

HIGHER ORDER COMPACT FINITE DIFFERENCE METHOD FOR SINGULARLY PERTURBED ONE DIMENSIONAL REACTION DIFFUSION PROBLEMS

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ABSTRACT. In this paper, a higher order numerical method based on finite difference scheme with uniform mesh is presented for solving singularly perturbed two-point boundary value problems of reaction diffusion type. An eighth order compact finite difference has been developed for solving the problem. To demonstrate the efficiency of the method, three test examples have been considered. The numerical results obtained by the present method are tabulated and compared with some results of the previous findings of others existing in the literature. Graphs are also depicted in support of the numerical results. The convergence of the method has been examined and the theoretical error bound has been established. The present method is simple and it approximates the exact solution very well.

Keywords and phrases: Singular perturbation; Compact finite difference; Reaction diffusion equations

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1. INTRODUCTION

The differential equations in which the highest order derivative term is multiplied by a small positive parameter ε where $0 < \varepsilon \ll 1$ are known to be singularly perturbed differential equations and the parameter is known as the perturbation parameter. In the intensive development of science and technology, many practical problems, such as the mathematical boundary layer theory or approximation of solutions of various problems described by differential equations involving large or small parameters become more complex. In some problems, the perturbations are active over a very narrow region across which the dependent variable undergoes very rapid changes. The solutions of these problems depend on a small positive parameter, where in such a way that the solution varies rapidly in some

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parts of the domain and varies slowly in some other parts of the domain. Typically, there are thin transition layers where the solution varies rapidly or jumps abruptly, while away from the layers the solution behaves regularly and varies slowly [1]. As a result, if we apply the existing classical numerical methods for solving such types of problems large oscillations may arise and pollute the solution in the entire interval because of the boundary layer behavior. So, most of the classical numerical methods are not effective for solving such problems because, as the singular perturbation parameter tends to zero, the errors in the numerical solutions increase and often becomes comparable in magnitude to the exact solution [2]. Such types of problems most frequently arises in many physical phenomena such as fluid dynamics, chemical reactor theory, nuclear reactor theory, plasma physics, aerodynamics, meteorology, oceanography, diffraction theory, reaction-diffusion process, non-equilibrium and other domains of the great world of fluid motion.

Owing to this, many researchers tried to develop both asymptotic and numerical methods to solve such problems. For detail discussions on the asymptotic methods one can refer [3-7] and for numerical methods such as finite difference and finite element methods, one can refer to [8-17]. The main objective of this study is to present the eighth order compact finite difference method for solving singularly perturbed one dimensional reaction diffusion problems. The paper is presented as follows. In section 2, we formulate and describe the proposed method. In section 3, we proved the convergence of the method and establish theoretical error bound. In section 4, some results are obtained using the present numerical method and these experiments illustrate the validity of the method. Finally, discussion and conclusion drawn is presented.

2. DESCRIPTION OF THE METHOD

Consider singularly perturbed one dimensional reaction diffusion problems of the type:

$$-\varepsilon y'' + g(x)y = f(x), 0 \leq x \leq 1 \quad (1)$$

subject to the boundary conditions

$$y(0) = \alpha, y(1) = \beta \quad (2)$$

where α, β are constants, ε is small positive parameter, $f(x)$ and $g(x)$ are sufficiently smooth functions. In order to develop the numerical method for finding the solution of differential equation

(1-2), the interval $[0, 1]$ is divided into equal n subintervals using the grid points $x_i = x_0 + ih, i = 0, 1, 2, \dots, n, x_0 = 0, x_n = 1$, and $h = 1/n$.

Let $y_i = y(x_i)$ denote the solution of problem in Eqs. (1-2), $y_i^{(n)} = y^{(n)}(x_i)$ and $f_i^{(n)} = f^{(n)}(x_i)$ denote its n^{th} derivative at $x = x_i$. Applying Taylor series expansion on y_{i-1} and y_{i+1} respectively and adding the two, we obtain second order central difference, δ_c^2 of the second derivative of y_i as:

$$\delta_c^2 y_i = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \tau_1 \quad (3)$$

where $\tau_1 = -\frac{h^2}{12}y_i^{(4)} + O(h^4)$.

Further, using the Taylor series expansion of y_{i+1} and y_{i-1} up to $O(h^{10})$ and Eq.(3), we obtain:

$$\delta_c^2 y_i = y_i'' + \frac{h^2}{12}y_i^{(4)} + \frac{h^4}{360}y_i^{(6)} + \frac{h^6}{20160}y_i^{(8)} + \tau_2 \quad (4)$$

where $\tau_2 = \frac{2h^8}{10!}y_i^{(10)} + O(h^{10})$. To obtain the eighth order compact finite difference scheme, we apply δ_c^2 to $y_i^{(6)}$ and we obtain:

$$y_i^{(8)} = \delta_c^2 y_i^{(6)} + \tau_3 \quad (5)$$

where $\tau_3 = \frac{h^2}{90}y_i^{(10)} + O(h^4)$.

Now, at any point x_i , Eq. (1) can be written as:

$$-y_i'' + u_i y_i = r_i \quad (6)$$

where $u_i = \frac{q_i}{\varepsilon}, r_i = \frac{f_i}{\varepsilon}$ and assume that $g(x_i) = g_i \geq g$ where g is positive constant [18]. Thus, differentiating Eq. (8) successively, we obtain:

$$y_i^{(4)} = u_i y_i'' - r_i'' \quad (7)$$

and

$$y_i^{(6)} = u_i y_i^{(4)} - r_i^{(4)} \quad (8)$$

Substituting Eqs. (7- 8) into Eq. (4), we obtain:

$$\begin{aligned} \delta_c^2 y_i &= (1 + \frac{h^2 u_i}{12} + \frac{h^4 u_i^2}{360} + \frac{h^6 u_i^2}{20160} \delta_c^2) y_i'' - \\ &(\frac{h^2}{12} + \frac{h^4 u_i}{360} + \frac{h^6 u_i}{20160} \delta_c^2) r_i'' - (\frac{h^4}{360} + \frac{h^6}{20160} \delta_c^2) r_i^{(4)} + \tau_4 \end{aligned} \quad (9)$$

where $\tau_4 = \frac{h^6}{20160} \tau_3 + \tau_2 = \frac{h^8}{907200} y_i^{(10)} + O(h^{10})$

Solving Eq. (9) for y_i'' , we obtain:

$$y_i'' = \frac{\delta_c^2 y_i + ((\frac{h^2}{12} + \frac{h^4 u_i}{360} + \frac{h^6 u_i}{20160} \delta_c^2) r_i'' + (\frac{h^4}{360} + \frac{h^6}{20160} \delta_c^2) r_i^{(4)} + \tau_5)}{1 + \frac{h^2 u_i}{12} + \frac{h^4 u_i^2}{360} + \frac{h^6 u_i^2}{20160} \delta_c^2} \quad (10)$$

Substituting Eq.(10) into Eq.(6), we obtain:

$$\begin{aligned} & -\delta_c^2 y_i - (\frac{h^2}{12} + \frac{h^4 u_i}{360}) r_i'' - \frac{h^6 u_i}{20160} \delta_c^2 r_i'' - \frac{h^4}{360} r_i^{(4)} - \frac{h^6}{20160} \delta_c^2 r_i^{(4)} - \tau_5 \\ & + u_i (1 + \frac{h^2 u_i}{12} + \frac{h^4 u_i^2}{360}) y_i + \frac{h^6 u_i^3}{20160} \delta_c^2 y_i = (1 + \frac{h^2 u_i}{12} + \frac{h^4 u_i^2}{360}) r_i + \frac{h^6 u_i^2}{20160} \delta_c^2 r_i \end{aligned} \quad (11)$$

Applying the central difference approximations and Eq.(3) for r_i, r_i' and $r_i^{(4)}$ in Eq.(11), we obtain:

$$\begin{aligned} & -(\frac{1}{h^2} - \frac{h^4 u_i^3}{20160}) y_{i-1} + (\frac{2}{h^2} + u_i (1 + \frac{h^2 u_i}{12} + \frac{3h^4 u_i^2}{1120})) y_i - (\frac{1}{h^2} - \frac{h^4 u_i^3}{20160}) y_{i+1} = \\ & \frac{h^4 u_i^2}{20160} r_{i-1} + (1 + \frac{h^2 u_i}{12} + \frac{3h^4 u_i^2}{1120}) r_i + \frac{h^4 u_i^2}{20160} r_{i+1} + \frac{h^4 u_i}{20160} r_{i-1}'' \\ & + (\frac{h^2}{12} + \frac{3h^4 u_i}{1120}) r_i'' + \frac{h^4 u_i}{20160} r_{i+1}'' + \frac{h^4}{20160} r_{i-1}^{(4)} + \frac{3h^4}{1120} r_i^{(4)} + \frac{h^4}{20160} r_{i+1}^{(4)} \end{aligned} \quad (12)$$

Eq.(12) can be written as a three term recurrence relation of the form:

$$-E_i y_{i-1} + F_i y_i - G_i y_{i+1} = H_i \quad (13)$$

where;

$$E_i = \frac{1}{h^2} - \frac{h^4 u_i^3}{20160} = G_i, \quad F_i = \frac{2}{h^2} + u_i (1 + \frac{h^2 u_i}{12} + \frac{3h^4 u_i^2}{1120}) \text{ and}$$

$$\begin{aligned} H_i = & \frac{h^4 u_i^2}{20160} r_{i-1} + (1 + \frac{h^2 u_i}{12} + \frac{3h^4 u_i^2}{1120}) r_i + \frac{h^4 u_i^2}{20160} r_{i+1} + \frac{h^4 u_i}{20160} r_{i-1}'' \\ & + (\frac{h^2}{12} + \frac{3h^4 u_i}{1120}) r_i'' + \frac{h^4 u_i}{20160} r_{i+1}'' + \frac{h^4}{20160} r_{i-1}^{(4)} + \frac{3h^4}{1120} r_i^{(4)} + \frac{h^4}{20160} r_{i+1}^{(4)} \end{aligned}$$

This gives us the tridiagonal system which can easily be solved by using the well known algorithm called Discrete Invariant Imbedding Algorithm.

3. CONVERGENCE ANALYSIS

Writing the tri-diagonal system in Eq. (13) in matrix vector form, we obtain:

$$AY = C \quad (14)$$

where $A = (m_{ij}), 1 \leq i, j \leq N-1$ is a tri-diagonal matrix of order N-1, with $m_{i,i+1} = -\frac{1}{h^2} + \frac{h^4 u_i^3}{20160}$, $m_{i,i} = \frac{2}{h^2} + u_i + \frac{h^2 u_i^2}{12} + \frac{3h^4 u_i^3}{1120}$,

$m_{i,i-1} = -\frac{1}{h^2} + \frac{h^4 u_i^3}{20160}$ and $C = (d_i)$ be a column vector with
 $d_i = \frac{h^4 u_i^2}{20160} r_{i-1} + (1 + \frac{h^2 u_i}{12} + \frac{3h^4 u_i^2}{1120}) r_i + \frac{h^4 u_i^2}{20160} r_{i+1} + \frac{h^4 u_i}{20160} r_{i-1}'' +$
 $(\frac{h^2}{12} + \frac{3h^4 u_i}{1120}) r_i'' + \frac{h^4 u_i}{20160} r_{i+1}'' + \frac{h^4}{20160} r_{i-1}^{(4)} + \frac{3h^4}{1120} r_i^{(4)} + \frac{h^4}{20160} r_{i+1}^{(4)}$
for $i = 1, 2, \dots, N$ with local truncation error which is given by:

$$\tau_i(h_i) = \frac{h^8}{907200} y_i^{(10)} + O(h^{10}) \quad (15)$$

we also have

$$A\bar{Y} - \tau(h) = C \quad (16)$$

where $\bar{Y} = (\bar{y}_0, \bar{y}_1, \dots, \bar{y}_N)^t$ and $\tau(h) = (\tau_1(h_0), \tau_2(h_1), \dots, \tau_N(h_N))^t$ stands for the exact solution and local truncation error respectively. From Eqs.(14) and (16), we obtain:

$$A(\bar{Y} - Y) = \tau(h) \quad (17)$$

Thus, we get an error equation

$$AE = \tau(h) \quad (18)$$

where $E = \bar{Y} - Y = (e_0, e_1, \dots, e_N)$

Let S_i be the sum of elements of the i^{th} row of the matrix A , i.e $S_i = \sum_{j=1}^{N-1} m_{ij}$, then we have:

For $i = 1$, $S_1 = B_1 + A_1 h^4 + O(h^4)$, where $B_1 = u_i + \frac{1}{h^2} + \frac{h^2 u_i^2}{12}$,

$A_1 = \frac{11u_i^3}{4032}$ and $|B_1| = \min S_1$

For $i = 2, 3, \dots, N-2$, $S_i = B_i + A_0 h^4 = B_i + O(h^4)$ where $B_i =$

$u_i + \frac{h^2 u_i^2}{12}$, $A_0 = \frac{u_i^3}{360}$ and $|B_i| = \min_{2 \leq i \leq N-2} S_i$

For $i = N-1$, $S_{N-1} = B_1 + A_1 h^4 = B_1 + O(h^4)$, where $B_1 =$

$u_i + \frac{1}{h^2} + \frac{h^2 u_i^2}{12}$, $A_1 = \frac{11u_i^3}{4032}$ and $|B_1| = \min S_{N-1}$

From the above we have $B_i \leq B_1$ which implies B_i is minimum value. Since $0 < \varepsilon \ll 1$, we can choose h sufficiently small so that the matrix A is irreducible and monotonic [19]. Then, it follows that A^{-1} exists and its elements are non-negative. Hence, from Eq.(18), we get:

$$E = A^{-1} \tau(h) \quad (19)$$

and

$$\|E\| = \|A^{-1}\| \|\tau(h)\| \quad (20)$$

Let $\bar{m}_{k,i}$ be the (k, i) elements of A^{-1} . Since $\bar{m}_{k,i} \geq 0$, by the definition of multiplication of matrices with its inverses (from the theory of matrices) we have

$$\sum_{i=1}^{N-1} \bar{m}_{k,i} S_i = 1, \quad k = 1, 2, \dots, N-1 \quad (21)$$

Therefore, it follows that

$$\sum_{i=1}^{N-1} \overline{m}_{k,i} S_i \leq \frac{1}{\min_{1 \leq i \leq N-1} S_i} = \frac{1}{|B_i|} \quad (22)$$

We define $\|A^{-1}\| = \max_{1 \leq i \leq N-1} \sum_{j=1}^{N-1} |\overline{m}_{k,i}|$ and $\|\tau(h)\| = \max_{1 \leq i \leq N-1} |\tau(h)|$.

Therefore, from Eqs.(15), (18) and (22), we obtain:

$$e_j = \sum_{i=1}^{N-1} \overline{m}_{k,i} \tau_i(h), \quad j = 1, 2, 3, \dots, N-1$$

$$e_j = \frac{1}{|B_i|} \cdot \tau_i(h) = \frac{1}{|B_i|} \frac{h^8}{907200} y_i^{(10)}$$

Therefore, $e_j \leq \frac{kh^8}{|B_i|}, j = 1, 2, 3, \dots, N-1$, where $k = \left(\frac{1}{907200}\right) |y_i^{(10)}|$,

which is a constant and independent of h . Therefore, $\|E\| \leq O(h^8)$.

Remark: The computational rate of convergence is obtained by using the double mesh principle described below.

Let

$$z_h = \max_j |y_j^h - y_j^{\frac{h}{2}}|, \quad j = 1, 2, 3, \dots, N-1,$$

where y_i^h is the computed solution on the mesh point $\{x_j\}_0^N$ at the nodal point of x_j for $x_j = x_{j-1} + h, j = 1, 2, \dots, N$ and $y_i^{\frac{h}{2}}$ is the computed solution at the nodal point x_j on the mesh $\{x_j\}_0^{2N}$, where $x_j = x_{j-1} + h/2, j = 1(1)2N$.

In the same case we can define $z_{h/2}$ by replacing h by $h/2$ and N by $N/2$, we obtain

$$z_{h/2} = \max_j |y_j^{h/2} - y_j^{h/4}|, \quad j = 1, 2, 3, \dots, N-1,$$

The computed order of convergence is evaluated as

$$Rate = \frac{\log Z_h - \log Z_{h/2}}{\log 2}.$$

Also the maximum absolute error based on double mesh principle is given by:

$$E_i^N = \max_j |y_j^N - y_{2j}^{2N}|, \quad j = 1, 2, 3, \dots, N.$$

and $y_j^{\frac{h}{2}}$ denotes that the value of y_i for mesh length $\frac{h}{2}$

4. TEST EXAMPLES AND NUMERICAL RESULTS

To test the applicability of the present method, we have considered the following model problems with and without exact solution.

Example 1: Consider the singularly perturbed problem:

$$-\varepsilon y'' + y = x$$

with the boundary conditions $y(0) = 1, y(1) = 1 + e^{(\frac{-1}{\sqrt{\varepsilon}})}$. The exact solution is given by: $y(x) = x + e^{(\frac{-x}{\sqrt{\varepsilon}})}$.

The numerical solutions in terms of maximum absolute errors are given in Table 1.

Example 2: Consider the singularly perturbed problem:

$$-\varepsilon y'' + y = -\cos^2(\pi x) - 2\varepsilon\pi^2 \cos(2\pi x), 0 \leq x \leq 1$$

with the boundary conditions: $y(0) = 0, y(1) = 0$, the exact solution is given by:

$$y(x) = \frac{e^{(\frac{x-1}{\sqrt{\varepsilon}})} + e^{(\frac{-x}{\sqrt{\varepsilon}})}}{1 + e^{(\frac{-1}{\sqrt{\varepsilon}})}} - \cos^2(\pi x)$$

The maximum absolute errors are given in Table 2.

Example 3: Consider the singularly perturbed problem:

$$-\varepsilon y'' + y = 1 - 3x \cos(\pi x)$$

with boundary condition: $y(0) = y(1) = 0$.

The exact solution of the problem is not known. The maximum absolute errors are tabulated in Table 3.

Table 1. The maximum absolute errors E_i^N for Example 1

ε	$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$
Our Method					
1/16	9.8908E-12	3.8192E-14	4.4298E-14	2.0206E-14	7.8404E-13
1/32	1.5796E-10	6.2705E-13	6.8834E-15	5.7732E-14	8.2823E-14
1/64	2.4930E-09	9.9758E-12	3.8691E-14	5.4956E-14	3.8081E-14
1/128	3.6637E-08	1.5803E-10	6.2672E-13	9.6589E-15	6.5503E-14
Rashidinia [13]					
1/16	2.96E-006	1.85E-007	1.15E-008	7.24E-010	4.56E-011
1/32	1.18E-005	7.54E-007	4.67E-008	2.96E-009	1.82E-010
1/64	4.74E-005	2.96E-006	1.86E-007	1.16E-008	7.30E-010
1/128	1.78E-004	1.18E-005	7.46E-007	4.67E-008	2.92E-009

Table 2. The maximum absolute errors E_i^N for Example 2

ε	$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$
Our Method					
1/16	9.0031E-10	3.5116E-12	7.2164E-15	1.8596E-15	1.0325E-13
1/32	4.8094E-10	1.8783E-12	7.6467E-15	1.2657E-14	2.3148E-14
1/64	2.6577E-09	1.0625E-11	4.2411E-14	2.4425E-14	1.2323E-14
1/128	3.6756E-08	1.5861E-10	6.2550E-13	3.9413E-15	4.1855E-14
Rashidinia [13]					
1/16	4.07E-005	2.53E-006	1.58E-007	9.87E-009	6.17E-010
1/32	2.00E-005	1.24E-006	7.74E-008	4.83E-009	3.02E-010
1/64	5.45E-005	3.42E-006	2.14E-007	1.34E-008	8.39E-010
1/128	1.83E-004	1.22E-005	7.68E-007	4.81E-008	3.01E-009
Surla et. al [14]					
1/16	1.20E-004	7.47E-006	4.67E-007	2.90E-008	4.39E-009
1/32	1.28E-004	8.00E-006	5.00E-007	3.14E-008	1.99E-009
1/64	1.60E-004	1.00E-005	6.26E-007	3.92E-008	2.31E-009
1/128	2.344E-004	1.47E-005	9.23E-007	5.77E-008	3.72E-009

Table 3. Maximum Absolute Errors E_i^N for Example 3

ε	$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$	$N = 512$
2^{-4}	2.2121E-11	8.9040E-14	2.2204E-15	7.1054E-15	5.1936E-13	6.3960E-13
2^{-5}	5.2890E-10	2.0908E-12	1.0436E-14	7.9936E-15	3.8858E-14	6.4393E-14
2^{-6}	8.9703E-09	3.5893E-11	1.4033E-13	7.9936E-15	1.1768E-14	3.1686E-13
2^{-7}	1.3813E-07	5.9595E-10	2.3554E-12	1.2434E-14	1.6431E-14	3.7970E-14
2^{-8}	2.2537E-06	9.6555E-09	3.8634E-11	1.4255E-13	1.5676E-13	4.7518E-14
2^{-9}	3.0463E-05	1.4388E-07	6.200E-10	2.4603E-12	6.6169E-14	2.4025E-13

Table 4. Numerical rate of convergence for Examples 1, 2 and 3 when $\varepsilon = 1/128$

	h	$h/2$	Z_h	$h/4$	$Z_{h/2}$	rate
Example 1:	2^{-4}	2^{-5}	3.6479E-008	2^{-6}	1.5740E-010	7.8565
	2^{-5}	2^{-6}	1.5740E-010	2^{-7}	6.1706E-013	7.9948
Example 2:	2^{-4}	2^{-5}	3.6597E-008	2^{-6}	1.5798E-010	7.8558
	2^{-5}	2^{-6}	1.5798E-010	2^{-7}	6.2156E-013	7.9897
Example 3:	2^{-4}	2^{-5}	1.3753E-007	2^{-6}	5.9359E-010	7.8561
	2^{-5}	2^{-6}	5.9359E-010	2^{-7}	2.3430E-012	7.9850

The following figures (Figures 1-4) show that the numerical solutions obtained by the present method for $h \geq \varepsilon$ as compared with exact solution.

5. DISCUSSION AND CONCLUSION

A higher order finite difference method, eighth order compact difference method, has been presented for solving singularly perturbed one dimensional reaction diffusion equations. Three examples are given to demonstrate the efficiency of the proposed method. The

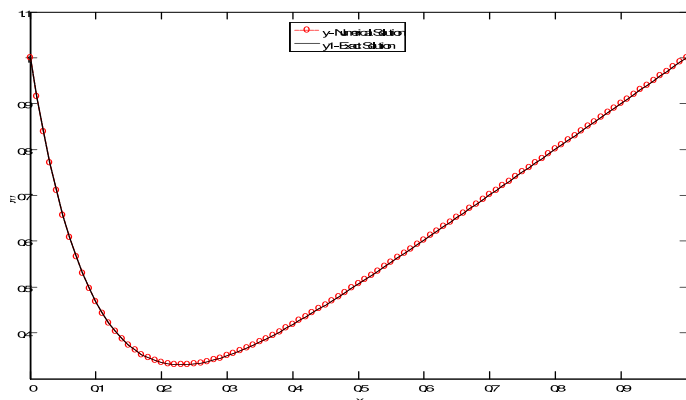


Fig. 1. Numerical Solution of Example 1 for $\varepsilon = 0.01$ and $h = 0.01$

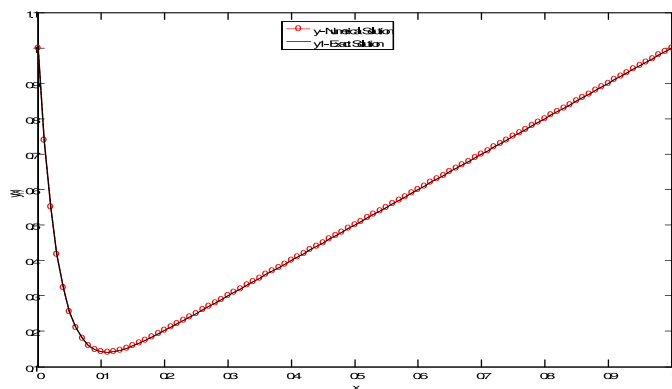


Fig. 2. Numerical Solution of Example 1 for $\varepsilon = 0.001$ and $h = 0.01$

maximum absolute errors are tabulated in the tables (Tables 1-3) for different values of the perturbation parameter ε and the number of mesh points N . The numerical results presented in Tables 1 and 2 clearly indicate that the proposed scheme is more efficient than the methods given in [13-14].

Tables 1- 3 also show that the maximum absolute error decreases as the mesh size h decreases, which in turn shows the convergence of the computed solution and it also substantiates the theoretical convergence analysis given. To further substantiate the applicability of the proposed method, graphs between exact solution and approximate solutions have been plotted (Figures 1-4) for the two

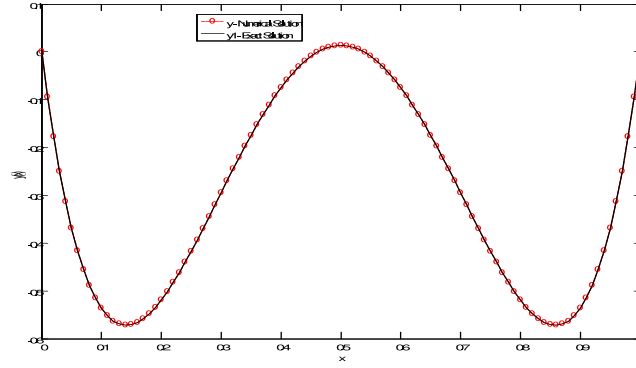


Fig. 3. Numerical Solution of Example 2 for $\varepsilon = 0.01$ and $h = 0.01$

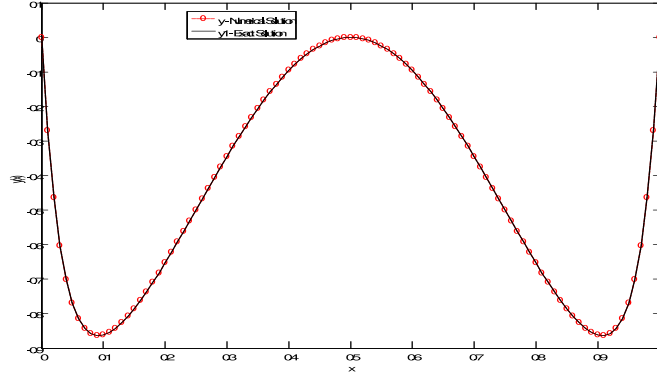


Fig. 4. Numerical Solution of Example 2 for $\varepsilon = 0.001$ and $h = 0.01$

examples for different values of $\varepsilon = 10^{-2}$, $\varepsilon = 10^{-3}$ and fixed value of $N = 100$. It is observed that the numerical solutions are in a very good agreement of the exact solution for small value of ε (i.e. $h \geq \varepsilon$) for which most of classical numerical methods fail to give good result. Further, the results obtained by the present method confirmed that the computational rate of convergence is in a good agreement with the theoretical estimates of order of convergence (Table 4). In a concise manner, the present method is simple and approximates the exact solution very well.

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