40	3.33834e-04	1.1681013956	4.53720e-05	1.8899776611
80	1.47578e-04	1.1776528864	1.27086e-05	1.8359933113
160	6.43087e-05	1.1983931954	3.73784e-06	1.7655324942

Example 3.2. [101] Let us consider problem (3.31)-(3.33) on the domain $(0,1) \times (0,1]$ with the assumption that the function $u(x,t) = \sin(\pi x) + x(x-1)t^2$ is the exact solution.

We have solved this problem taking $\alpha = 0.85$, $p(t) = 1$, and $q(t) = 0$, and display

TABLE 3.4: (Example 3.2) Comparison with method in [101] taking $\alpha = 0.85$ and $N_x = 512$.

N_t	$NS2$ scheme[101] $\mathcal{L}_\infty$-error	cov.order$_t$	CFD$_2$ scheme $\mathcal{L}_\infty$-error	cov.order$_t$
20	1.38449e-04	-	2.3980e-05	-
40	3.80566e-05	1.863134649	1.0177e-05	1.232051516
80	1.06408e-05	1.838532264	3.5290e-06	1.527988936
160	3.10503e-06	1.776936275	1.0938e-06	1.689906557

the results in Tables 3.3, 3.4, and 3.5. In Table 3.3, we compare the proposed scheme CFD$_1$ with the scheme $NS1$ in [101] and show that the temporal order of convergence obtained using the CFD$_1$ scheme is at least $2-\alpha$, which is the same as in [101], but order of accuracy has been increased in our work. Similarly, Table 3.4 displays the temporal order of convergence obtained using the CFD$_2$ scheme. The table shows that the convergence order for both NS2 and CFD$_2$ schemes falls below $3-\alpha$, primarily due to the unmet conditions on u. However, the comparison does indicate a noticeable enhancement in the error accuracy achieved within our study. In Table 3.5, we present the $\mathcal{L}_\infty$-error obtained using the CFD$_1$ and CFD$_2$ schemes for different values of discretization parameter N_x with $N_t = 600$ and compare with $NS1$ and $NS2$ schemes. From this table, we see that the error decreases as N_x increases and error accuracy has been improved in the CFD$_1$ and CFD$_2$ schemes as compared to the $NS1$ and $NS2$ schemes. Further, Table 3.6 shows the $\mathcal{L}_2$-error and spatial order of convergence obtained using the CFD$_1$ and CFD$_2$ schemes for different fractional orders. Analyzing this table, it becomes apparent that both the CFD$_1$ and CFD$_2$ schemes exhibit fourth-order accuracy in the spatial direction. In contrast, the $NS1$ and $NS2$ schemes proposed in [101] are limited to second-order accuracy.

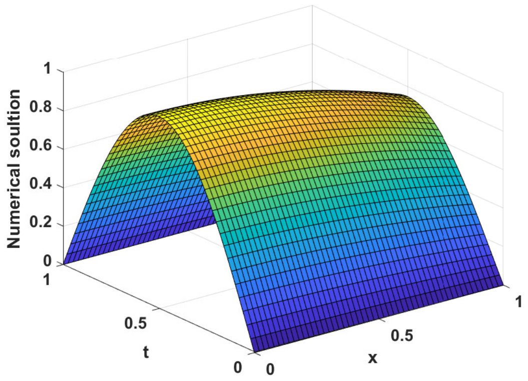
Table 3.5: (Example 3.2) Comparison with method in [101] taking $N_t = 600$ and $\alpha = 0.85$.

N_x	$NS1$ scheme[101]	CFD$_1$ scheme	$NS2$ scheme[101]	CFD$_2$ scheme
10	8.00858e-03	3.96655e-05	8.02309e-03	3.92385e-05
20	1.98427e-03	2.87219e-06	1.99880e-03	2.44541e-06
40	4.84736e-04	5.79700e-07	4.99266e-04	1.52932e-07
80	1.10259e-04	4.36530e-07	1.24789e-04	9.87363e-08
160	1.66651e-05	4.27583e-07	3.11959e-05	9.81658e-08

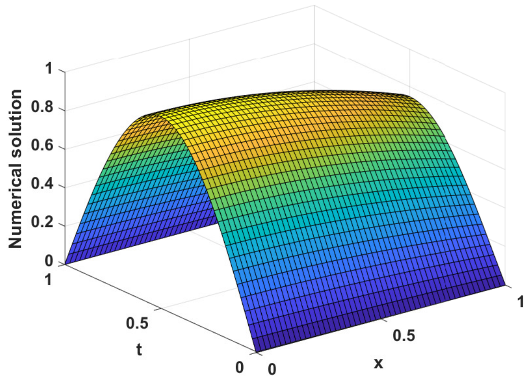
Table 3.6: (Example 3.2) $\mathcal{L}_2$-error, $\mathcal{L}_\infty$-error and respective spatial orders of convergence taking different α and $N_t = 7000$.

		CFD$_1$ scheme		CFD$_2$ scheme	
α	N_x	$\mathcal{L}_2$-error	cov.order$_x$	$\mathcal{L}_2$-error	cov.order$_x$
0.2	2^2	1.0172e-03	-	1.4385e-03	-
	2^3	6.2415e-05	4.0266	8.8267e-05	4.0265
	2^4	3.8834e-06	4.0065	5.4914e-06	4.0066
	2^5	2.4272e-07	3.9999	3.4282e-07	4.0017
0.5	2^2	1.0508e-03	-	1.4860e-03	-
	2^3	6.4473e-05	4.0266	9.1177e-05	4.0266
	2^4	4.0119e-06	4.0063	5.6725e-06	4.0066
	2^5	2.5131e-07	3.9968	3.5412e-07	4.0017
0.8	2^2	1.0972e-03	-	1.5517e-03	-
	2^3	6.7325e-05	4.0266	9.5204e-05	4.0267
	2^4	4.1940e-06	4.0048	5.9230e-06	4.0066
	2^5	2.6725e-07	3.9721	3.6976e-07	4.0017

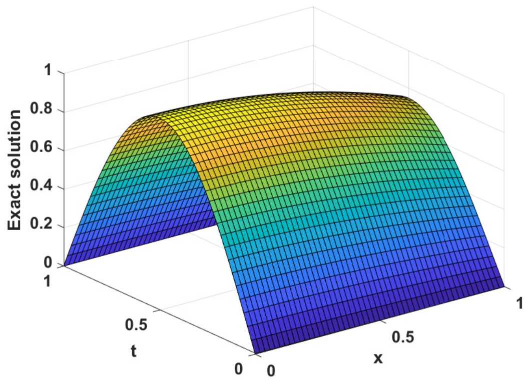
Moreover, in Figure 3.1, we plot the three-dimensional graphics of numerical solutions obtained using the CFD$_1$ and CFD$_2$ schemes and the exact solution of Example 3.2 taking $p(t) = 1$, and $q(t) = 0$. Obviously, this figure compares the numerical and exact solutions and we see good approximations using the CFD$_1$ and CFD$_2$ schemes.



(a) CFD$_1$ scheme



(b) CFD$_2$ scheme

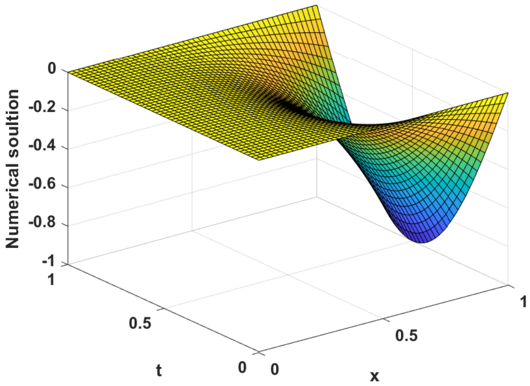


(c) Exact solution

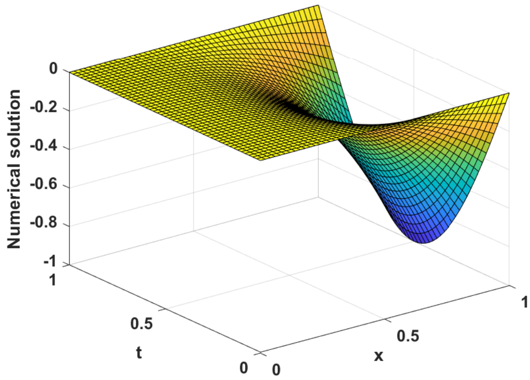
FIGURE 3.1: Comparing numerical and exact solutions of Example 3.2 with $\alpha = 0.6$ $M = N = 50$.

Example 3.3. Let us consider problem (3.31)-(3.33) on the domain $(0, 1) \times (0, 1]$ with the assumption that the function $u(x, t) = t^3 \cos\left(\pi x + \frac{\pi}{2}\right)$ is the exact solution.

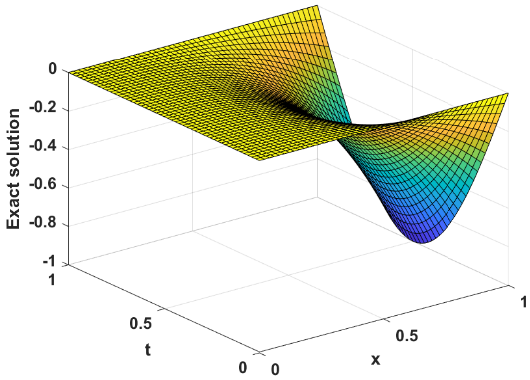
We have solved this problem taking $p(t) = t$, $q(t) = 1 - \sin(t)$, with the outcomes being showcased in Tables 3.7 and 3.8. Table 3.7 shows the $\mathcal{L}_2$-errors, temporal and spatial order of convergence for different fractional orders obtained using the CFD$_1$ scheme. From this table, we observe that the temporal and spatial orders of convergence are at least $2 - \alpha$ and 4, respectively, the same as the theoretical orders. Similarly, Table 3.8 displays $\mathcal{L}_\infty$-error, temporal and spatial convergence orders obtained using the CFD$_2$ scheme. This table indicates that the temporal



(a) CFD_1 scheme



(b) CFD_2 scheme



(c) Exact solution

FIGURE 3.2: Comparing numerical and exact solutions of Example 3.3 with $\alpha = 0.4$ $M = N = 50$.

and spatial orders of convergence are almost $3 - \alpha$ and 4, respectively, which are in agreement with the theory.

Moreover, Figure 3.2 compares the exact and numerical solutions using the CFD_1 and CFD_2 methods for Example 3.3. The graph illustrates close agreement between the two, highlighting the effective approximation of the proposed schemes.

TABLE 3.7: (Example 3.3) $\mathcal{L}_2$-error and corresponding order of convergence using CFD_1 scheme.

α	N_x	N_t	$\mathcal{L}_2$-error	cov.order$_t$	N_t	N_x	$\mathcal{L}_2$-error	cov.order$_x$
0.2	500	20	4.1356e-04	-	5000	2^2	9.6170e-04	-
		40	1.0259e-04	2.0112		2^3	5.9008e-05	4.0266
		80	2.5456e-05	2.0108		2^4	3.6646e-06	4.0092
		160	6.3247e-06	2.0089		2^5	2.2226e-07	4.0434
0.5	500	20	9.0712e-04	-	5000	2^2	8.9759e-04	-
		40	2.3608e-04	1.9420		2^3	5.5068e-05	4.0268
		80	6.1976e-05	1.9295		2^4	3.4085e-06	4.0140
		160	1.6442e-05	1.9143		2^5	1.9525e-07	4.1258
0.8	500	20	1.5779e-03	-	5000	2^2	8.1419e-04	-
		40	4.7199e-04	1.7412		2^3	4.9879e-05	4.0289
		80	1.4717e-04	1.6813		2^4	3.0073e-06	4.0519
		160	4.7815e-05	1.6219		2^5	1.6228e-07	4.2119

TABLE 3.8: (Example 3.3) $\mathcal{L}_\infty$-error and corresponding order of convergence using CFD_2 scheme.

α	N_x	N_t	$\mathcal{L}_\infty$-error	cov.order$_t$	N_t	N_x	$\mathcal{L}_\infty$-error	cov.order$_x$
0.2	500	20	1.3165e-05	-	5000	2^2	1.3601e-03	-
		40	2.2132e-06	2.5725		2^3	8.3460e-05	4.0264
		80	3.5867e-07	2.6254		2^4	5.1924e-06	4.0066
		160	5.6396e-08	2.6690		2^5	3.2415e-07	4.0016
0.5	500	20	9.0651e-05	-	5000	2^2	1.2694e-03	-
		40	1.7347e-05	2.3857		2^3	7.7905e-05	4.0263
		80	3.2115e-06	2.4333		2^4	4.8468e-06	4.0066
		160	5.8216e-07	2.4638		2^5	3.0263e-07	4.0014
0.8	500	20	4.0463e-04	-	5000	2^2	1.1516e-03	-
		40	9.1946e-05	2.1377		2^3	7.0685e-05	4.0261
		80	2.0365e-05	2.1747		2^4	4.3989e-06	4.0062
		160	4.4496e-06	2.1943		2^5	2.7581e-07	3.9954

3.5 Conclusion

In this chapter, we have introduced two novel difference approximations for the Caputo-Prabhakar time-fractional derivative, namely CPL2-1_σ and CPL-2, with approximation orders $\mathcal{O}\left(\Delta t^{2-\alpha}\right)$ and $\mathcal{O}\left(\Delta t^{3-\alpha}\right)$, respectively. The fundamental features of these difference operators are discussed. Subsequently, we constructed two novel discrete schemes, namely CFD_1 and CFD_2, for solving the Caputo-Prabhakar fractional reaction-diffusion equation with variable coefficients. These schemes possess temporal orders of $2-\alpha$ and $3-\alpha$, respectively, while simultaneously maintaining a spatial accuracy of order four. The theoretical analysis, including the stability and convergence of both schemes, has been rigorously discussed using the discrete energy method. The convergence orders $\mathcal{O}(\Delta t^{2-\alpha}, \Delta t^2, h^4)$ and $\mathcal{O}(\Delta t^{3-\alpha}, h^4)$, respectively, of the CFD_1 and CFD_2 schemes have improved the existing works and are best to date for the variable coefficients Caputo-Prabhakar fractional reaction-diffusion equation. Finally, the current schemes have been implemented on three test problems, thus confirming the theoretical results and showing the viability of the proposed schemes.