Sixth-order compact finite difference method for singularly perturbed 1D reaction diffusion problems

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Received 3 July 2015; received in revised form 8 December 2015; accepted 28 December 2015

Abstract

In this paper, the sixth-order compact finite difference method is presented for solving singularly perturbed 1D reaction–diffusion problems. The derivative of the given differential equation is replaced by finite difference approximations. Then, the given difference equation is transformed to linear systems of algebraic equations in the form of a three-term recurrence relation, which can easily be solved using a discrete invariant imbedding algorithm. To validate the applicability of the proposed method, some model examples have been solved for different values of the perturbation parameter and mesh size. Both the theoretical error bounds and the numerical rate of convergence have been established for the method. The numerical results presented in the tables and graphs show that the present method approximates the exact solution very well.

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Keywords: Compact finite difference method; Singular perturbation problem; Reaction–diffusion equation

1. Introduction

Singular perturbation problems containing a small parameter, ε, multiplied by their highest derivative term arise frequently in many fields of applied mathematics and engineering, for instance, fluid mechanics, elasticity, hydrodynamics, chemical-reactor theory, reaction–diffusion processes and many other allied areas. The solution of singular perturbation problems exhibits a multi-scale character, that is, there are thin transition layer(s) where the solution varies rapidly or jumps abruptly within a narrow region called the boundary layer, whereas away from the layer(s), the solution behaves regularly and varies slowly, called the outer region.

Thus, the treatment of such problems is not trivial because of the boundary layer behaviour of their solutions. Classical computational approaches for singularly perturbed problems are inadequate because they require extremely large numbers of mesh points to produce satisfactory computed solutions [1,2]. Therefore, the treatment of singularly perturbed problems presents severe difficulties that have to be addressed to ensure accurate numerical solutions [3–5]. Various scholars have tried to design efficient numerical methods for solving singular perturbation problems. The authors in

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Peer review under responsibility of Taibah University.

http://dx.doi.org/10.1016/j.jtusci.2015.12.010
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Please cite this article in press as: F.W. Gelu, et al. Sixth-order compact finite difference method for singularly perturbed 1D reaction diffusion problems, J. Taibah Univ. Sci. (2016), http://dx.doi.org/10.1016/j.jtusci.2015.12.010
where

\[ y(0) = \alpha, \quad y(1) = \beta \]  

with the boundary conditions

Using the Taylor series expansion, we obtain:

\[ y_{i+1} = y_i + h y_i' + \frac{h^2}{2!} y_i'' + \frac{h^3}{3!} y_i''' + \frac{h^4}{4!} y_i^{(4)} + \frac{h^5}{5!} y_i^{(5)} + O(h^6) \]  

Similarly, by adding Eqs. (3) and (4), we obtain the second-order finite difference approximation \((\delta_y^2 y_i)\) for the second derivative of \(y_i\):

\[ \delta_y^2 y_i = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + T_2 \]  

By substituting Eqs. (3) and (4) into Eq. (5) yields:

\[ \delta_y^1 y_i = y_i' + \frac{h^2}{6} y_i^{(3)} + \frac{h^4}{120} y_i^{(5)} + T_3 \]  

where \(T_3 = \frac{h^6}{120} y_i^{(7)} + T_1\).

By applying \(\delta_y^2\) to \(y_i^{(4)}\) in Eq. (6), we obtain

\[ y_i^{(6)} = \delta_y^2 y_i^{(4)} - T_4 \]  

By substituting Eq. (9) into Eq. (8), we obtain:

\[ \delta_y^2 y_i = y_i'' + \frac{h^2}{12} y_i^{(4)} + \frac{h^4}{360} y_i^{(6)} + T_4 \]  

where \(T_4 = \frac{h^6}{21600} y_i^{(8)} - \frac{h^4}{72} y_i^{(4)}\).

By applying \(\delta_y^2\) to \(y_i^{(4)}\) in Eq. (6), we obtain

\[ \delta_y^2 y_i = \frac{y_i''}{h^2} + h^2 y_i^{(4)} + \frac{h^4}{360} y_i^{(6)} + T_4 \]  

where \(T_4 = \frac{h^6}{21600} y_i^{(8)} - \frac{h^4}{72} y_i^{(4)}\).

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where \(T_4 = \frac{h^6}{21600} y_i^{(8)} - \frac{h^4}{72} y_i^{(4)}\).

For Eq. (1) at discretized mesh points, we obtain:

\[ -\varepsilon y_i'' + a y_i = f_i \]
Differentiating Eq. (11) twice and solving for \( y_i^{(4)} \), we get:
\[
y_i^{(4)} = \frac{a_i}{\varepsilon} y_i'' - \frac{f_i''}{\varepsilon}
\] (12)

Substituting Eq. (12) into Eq. (10) and solving for \( y_i'' \) is given by:
\[
y_i'' = \frac{\delta^2_i y_i + \left( \frac{h^2}{12\varepsilon} + \frac{h^4}{360\varepsilon^2} \right) f_i'' - T_5}{1 + \frac{a_i h^2}{12\varepsilon} + \frac{a_i^2 h^4}{360\varepsilon^2}}
\] (13)

Substituting Eq. (13) into Eq. (1) for \( y_i'' \) and rearranging yields:
\[
\begin{aligned}
& -\varepsilon + \frac{a_i^2 h^4}{360\varepsilon} \delta^2_i y_i + \left( a_i + \frac{a_i^2 h^2}{12\varepsilon} \right) y_i = \left( 1 + \frac{a_i h^2}{12\varepsilon} \right) f_i \\
& + \frac{h^2}{12} f''_i + \frac{h^4}{360\varepsilon^2} f''_i + \frac{a_i h^4}{360\varepsilon^2} f_i - \varepsilon T_5
\end{aligned}
\] (14)

Substituting Eq. (6) into Eq. (14) for \( \delta^2_i y_i \) and making use of \( \delta^2_i f_i = \frac{f_{i+1} - 2 f_i + f_{i-1}}{h^2} \) and \( \delta^2_i f''_i = \frac{f_{i+1} - 2 f_i + f_{i-1}}{h^2} \) we obtain:
\[
\begin{aligned}
& -\varepsilon + \frac{a_i^2 h^2}{360\varepsilon} y_{i-1} + \left( \frac{2\varepsilon}{h^2} + a_i + \frac{7a_i^2 h^2}{90\varepsilon} \right) y_i \\
& + \left( \frac{\varepsilon}{h^2} + \frac{a_i^2 h^2}{360\varepsilon} \right) y_{i+1} = \frac{a_i h^2}{360\varepsilon} f_i - \varepsilon f_{i-1} \\
& + \left( 1 + \frac{7a_i h^2}{90\varepsilon} \right) f_i + \frac{a_i h^2}{360\varepsilon} f_{i+1} + \frac{h^2}{360} f''_{i-1} \\
& + \frac{7h^2}{90} f''_{i-1} + \frac{h^2}{360} f''_{i+1} + T
\end{aligned}
\] (15)

where \( T = \frac{a_i^2 h^6}{4320\varepsilon^5} y_i^{(4)} - \frac{17h^6}{60,480} y_i^{(8)} \) is the local truncation error.

From Eq. (15), we obtain the three-term recurrence relation of the form:
\[
-E_i y_{i-1} + F_i y_i - G_i y_{i+1} = H_i, \quad i = 1, 2, \ldots, N - 1
\] (16)

where \( E_i = \frac{\varepsilon}{h^2} - \frac{a_i^2 h^2}{360\varepsilon} \), \( F_i = \frac{2\varepsilon}{h^2} + a_i + \frac{7a_i^2 h^2}{90\varepsilon} \), \( G_i = \frac{\varepsilon}{h^2} - \frac{a_i^2 h^2}{360\varepsilon} \), \( H_i = \frac{a_i h^2}{360\varepsilon} f_{i-1} + \left( 1 + \frac{7a_i h^2}{90\varepsilon} \right) f_i + \frac{a_i h^2}{360\varepsilon} f_{i+1} + \frac{h^2}{360} f''_{i-1} \\
+ \frac{7h^2}{90} f''_{i-1} + \frac{h^2}{360} f''_{i+1} + T \)

Eq. (16) gives us the tri-diagonal system, which can easily be solved by the Thomas Algorithm.

3. Convergence analysis

Writing Eq. (16) in matrix vector form, we obtain:
\[
BY = C
\] (17)

where \( B = (m_{ij}) \), \( 1 \leq i, j \leq N - 1 \) is a tri-diagonal matrix of order \( N \), with
\[
m_{ii+1} = -\frac{\varepsilon}{h^2} + \frac{a_i^2 h^2}{360\varepsilon}
\]
\[
m_{ii} = \frac{2\varepsilon}{h^2} + a_i + \frac{7a_i^2 h^2}{90\varepsilon}
\]
\[
m_{ii-1} = -\frac{\varepsilon}{h^2} + \frac{a_i^2 h^2}{360\varepsilon}
\]

and \( C = (d_{ij}) \) is a column vector with
\[
d_{ii} = \frac{a_i h^2}{360\varepsilon} f_{i-1} + \left( 1 + \frac{7a_i h^2}{90\varepsilon} \right) f_i + \frac{a_i h^2}{360\varepsilon} f_{i+1} + \frac{h^2}{360} f''_{i-1} \\
+ \frac{h^2}{360} f''_{i-1} + \frac{7h^2}{90} f''_{i+1} + \frac{h^2}{360} f''_{i+1} + T, \quad i = 1, 2, \ldots, N - 1
\]

and with the local truncation error
\[
T_i(h) = \frac{a_i h^6}{4320\varepsilon^5} y_i^{(4)} - \frac{17h^6}{60,480} y_i^{(8)}
\] (18)

We also have
\[
B\bar{Y} - T(h) = C
\] (19)

where \( \bar{Y} = (\bar{y}_0, \bar{y}_1, \bar{y}_2, \ldots, \bar{y}_N)^T \) denotes the exact solution and \( T(h) = (T_1(h), T_2(h_1), \ldots, T_N(h_N))^T \) denotes the local truncation error.

Making use of Eqs. (17) and (19), we obtain an error equation:
\[
BE = T(h)
\] (20)

where \( E = \bar{Y} - Y = (e_0, e_1, e_2, \ldots, e_N)^T \)

Let \( S_i \) be the sum of elements of the \( i \)th row of the matrix \( B \), then
\[
S_i = \sum_{j=1}^{N-1} m_{ij}, \quad \text{for} \quad i = 1.
\]

Therefore, \( S_1 = \frac{\varepsilon}{h^2} + a_1 + \frac{29a_1^2 h^2}{360\varepsilon}, \quad \text{for} \quad i = 1 \)
\[
S_i = \sum_{j=1}^{N-1} m_{ij}, \quad \text{for} \quad i = 2, 3, \ldots, N - 2
\]
Therefore, $S_i = a_i + B_0 h^2$, where $B_0 = a_i^2 / 12 \varepsilon$ for $|a_i| = \min_{2 \leq i \leq N-2} S_i$, for $i = 2, 3, \ldots, N - 2$.

$$S_{N-1} = \sum_{j=1}^{N-1} m_{N-1,j}, \quad \text{for} \quad i = N - 1$$

Therefore, $S_{N-1} = \frac{\varepsilon}{h} + a_i + \frac{2 a_i^2 h^2}{50 \varepsilon}$ for $i = N - 1$.

Because $0 < \varepsilon \ll 1$, we can choose $h$ sufficiently small so that the matrix $B$ is irreducible and monotone [8]. Then, it follows that $B^{-1}$ exists and its elements are non-negative. Hence, from Eq. (20), we get

$$E = B^{-1} \cdot T(h)$$

and

$$||E|| = ||B^{-1}|| \cdot ||T(h)||$$

Let $m_{k,i}$ be the $(k, i)$th elements of $B^{-1}$. Because $m_{k,i} \geq 0$, by the definition of multiplication of a matrix with its inverses, we have

$$\sum_{i=1}^{N-1} m_{k,i} S_i = 1, \quad k = 1, 2, \ldots, N - 1$$

Therefore, it follows that

$$\sum_{i=1}^{N-1} m_{k,i} \leq \frac{1}{1 \leq i \leq N-1} S_i = \frac{1}{|a_i|}$$

We define $||B^{-1}|| = \max_{1 \leq i \leq N-1} \sum_{i=1}^{N-1} |m_{k,i}|$

and $||T(h)|| = \max_{1 \leq i \leq N-1} |T_i(h)|$.

From Eqs. (18), (21), (22) and (24), we obtain:

$$\varepsilon_j \leq \frac{1}{|a_i|} \cdot T_i(h)$$

Therefore, $\varepsilon_j \leq \frac{kh^6}{\ln^4}$, $j = 1, 2, \ldots, N - 1$ where

$$k = \frac{a_i^2}{12 \varepsilon} \left| \begin{array}{c} \varepsilon \left( 6 \right) \\ \varepsilon \left( 8 \right) \end{array} \right|, \quad \text{which is a constant and is independent of } h$$

Therefore, $||E|| \leq o(h^6)$. This implies that the method has sixth-order convergence.

4. Thomas Algorithm

A brief description for solving the tri-diagonal system using the discrete invariant imbedding algorithm, also called the Thomas Algorithm, is presented as follows.

Consider the scheme above:

$$-E_i y_{i-1} + F_i y_i - G_i y_{i+1} = H_i, \quad i = 1, 2, \ldots, N - 1$$

subject to the boundary conditions

$$y_0 = y(0) = \alpha$$

$$y_N = y(1) = \beta$$

Therefore, the solution of Eq. (1) can be written as:

$$y_i = W_i y_{i+1} + T_i, \quad i = N - 1, N - 2, \ldots, 2, 1$$

where $W_i = W(x_i)$ and $T_i = T(x_i)$ are to be determined.

By evaluating Eq. (28) at $x_i = x_{i-1}$, we have

$$y_{i-1} = W_{i-1} y_i + T_{i-1}$$

Substituting Eq. (29) into Eq. (25) gives:

$$y_i = \frac{G_i}{F_i - E_i W_{i-1}} y_{i+1} + \frac{H_i}{F_i - E_i W_{i-1}} T_{i-1}$$

Comparing Eq. (28) with Eq. (30), we obtain the recurrence relations:

$$W_i = \frac{G_i}{F_i - E_i W_{i-1}}$$

$$T_i = \frac{H_i}{F_i - E_i W_{i-1}}$$

To solve these recurrence relations for $i = 2, 3, \ldots, N - 1$, we need the initial conditions for $W_0$ and $T_0$. We take $y_0 = y(0) = W_0 y(1) + T_0$. For $W_0 = 0$, the value of $T_0 = y(0) = \alpha$. With these initial values, we compute $W_i$ and $T_i$ for $i = 2, 3, \ldots, N - 1$ from Eqs. (31) and (32) in the forward process, and then obtain $y_j$ in the backward process from Eqs. (27) and (28).

Further, the conditions for the discrete invariant imbedding algorithm to be stable, see [9,10]:

$$E_i > 0, G_i > 0, F_i \geq E_i + G_i \text{ and } |E_i| \leq |G_i|$$

For our method, Eq. (16) satisfies the conditions given in Eq. (33); hence, the Thomas Algorithm is stable for the proposed method.

5. Numerical examples

To validate the applicability of the method, two model singularly perturbed problems are considered.

**Example 1.** Consider the following singularly perturbed problem:

$$-\varepsilon y'' + y = x, \quad 0 \leq x \leq 1, \quad \text{with } y(0) = 1,$$

$$y(1) = 1 + \exp \left( -\frac{1}{\sqrt{\varepsilon}} \right).$$

The exact solution is given by:

$$y(x) = x + \exp \left( -\frac{x}{\sqrt{\varepsilon}} \right).$$
Table 1
Maximum absolute errors for Example 1.

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$N=16$</th>
<th>$N=32$</th>
<th>$N=64$</th>
<th>$N=128$</th>
<th>$N=256$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Our method</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1/16</td>
<td>8.037E-009</td>
<td>1.2628E-010</td>
<td>1.9704E-012</td>
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<td>1/64</td>
<td>5.0661E-007</td>
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<td>1.2737E-010</td>
<td>1.9886E-012</td>
<td>4.4076E-014</td>
</tr>
<tr>
<td>Rashidinia et al. [11]</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1/16</td>
<td>2.96E-006</td>
<td>1.85E-007</td>
<td>1.15E-008</td>
<td>7.24E-010</td>
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</tr>
<tr>
<td>1/32</td>
<td>1.18E-005</td>
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<td>2.96E-009</td>
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</table>

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

Example 2. Consider the following singularly perturbed problem:

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

$$0 \leq x \leq 1,$$ with $y(0) = y(1) = 0.$

The exact solution for this example is given by:

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

Table 2
Maximum absolute errors for Example 2.

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$N=16$</th>
<th>$N=32$</th>
<th>$N=64$</th>
<th>$N=128$</th>
<th>$N=256$</th>
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</thead>
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<tr>
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<td>Rashidinia et al. [11]</td>
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</table>

The numerical results of the maximum absolute errors are tabulated in Table 2 for different values of the perturbation parameters $\varepsilon$ and $N$. The effect of the perturbation parameter on the solution of the problem is also shown in Figs. 1(a)–2(b) for fixed $h$ and different values of the perturbation parameter $\varepsilon$, that is, Figs. 1(a)–2(b) show the comparison of the exact and numerical solutions for $h \geq \varepsilon$.

6. Numerical results

The computational rate of convergence can also be obtained using the double mesh principle defined below. Let

$$Z_h = \max_i \left| y_i^h - y_i^{h/2} \right|,$$

$i = 1, 2, \ldots, N - 1$
where \( y_i^h \) is the numerical solution on the mesh \( \{x_i\}_{i=1}^{N-1} \) at the nodal point \( x_i \) where

\[ x_i = x_0 + ih, \quad i = 1, 2, \ldots, N - 1 \]

and

where \( y_{i/2}^h \) is the numerical solution at the nodal point \( x_i \) on the mesh \( \{x_i\}_{i=1}^{2N-1} \) where

\[ x_i = x_0 + ih/2, \quad i = 1, 2, \ldots, 2N - 1. \]

In the same way, one can define \( Z_{h/2} \) by replacing \( h \) by \( h/2 \) and \( N-1 \) by \( 2N-1 \). That is, \( Z_{h/2} = \max_i \left| y_i^{h/2} - y_i^{h/4} \right|, \quad i = 1, 2, \ldots, 2N - 1. \)

The computed rate of convergence is defined as

\[
\text{Rate} = \frac{\log Z_h - \log Z_{h/2}}{\log 2}.
\]

Figs. 1(a)–2(b) show the numerical solutions obtained by the present method for \( h \geq \varepsilon \) compared to the exact solutions.

7. Discussion and conclusion

In this paper, we described the sixth-order compact finite difference method to solve singularly perturbed reaction–diffusion equations. To demonstrate the efficiency of the method, we implemented two model examples by taking different values for the perturbation parameter, \( \varepsilon \), and mesh size, \( h \). The numerical results obtained by the present method have been compared with numerical results obtained by [11–13] from the literature, and the results are summarized in Tables 1 and 2 for different values of the perturbation parameter, \( \varepsilon \), and different numbers of mesh points, \( N \).

Further, as shown in Figs. 1(a)–2(b), the proposed method approximates the exact solution very well for \( h \geq \varepsilon \), for which most of the existing methods fail to give good results. Moreover, the maximum absolute errors decrease rapidly as \( N \) increases.

To further corroborate the applicability of the proposed method, graphs were plotted for Examples 1 and 2 for exact solutions versus the numerical solutions obtained for different values of \( \varepsilon \). Figs. 1(a)–2(b) indicate good agreement of the results, presenting exact as
well as numerical solutions, which proves the reliability of the compact finite difference method. Further, the numerical results presented in this paper demonstrate the improvement of the proposed method over some of the existing methods reported in the literature.

Both the theoretical and numerical error bounds have been established for the sixth-order compact finite difference method. The results confirmed that the computational rate of convergence and theoretical estimates are in agreement (Tables 3 and 4). The present method is conceptually simple, easy to use and readily adaptable for computer implementation for solving singularly perturbed reaction–diffusion equations.

Acknowledgments

The authors would like to thank Jimma University for the financial and material support of the work as part of the MSc Thesis of Mr Fasika Wondimu Gelu.

References


