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A Numerical Iterative Scheme for Solving Nonlinear Boundary Value Problems of Fractional Order $0 < \alpha < 1$

Muhammad Adnan Anwar
Department of Mathematics,
University of Engineering and Technology, Lahore, Pakistan.
Email: bssm.10.20@gmail.com

Shafiq Ur Rehman
Department of Mathematics,
University of Engineering and Technology, Lahore, Pakistan.
Email: srehman@uet.edu.pk

Fayyaz Ahmad
Department de Física i Enginyeria Nuclear,
Universitat Politècnica de Catalunya, Eduard Maristany 10, Barcelona 08019, Spain.
Dipartimento di Scienza e Alta Tecnologia,
Universita dell'Insubria, Via Valleggio 11, Como 22100, Italy.
Email: fahmad@uninsubria.it

Muhammad Irfan Qadir
Department of Mathematics,
University of Engineering and Technology, Lahore, Pakistan.
Email: mirfan@uet.edu.pk

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Abstract. Accurate numerical approximations for solving non linear fractional order boundary value problems are presented in this paper. To accomplish this goal, first- and second-order derivatives involved in the developed scheme are approximated by central finite difference scheme of order four. Whereas, integrals in this work are approximated by the composite Simpson's rule in the Caputo's definition. The performance of the proposed iterative scheme is demonstrated by solving nonlinear fractional order boundary value problems of order $0 < \alpha < 1$.

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Key Words: Fractional differential equation, boundary value problem, central difference scheme, Simpson's rule, iterative scheme.

1. INTRODUCTION

Many real world problems are extensively modeled as differential equations (DEs). Ordinary differential equations (ODEs) have been applied in many areas of science and engineering, such as, physics, electronic engineering, and population dynamics. Partial differential equations (PDEs) are also encountered in several areas of engineering, applied sciences, and finance. In some cases, differential equations can be solved analytically, but mostly the differential equations are too-complicated to solve analytically, necessitating the use of numerical techniques to obtain numerical approximate solution. There are many methods for the discretization of differential equations, for instance, perturbation method [9, 19, 28]. Many numerical and analytical methods have been developed and illustrated to examine the solution of PDEs, such as, adomian decomposition method [1, 14], variational iterative method [18], homotopy perturbation method [2, 31]. For nonlinear PDEs, perturbation iteration technique, modified, and improved perturbation iteration technique have been developed [10]. A special type of nonlinear differential equations, namely, Lane-Emden, have been solved by optimal perturbation iterative method [13].

Fractional calculus (FC) presents a highly endorsement tool to evoke natural phenomena more realistically by making classy modeling of physical phenomena [25]. Much of the literature survey is available which cope with the theory and applications of fractional differential equations [8, 20, 23, 26, 30, 33, 34, 39]. Fractional differential equations arises in many scientific and engineering disciplines including: chemistry, physics, viscoelasticity, signal processing, mathematical biology, and fluid mechanics, as the mathematical modeling of structures and mechanisms in these fields involves derivatives of fractional order, see, for example [5, 7, 21, 41, 42]. Not only in applied mathematics, FC also has great applications in pure mathematics [35].
The idea of FC is almost as old as calculus itself. Basically, FC deals with the properties of derivatives and integrals of fractional order over real and complex domains. Simply, we can say FC is generalization of classical calculus. Particularly, it involves the study of fractional differential equations and their applications in daily life. Leibniz was the first person who gave the idea of generalizing the derivatives to fractional order in 1695 [26]. L'Hospital asked him, what if the order of a derivative is $1/2$? Leibniz replied, it will lead to a paradox, from which one day useful consequences will be drawn.
The first paper in which fractional derivative was mentioned, published in 1819 by S. F. Lacroix [38]. F. Lacroix started with $y = x^n$, for positive n and found its mth derivative

$$D_x^m y = \frac{d^m y}{dx^m} = \frac{n!}{(n-m)!} x^{n-m}. \tag{1. 1}$$

Using Legendre's symbol Γ which denotes the generalized factorial given in equation (2. 6) and by taking α, a constant, he obtained

$$D_x^m x^\alpha = \frac{d^m x^\alpha}{dx^m} = \frac{\Gamma(\alpha+1)}{\Gamma(\alpha-m+1)} x^{\alpha-m}. \tag{1. 2}$$

Then S. F. Lacroix put $\alpha = 1$ and $m = 1/2$ and obtained

$$D_x^{1/2} x = \frac{d^{1/2} x}{dx^{1/2}} = \frac{2\sqrt{x}}{\sqrt{\pi}}. \tag{1. 3}$$

Note that, the definition in equation (1. 2) gives a nonzero value for the fractional order derivative of a constant function, i.e., for $\alpha = 0$

$$D_x^m x^0 = \frac{d^m 1}{dx^m} = \frac{1}{\Gamma(1-m)} x^{-m} \neq 0. \tag{1. 4}$$

These are the basic developments of FC. These theoretical developments causes to bring revolution in FC. The first practical application of FC is due to Abel [3, 4].
Now a days, fractional differential equations with boundary conditions have become one of the crucial question of FC, because fractional order boundary value problems arise in the modeling of many complex systems, including: blood flow, thermo-elasticity, population dynamic, and underground water flow, see, for example [6, 11, 24, 40, 45]. These types of problems also arise in various physical process of stochastic transport and many applications in the liquid filtration in a strongly porous medium [46] .
Recently, various strategies have been introduced for the numerical approximation of fractional order differential equations, see, for example [15, 16, 17, 22, 27, 32, 36, 37, 43]. Several new techniques are created for the numerical approximation of linear fractional order boundary value problems [29]. In this paper, we develop a numerical iterative scheme for the approximation of nonlinear fractional order boundary value problems.
In the next section, we provide some preliminaries which are vital in the development of the proposed iterative scheme. In Section 3, the construction of the proposed scheme is discussed. Whereas, Section 4 describes the experimental framework used to illustrate the performance of the proposed iterative scheme. Finally, Section 5 presents overall conclusions based upon the numerical testing performed in Section 4. We also provide future directions in Section 5.

2. Notations and Preliminaries

We begin this section with some preliminaries of FC, in-particular, fractional derivatives and their formula which are used to develop the proposed iterative scheme for the numerical approximation of nonlinear fractional order boundary value problems.

Definition 2.1. *Suppose α is a positive real number. Then the fractional integral*

$$I_{a,x}^{-m} f(x) = \frac{1}{\Gamma(m)} \int_a^x \frac{f(t)}{(x-t)^{1-m}} dt, \tag{2. 5}$$

is called Riemann-Liouville integral of fractional order m. And Γ is a gamma function [44] *which is defined as*

$$\Gamma(w) = \int_0^\infty x^{w-1} e^{-x} dx, \quad \Re(w) > 0. \tag{2. 6}$$

Definition 2.2. *The Riemann-Liouville derivative of fractional order* α*, where* $(n-1 < \alpha < n)$ *and* n *is a positive integer, i.e.,* $n \in \mathbb{Z}^+$*, of the function* $f(t)$ *is given by*

$$\begin{aligned} {}_{RL}D^{\alpha}_{0,t} f(t) &= \frac{d^n}{dt^n} D^{-(n-\alpha)}_{0,t} f(t), \\ &= \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_0^t (t-\tau)^{n-(\alpha+1)} f(\tau) d\tau. \end{aligned} \tag{2. 7}$$

Definition 2.3. *In 1967, Italian mathematician M. Caputo introduced Caputo fractional derivative* [12] *which is defined as*

$$\begin{aligned} D^{\alpha}_{c} f(t) &= D^{-(n-\alpha)}_{c} \frac{d^n}{dt^n} f(t), \\ &= \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{f^{(n)}(\tau)}{(t-\tau)^{-(n-\alpha-1)}} d\tau. \end{aligned} \tag{2. 8}$$

A beautiful property of Caputo fractional derivative is that, it allows standard initial and boundary conditions in the modeling. Whereas, models based on other fractional derivatives could also require the values of fractional derivative terms at the initial time.

2.4. **Derivative approximation.** We approximate derivatives in the developed iterative scheme (Section 3) using central difference formulas.

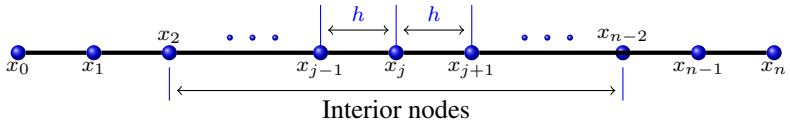


FIGURE 1. Nodes for central difference scheme

The stencil of fourth order central difference scheme used to approximate the first- and second-order derivatives for the interior nodes is

$$\{x_{j-1}, x_j, x_{j+1}\}, \quad for\ j = 2, 3, ..., n-2. \tag{2. 9}$$

It means that if we are at location j, then we need one grid node to the left of j and one grid point to the right of it. It is noticeable that, mutual distance between nodes is equal to $h = (b-a)/(n-1)$. We consider the following compact finite difference scheme

$$\kappa_1 f''_{j-1} + f''_j + \kappa_2 f''_{j+1} = \frac{1}{h^2} \left(\tau_1 f_{j-1} + \tau_2 f_j + \tau_3 f_{j+1} \right). \tag{2. 10}$$

We are interested to obtain the values of unknowns in such a way that the fourth order accurate approximation of second-order derivative is achieved. By expanding equation

(2. 10) around x_1, we have the following system of algebraic equations:

$$\begin{aligned} &\tau_1 + \tau_2 + \tau_3 = 0, \\ &\tau_1 - \tau_3 = 0, \\ &-\tau_1/2 - \tau_3/2 + \kappa_1 + \kappa_2 + 1 = 0, \\ &\tau_1/6 - \tau_3/6 - \kappa_1 + \kappa_2 = 0, \\ &-\tau_1/24 - \tau_3/24 + \kappa_1/2 + \kappa_2/2 = 0. \end{aligned} \tag{2. 11}$$

By solving the above system of equations, we have

$$\left\{\kappa_1 = \frac{1}{10}, \quad \kappa_2 = \frac{1}{10}, \quad \tau_1 = \frac{6}{5}, \quad \tau_2 = -\frac{12}{5}, \quad \tau_3 = \frac{6}{5}\right\}. \tag{2. 12}$$

To find the approximations of first derivatives at the interior nodes, we consider the following prototype

$$\kappa_1 f'_{i-1} + f'_i + \kappa_2 f'_{i+1} = \frac{1}{h^2}(\tau_1 f_{i-1} + \tau_2 f_i + \tau_3 f_{i+1}). \tag{2. 13}$$

By expanding equation (2. 13), we get the following system of algebraic equations:

$$\begin{aligned} &\tau_1 + \tau_2 + \tau_3 = 0, \\ &\tau_1 - \tau_3 + \kappa_1 + \kappa_2 = 0, \\ &-\tau_1/2 - \tau_3/2 - \kappa_1 + \kappa_2 = 0, \\ &\tau_1/6 - \tau_3/6 + \kappa_1/2 + \kappa_2/2 = 0, \\ &-\tau_1/24 - \tau_3/24 - \kappa_1/6 + \kappa_2/6 = 0. \end{aligned} \tag{2. 14}$$

Solving the above system, we get

$$\left\{\kappa_1 = \frac{1}{4}, \quad \kappa_2 = \frac{1}{4}, \quad \tau_1 = -\frac{3}{4}, \quad \tau_2 = 0, \quad \tau_3 = \frac{3}{4}\right\}. \tag{2. 15}$$

Similarly, one sided approximations for nodes adjacent to boundary nodes and solving system of equations, we obtain the following coefficients:

For second-order derivative, we use the following scheme

$$f''_1 + \kappa\, f''_2 = \frac{1}{h^2}\left(\tau_1\, f_1 + \tau_2\, f_2 + \tau_3\, f_3 + \tau_4\, f_4 + \tau_5\, f_5\right),$$

where, we have

$$\left\{\kappa = 10, \quad \tau_1 = \frac{145}{12}, \quad \tau_2 = -\frac{76}{3}, \quad \tau_3 = \frac{29}{2}, \quad \tau_4 = -\frac{4}{3}, \quad \tau_5 = \frac{1}{12}\right\}. \tag{2. 16}$$

For first-order derivative, we use

$$f'_1 + \kappa\, f'_2 = \frac{1}{h}\left(\tau_1\, f_1 + \tau_2\, f_2 + \tau_3\, f_3 + \tau_4\, f_4 + \tau_5\, f_5\right),$$

where, we have

$$\left\{\kappa = 4, \quad \tau_1 = -\frac{37}{12}, \quad \tau_2 = \frac{2}{3}, \quad \tau_3 = 3, \quad \tau_4 = -\frac{2}{3}, \quad \tau_5 = \frac{1}{12}\right\}. \tag{2. 17}$$

2.5. **Integral approximation.** For the numerical computation of the integrals used in this work, we have applied the following Simpson's rule

$$\int_1^{x_{n-1}} \zeta(s)ds \approx \frac{h}{3}\left(\zeta_1 + 4\sum_{i=2,4,6}^{n-2}\zeta_i + 2\sum_{i=3,5,7}^{n-3}\zeta_i + \zeta_{n-1}\right), \tag{2. 18}$$

where $\zeta_i = \zeta(x_i)$ and $h(= x_n - x_{n-1})$ is uniform step-size.

3. Proposed scheme

For the construction of the proposed iterative scheme, consider the following non homogeneous nonlinear fractional order boundary value problem

$$D^{-\alpha}y'' + p(x)f(y) = g(x), \quad x \in (0,1), \quad 0 < \alpha < 1, \tag{3. 19}$$

with the boundary conditions:

$$y(0) = 0,\ y(1) = 0. \tag{3. 20}$$

Here, $D^{-\alpha}$ is fractional order derivative in Caputo sense and $f(\cdot)$ is a nonlinear function. The fractional order differential equation (3. 19) can also be written as

$$y''(x) = D^{\alpha}(g(x) - p(x)f(y)). \tag{3. 21}$$

For a given smooth function $w(\cdot)$, we describe

$$\begin{aligned} D^{\alpha}w(x) &= \tfrac{1}{\Gamma(1-\alpha)}\int_0^x (x-s)^{-\alpha}w'(s)ds, \quad \alpha > 0, \\ &= \tfrac{1}{(1-\alpha)\Gamma(1-\alpha)}\left(x^{1-\alpha}w'(0) + \int_0^x (x-s)^{1-\alpha}w''(s)ds\right). \end{aligned} \tag{3. 22}$$

We can write equation (3. 21) with the help of equation (3. 22) as

$$\begin{aligned} y''(x) = \frac{1}{\Gamma(1-\alpha)}\Bigg[&\frac{x^{1-\alpha}}{1-\alpha}\Big(g'(0) - p'(0)y(0) - p(0)y'(0)\Big) \\ &+ \int_0^x \frac{(x-s)^{1-\alpha}}{1-\alpha}\Big(g''(s) - p''(s)y(s) - 2p'(s)y'(s) - p(s)y''(s)\Big)ds\Bigg]. \end{aligned} \tag{3. 23}$$

For a given n number of nodes, we discretize $[0,1]$ and compute uniform step size $h = (1-0)/(n-1) = 1/(n-1)$. Furthermore, we use central finite difference approximation of order four for the approximation of first- and second-order derivatives as described in subsection 2.4. Whereas, integrals in our work are approximating by using Simpson's rule (2. 18). The equation (3. 23) can also be written as

$$\begin{aligned} y''(x_i) = \frac{1}{\Gamma(2-\alpha)}\Bigg[&x_i^{1-\alpha}\Big(g'(0) - p'(0)y(0) - p(0)y'(0)\Big) \\ &+ A(x_i) - B(x_i) - C(x_i) - D(x_i)\Bigg], \end{aligned} \tag{3. 24}$$

where,

$$A(x_i) = \int_0^{x_i} (x_i - s)^{1-\alpha} g''(s) ds,$$

$$B(x_i) = \int_0^{x_i} (x_i - s)^{1-\alpha} p''(s) f ds,$$

$$C(x_i) = \int_0^{x_i} (x_i - s)^{1-\alpha} 2p'(s) f' ds,$$

$$D(x_i) = \int_0^{x_i} (x_i - s)^{1-\alpha} p(s) f'' ds.$$

Here, we have applied a very vigorous iterative scheme. The equation (3. 23) can also be written as

$$y_{n+1} = \Psi(y_n), \tag{3. 25}$$

where, $y = [y_1, y_2, ..., y_n]^T$ is the n^{th} numerical approximation to the solution of discretized form of equation (3. 23) and $\Psi(y)$ is the right hand side.

4. NUMERICAL TESTING

To illustrate the performance, in-terms of convergence and accuracy, of the above constructed iterative scheme, we perform numerical testing on a collection of test problems. In all our numerical testing, we approximate the numerical solution of two non-linear fractional order $(0 < \alpha < 1)$ boundary value problems by solving iteratively the equation (3. 25) to obtain a sequence of probably convergent vectors $y_0, y_1, y_2, ...,$ till $||y_{n+1} - y_n|| \leq$ some pre-defined tolerance.

Problem 4.1. *Assume a solution* $y(x) = x^4(x-1)(1-(1-x)^3)$ *to the equation* (3. 19). *We can compute* $g(x)$ *from the equation* (3. 19) *as*

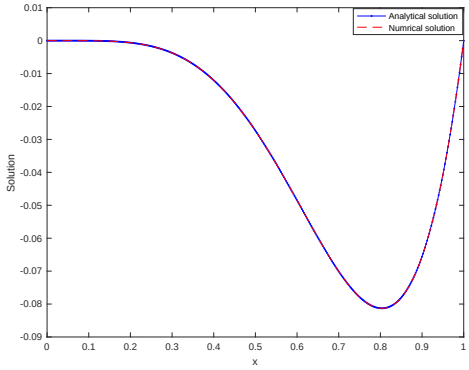
$$g(x) = \frac{128}{3003} \frac{x^{7/2}\left(896\,x^3 - 1287 + 3432\,x - 2912\,x^2\right)}{\sqrt{\pi}} + x^{18}\,(x-1)^4\left(1-(1-x)^3\right)^4.$$

We have performed the first set of numerical experiments with $f(x) = x^4$ and $p(x) = x^2$. Table 1 shows maximum of the absolute error for different values of α and n. The maximum of the absolute error is defined as the maximum absolute of the error evaluated at n evenly spaced data points. That is, we estimate the maximum absolute error by sampling $|y_{num}(x) - y_{true}(x)|$ over the complete interval of integration and using the maximum over all sampled values to be the estimate of $|y_{num}(x) - y_{true}(x)|$. It has been observed that as we increase the value of n and decrease the value of α, the maximum absolute error is decreased. The best observed accuracy (smallest maximum absolute error) is obtained at $\alpha = 1/8$ and with $n = 400$.

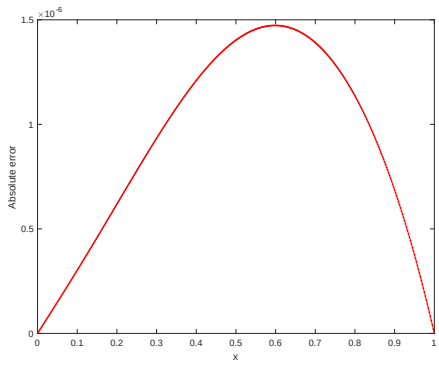
TABLE 1. Maximum absolute error for different values of α and n.

n	Max Absolute Error		
	$\alpha = 1/2$	$\alpha = 1/5$	$\alpha = 1/8$
100	2.6218×10^{-4}	3.9828×10^{-5}	2.3866×10^{-5}
150	1.4086×10^{-4}	1.8096×10^{-5}	1.0479×10^{-5}
200	9.0898×10^{-5}	1.0405×10^{-5}	5.8719×10^{-6}
250	6.4789×10^{-5}	6.7948×10^{-6}	3.7554×10^{-6}
300	4.9160×10^{-5}	4.8052×10^{-6}	2.6099×10^{-6}
350	3.8941×10^{-5}	3.5889×10^{-6}	1.9203×10^{-6}
400	3.1828×10^{-5}	2.7893×10^{-6}	1.4729×10^{-6}

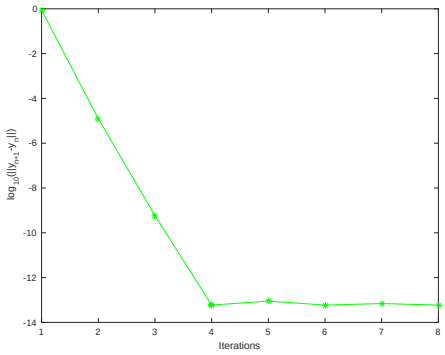
We performed a second set of experiments with $n = 400$, $f(x) = x^4$, $p(x) = x^2$, and $\alpha = 1/8$. In Figure 2(a), the approximated and exact solutions are plotted. One can observe that, the exact values and the numerical approximated values are very close to each other as both plots go side by side. The absolute of the error for different values of x is shown in Figure 2(b). It has been observed that near the boundary points, the value of absolute error is quit small and the maximum absolute error at the interior nodes in this case is approximately 1.4729×10^{-6}. Figure 2(c) shows number of iterations (Nit) against the $\log_{10}(||y_{n+1} - y_n||)$. We observe that as n increases $\log_{10}(||y_{n+1} - y_n||)$ is reduced significantly till a value of approximately 5.9845×10^{-14} for $Nit = 4$, which is very small compared to the maximum absolute error obtained in this case. This is an optimal achieved accuracy which cannot be improved with further iterations.



(A) Comparison between analytical and numerical solutions.



(B) Absolute of the error in numerical approximation



(C) Number of iterations against the $\log_{10}(||y_{n+1} - y_n||)$

FIGURE 2. with $n = 400$, $f(x) = x^4$, $p(x) = x^2$, and $\alpha = 1/8$

Problem 4.2. *Assume a solution* $y(x) = 10x^6(1 - x^2)$ *to the equation* (3. 19)*. We can compute* $g(x)$ *from the equation* (3. 19) *as*

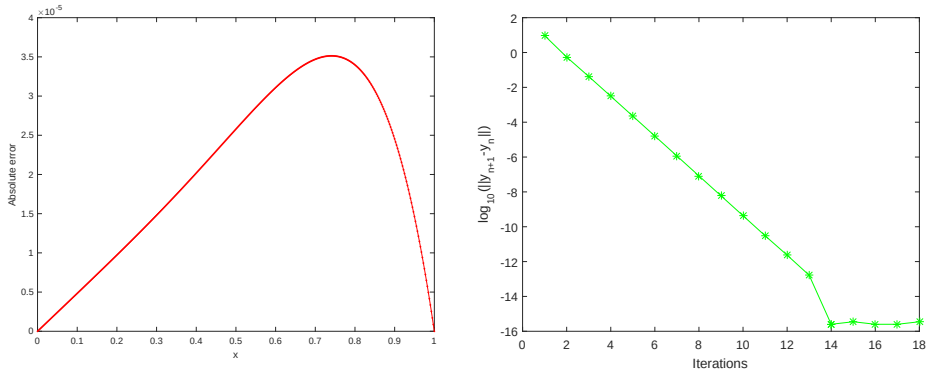
$$g(x) = -\frac{5120}{3003}\frac{x^{9/2}\left(-143 + 224\,x^2\right)}{\sqrt{\pi}} + x^2 e^{10\,x^6\left(1-x^2\right)}$$

The next set of experiments is performed for the second test problem with same parameters as described in Table 1 except for f which is $f(x) = e^x$ in this case. Table 2 shows maximum of the absolute error for different values of α and n. From Table 2, we observe that as we increase the value of n and decrease the value of α, the maximum absolute error is decreased. As before, the best observed accuracy is again obtained at $\alpha = 1/8$ and with $n = 400$.

For the final set of experiments performed using the developed iterative scheme, absolute of the error and number of iterations against the $\log_{10}(||y_{n+1} - y_n||)$ are plotted in Figures 3(a) and 3(b), respectively. Figure 3(a) illustrates that estimated maximum error occurs for this problem using the proposed scheme is approximately 3.5130×10^{-5}. We can observe from the Figure 3(b) that, also in this case, as n increases $\log_{10}(||y_{n+1} - y_n||)$ is reduced significantly. In this case, $\log_{10}(||y_{n+1} - y_n||)$ is approximately 4.9014×10^{-15} for $Nit = 14$, which is, again, very small compared to the maximum absolute error.

TABLE 2. Maximum absolute error for different values of α and n.

n	Max Absolute Error		
	$\alpha = 1/2$	$\alpha = 1/5$	$\alpha = 1/8$
100	8.4154×10^{-3}	1.0767×10^{-3}	5.0025×10^{-4}
150	4.5308×10^{-3}	5.0817×10^{-4}	2.2772×10^{-4}
200	2.9266×10^{-3}	2.9971×10^{-4}	1.3114×10^{-4}
250	2.0871×10^{-3}	1.9937×10^{-4}	8.5694×10^{-5}
300	1.5841×10^{-3}	1.4303×10^{-4}	6.0592×10^{-5}
350	1.2551×10^{-3}	1.0807×10^{-4}	4.5235×10^{-5}
400	1.0261×10^{-3}	8.4806×10^{-5}	3.5130×10^{-5}



(A) Absolute of the error in numerical approximation

(B) Number of iterations against the $\log_{10}(||y_{n+1} - y_n||)$

FIGURE 3. with $n = 400$, $f(x) = e^x$, $p(x) = x^2$, and $\alpha = 1/8$

5. CONCLUSION

In this paper, a new iterative scheme is developed for the numerical approximation of nonlinear boundary value problems of fractional order $0 < \alpha < 1$. The proposed scheme is developed by using central finite difference scheme of order four for the approximation of first- and second-order derivatives and using Simpson's rule for the numerical computation of the integrals used in this work. For the sets of experiments performed to obtain the maximum of the absolute error for different values of α and n, it has been observed that as we increase the value of n and decrease the value of α, the maximum absolute error

is decreased. The best observed accuracy (smallest maximum absolute error) for the test problem 1 and 2 is obtained at $\alpha = 1/8$ and with $n = 400$. Moreover, for the problems considered in this paper, convergence of the proposed iterative scheme till reaching optimal accuracy is achieved after no more than 14 iterations.

We believe that the optimal accuracy can further be improved by using more higher order finite difference schemes for the derivatives involved and using other numerical integration techniques for numerical computation of the integrals.

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