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An Efficient Third-Derivative Hybrid Block Method for the Solution of Second-Order BVPs

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Abstract: A new one-step hybrid block method with two-point third derivatives is developed to solve the second-order boundary value problems (BVPs). The mathematical derivation of the proposed method is based on the interpolation and collocation methods. The theoretical properties of the proposed method, such as consistency and convergence, are well analysed. Some BVPs with different boundary conditions are solved to demonstrate the efficiency and feasibility of the suggested method. The numerical results of the proposed method are much closer to the exact solutions and more competitive than other numerical methods in the available literature.

Keywords: hybrid block method; boundary value problems; ordinary differential equations; convergence analysis; collocation and interpolation methods

MSC: 65L10; 65L20; 65L60

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1. Introduction and Description of the Problem

Numerous real-life application problems frequently lead to ODEs in which the dependent variable or its derivative are specified at more than one point. For second-order problems of the form

$$q''(x) = f(x, q(x), q'(x)), \qquad x \in [a, b] \subset \mathbb{R}, \tag{1}$$

we have the following types of boundary conditions :

(i)

$$q(a) = q_a, \qquad q(b) = q_b\,. \tag{2}$$

(ii)

$$q'(a) = q'_a, \qquad q'(b) = q'_b\,. \tag{3}$$

(iii)

$$m_1(q(a), q'(a)) = v_a, \qquad m_2(q(b), q'(b)) = v_b\,. \tag{4}$$

Hence, when the ODEs, together with any form of the boundary conditions given above, are specified, one obtains a second-order boundary value problem (BVP) of ODEs. Here, I assume that the function f is continuous on $[a, b] \times \mathbb{R}^2$ and fulfills the Lipchitz's conditions to satisfy the uniqueness and existence theorem (see Keller et al. [1] and Soetaert et al. [2]).

The quest to tackle the class of BVP problems in Equations (1)–(4) theoretically or numerically has been of significant importance to scholars in the field of numerical solutions of the differential equations due to multiple practical applications of this problem in real-life modeling problems in various fields of applied and physical sciences and engineering.

The theoretical solution to the problem under consideration may be unknown or difficult to obtain due to the arbitrary nonlinearities of some of the problems of the form (1)–(4). Because of this reason, many research activities are are carried to develop numerical approaches for solving Equations (1)–(4).

There are many approximation methods for solving BVPs of ODEs in the literature. One of them is the shooting method. The shooting method (SM) is one of the existing methods for solving the class of BVPs in Equations (1)–(4). The SM gives a solution to Equations (1)–(4) by transforming them into a system of first-order IVPs of ODEs, which some initial-value solvers available for integrating first-order IVPs can solve. These solvers then find solutions to the obtained system of first-order IVPs for various initial conditions until one gets the solution that fulfills the desired boundary conditions (BCs) of the BVP.

One type of shooting method is the single shooting method (SSM). The SSM is easy to compute and implement. It is further compelling if the integration interval is small. However, a considerable large interval of integration needs a vast number of iterations, which is one of the demerits of the SSM. In addition, the SSM may be unstable for some BVPs, particularly the highly non-linear BVP of ODEs of the form (1)–(4). In the non-linear case, if the initial values are far from correct, the single SM always fails to obtain a correct solution.

Other types of shooting techniques have been proposed to overcome the the limitation associated with the SSM. One of the available shooting methods for increasing the accuracy of the SSM is the multiple SM, which decreases the distance of the growth of errors by partitioning the interval of integration. Multiple SM always gives better results than SSM. In addition, multiple SM can control the problem of instability for large intervals associated with the single SM by decreasing the growth of the solutions of the obtained systems of IVPs and partitioning the interval into several subintervals and then simultaneously improving the initial value to satisfy the boundary condition.

The SM can be applied effectively to the general non-linear second-order BVP of the form (1), with any of the boundary conditions given in Equations (3) and (4), where the non-linear terms pose no particular problems, and this is the main merit of utilising a shooting strategy as opposed to the finite difference method, in which a solution of finite difference equations is needed. However, the SM's main drawback is that shooting for more than one BC requires high computational time to obtain good accuracy.

For more explanation on shooting methods theory, see Ascher et al. [3], Ascher and Petzold [4], Atkinson et al. [5], Keskin [6], and Hoffman [7].

Several scholars have developed and used various approximate techniques for numerically integrating the type of problems under consideration. Some of these methods are the finite difference method, collocation method, spectral method, Galerkin method, variational iteration method, the Rayleigh–Ritz method, B-spline technique, the Adomian decomposition method, a fixed-point iteration with Green's functions method, finite-element technique, B-spline linear multistep method, block method, the simple Homotopy perturbation method, higher derivative hybrid block techniques, or the trigonometrically fitted predictor–corrector method (see [8–26]).

The research on BVPs is one of the important areas in applied and computational mathematics because it plays an essential role in modeling real-life problems in astrophysics, heat transfer, fluid mechanics and dynamics and physical and chemical phenomena such as electromagnetic radiation reactions, chemical reactor theory, isothermal packed-bed reactor and numerous other real-world differential problems, which can be modeled by Equations (1)–(4). For more details about the application of BVPs for modeling real-life differential problems, see [27–30]. Motivated by the different applications of the BVPs in real-world modeling problems in applied sciences and engineering mentioned above and with the aims of improving the accuracy of some existing methods for solving Equations (1)–(4), in this research paper, a new two-point third-derivative hybrid block method (TDHBM) is proposed to provide a better numerical solution to BVP in Equations (1)–(4).

2. Derivation of the TDHBM

This section aims to derive a TDHBM with two intermediate points on the interval $[x_n, x_{n+1}]$. To derive the proposed TDHBM, I assume that the theoretical solution $q(x)$ is approximated by a polynomial $p(x)$, i.e.,

$$q(x) \simeq p(x) = \sum_{n=0}^{7} k_n \, x^n, \tag{5}$$

from the above equation, we obtain

$$q'(x) \simeq p'(x) = \sum_{n=1}^{7} k_n n x^{n-1} \tag{6}$$

$$q''(x) \simeq p''(x) = \sum_{n=2}^{7} k_n n(n-1) x^{n-2} \tag{7}$$

$$q'''(x) \simeq p'''(x) = \sum_{n=3}^{7} k_n n(n-1)(n-2) x^{n-3}, \tag{8}$$

in which $k_n \in \mathbb{R}$ are real unknown coefficients that will be evaluated using collocation conditions at specific points. Consider the two off-grid points $x_n + (c_1)h$ and $x_n + (c_2)h$ on $[x_n, x_{n+1}]$ and the approximations in Equations (5) and (6) evaluated at the point x_n; its second derivative in Equation (7) is applicable to the points $x_n, x_{n+c_1}, x_{n+c_2}, x_{n+1}$, and its third derivative in Equation (8) is applicable to the points x_n, x_{n+1}. As a result, I obtain a system of eight equations with eight real unknowns, $k_n, n = 0(1)7$, written in matrix form as

$$\begin{pmatrix}
1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 & x_n^6 & x_n^7 \\
0 & 1 & 2x_n & 3x_n^2 & 4x_n^3 & 5x_n^4 & 6x_n^5 & 7x_n^6 \\
0 & 0 & 2 & 6x_n & 12x_n^2 & 20x_n^3 & 30x_n^4 & 42x_n^5 \\
0 & 0 & 2 & 6x_{n+c_1} & 12x_{n+c_1}^2 & 20x_{n+c_1}^3 & 30x_{n+c_1}^4 & 42x_{n+c_1}^5 \\
0 & 0 & 2 & 6x_{n+c_2} & 12x_{n+c_2}^2 & 20x_{n+c_2}^3 & 30x_{n+c_2}^4 & 42x_{n+c_2}^5 \\
0 & 0 & 2 & 6x_{n+1} & 12x_{n+1}^2 & 20x_{n+1}^3 & 30x_{n+1}^4 & 42x_{n+1}^5 \\
0 & 0 & 0 & 6 & 24x_n & 60x_n^2 & 120x_n^3 & 210x_n^4 \\
0 & 0 & 0 & 6 & 24x_{n+1} & 60x_{n+1}^2 & 120x_{n+1}^3 & 210x_{n+1}^4
\end{pmatrix}
\begin{pmatrix} k_0 \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ k_5 \\ k_6 \\ k_7 \end{pmatrix}
=
\begin{pmatrix} q_n \\ q'_n \\ f_n \\ f_{n+c_1} \\ f_{n+c_2} \\ f_{n+1} \\ g_n \\ g_{n+1} \end{pmatrix}.$$

I obtain the values of the coefficients k_n, $n = 0(1)7$ by solving the above system of equations using the Gaussian elimination method. Then, after mathematical simplifications, I rewrite the polynomial in Equation (5) as follows

$$\begin{aligned} p(x_n + th) \quad = \quad & \alpha_0(t) q_n + h\alpha_1(t) q'_n + h^2(\beta_0(t) f_n + \beta_{c_1}(t) f_{n+c_1} + \beta_{c_2}(t) f_{n+c_2} + \beta_1(t) f_{n+1}) \\ & + h^3(\gamma_0(t) g_n + \gamma_1(t) g_{n+1}), \end{aligned} \tag{9}$$

where the coefficients of the continuous scheme in the above equation is given by

$$
\begin{aligned}
\alpha_0(t) &= 1,\\
\alpha_1(t) &= t,\\
\beta_0(t) &= \frac{125t^7}{224} - \frac{223t^6}{96} + \frac{1137t^5}{320} - \frac{413t^4}{192} + \frac{t^2}{2},\\
\beta_{c_1}(t) &= -\frac{405t^7}{392} + \frac{81t^6}{20} - \frac{3159t^5}{560} + \frac{81t^4}{28},\\
\beta_{c_2}(t) &= \frac{3125t^7}{1568} - \frac{625t^6}{96} + \frac{3125t^5}{448} - \frac{3125t^4}{1344},\\
\beta_1(t) &= -\frac{85t^7}{56} + \frac{287t^6}{60} - \frac{391t^5}{80} + \frac{19t^4}{12},\\
\gamma_0(t) &= \frac{5t^7}{56} - \frac{47t^6}{120} + \frac{53t^5}{80} - \frac{25t^4}{48} + \frac{t^3}{6},\\
\gamma_1(t) &= \frac{5t^7}{28} - \frac{8t^6}{15} + \frac{21t^5}{40} - \frac{t^4}{6}.
\end{aligned}
$$

The following main formulas that approximate the solutions $q(x_{n+1})$ and $q'(x_{n+1})$ are obtained by evaluating (5) and (6) at the point $x_{n+1} = x_n + h$:

$$
\begin{aligned}
q_{n+1} &= q_n + hq'_n + h^2\left(\tfrac{1053f_{n+c_1}}{3920} + \tfrac{625f_{n+c_2}}{4704} + \tfrac{461f_n}{3360} - \tfrac{13f_{n+1}}{336}\right)\\
&\quad + h^3\left(\tfrac{g_n}{168} + \tfrac{g_{n+1}}{280}\right).
\end{aligned} \tag{10}
$$

$$
\begin{aligned}
hq'_{n+1} &= hq'_n + h^2\left(\tfrac{243f_{n+c_1}}{560} + \tfrac{625f_{n+c_2}}{1344} + \tfrac{25f_n}{192} - \tfrac{7f_{n+1}}{240}\right)\\
&\quad + h^3\left(\tfrac{g_n}{240} + \tfrac{g_{n+1}}{120}\right).
\end{aligned} \tag{11}
$$

The evaluations of $p(x)$ and $p'(x)$ at the points x_{n+c_1}, x_{n+c_2} are also considered in order to produce a total of six formulas that form the TDHBM. The obtained four formulas after the evaluation and simplification are listed below

$$
\begin{aligned}
q_{n+c_1} &= q_n + \tfrac{h}{3}q'_n + h^2\left(\tfrac{1861f_{n+c_1}}{105{,}840} - \tfrac{6875f_{n+c_2}}{857{,}304} + \tfrac{24{,}917f_n}{612{,}360} + \tfrac{6493f_{n+1}}{1{,}224{,}720}\right)\\
&\quad + h^3\left(\tfrac{151g_n}{76{,}545} - \tfrac{67g_{n+1}}{122{,}472}\right),\\
q_{n+c_2} &= q_n + \tfrac{4h}{5}q'_n + h^2\left(\tfrac{694{,}656f_{n+c_1}}{3{,}828{,}125} + \tfrac{164f_{n+c_2}}{3675} + \tfrac{36{,}524f_n}{328{,}125} - \tfrac{28{,}544f_{n+1}}{1{,}640{,}625}\right)\\
&\quad + h^3\left(\tfrac{8432g_n}{1{,}640{,}625} + \tfrac{768g_{n+1}}{546{,}875}\right),
\end{aligned} \tag{12}
$$

$$
\begin{aligned}
hq'_{n+c_1} &= hq'_n + h^2\left(\tfrac{859f_{n+c_1}}{5040} - \tfrac{18{,}125f_{n+c_2}}{326{,}592} + \tfrac{8491f_n}{46{,}656} + \tfrac{2123f_{n+1}}{58{,}320}\right)\\
&\quad + h^3\left(\tfrac{611g_n}{58{,}320} - \tfrac{109g_{n+1}}{29{,}160}\right),\\
hq'_{n+c_2} &= hq'_n + h^2\left(\tfrac{47{,}952f_{n+c_1}}{109{,}375} + \tfrac{8f_{n+c_2}}{21} + \tfrac{1204f_n}{9375} - \tfrac{6928f_{n+1}}{46{,}875}\right)\\
&\quad + h^3\left(\tfrac{184g_n}{46{,}875} + \tfrac{608g_{n+1}}{46{,}875}\right).
\end{aligned} \tag{13}
$$

3. Theoretical Analysis

In this section, the characteristics of the suggested TDHBM are investigated; one of the most difficult tasks is to analyse the convergence of the proposed method.

3.1. Consistency and Order of the TDHBM

I obtain the local truncation error for each of the formulas given in Equations (10)–(13) by transferring all of the terms to the left, replacing the approximate solution with the true

solutions, and expanding the obtained expression by Taylor series in powers of h. By doing this, I obtain the order (p) and the LTEs reported in the following Table 1.

Table 1. Order (p) and local truncation errors (LTEs) for the TDHBM method.

Scheme	Order	Local Truncation Error
q_{n+c_1}	6	$\frac{1697h^8q^{(8)}(x_n)}{19,840,464,000} + \mathcal{O}(h^9)$
q_{n+c_2}	6	$\frac{32h^8q^{(8)}(x_n)}{1,107,421,875} + \mathcal{O}(h^9)$
q_{n+1}	6	$-\frac{h^8q^{(8)}(x_n)}{9,072,000} + \mathcal{O}(h^9)$
q'_{n+c_1}	6	$\frac{1861h^7q^{(8)}(x_n)}{3,306,744,000} + \mathcal{O}(h^8)$
q'_{n+c_2}	6	$-\frac{164h^7q^{(8)}(x_n)}{221,484,375} + \mathcal{O}(h^8)$
q'_{n+1}	6	$-\frac{h^7q^{(8)}(x_n)}{1,512,000} + \mathcal{O}(h^8)$

Table 1 shows that each of the above formulas is of order 6. Since the order of the formulas is greater than one, the TDHBM method is consistent.

3.2. Convergence Analysis

This subsection focuses on the convergence analysis of the suggested TDHBM method.

Theorem 1 (Convergence Theorem [20]). *Let $q(x)$ denote the true solution to problem (1) along with the boundary conditions in (2), and $\{q_j\}_{j=1}^{N}$ denote the discrete solution provided by the proposed method. Then, the proposed method is convergent of order six.*

Proof. I begin the proof by letting A denote the $6N \times 6N$ matrix indicated by

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,2N} \\ \vdots & \vdots & & \vdots \\ A_{2N,1} & A_{2N,2} & \dots & A_{2N,2N} \end{bmatrix},$$

where the components $A_{i,j}$ are 3×3 submatrices, with the exception of the $A_{i,N}$, $i = 1, \dots, 2N$ which has 3×2 elements, and the $A_{i,2N}$, $i = 1, \dots, 2N$ with the size 3×4. These submatrices are provided below

$$A_{i,i} = I, i = 1, \dots, N-1, \text{ where } I \text{ is the identity matrix,}$$

$$A_{N,N} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}; \qquad A_{i,i-1} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & -1 \\ 0 & 0 & -1 \end{bmatrix}, \ i = 2, \dots, N;$$

$$A_{i,i} = h \begin{bmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}, \ i = N+1, \dots, 2N-1; \qquad A_{2N,2N} = h \begin{bmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix};$$

$$A_{i,i+1} = h \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \ i = N+1 \dots, 2N-2; \qquad A_{2N-1,2N} = h \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix};$$

$$A_{i,N+i} = h\begin{bmatrix} -\frac{1}{3} & 0 & 0 \\ -\frac{4}{5} & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix},\ i = 1\ldots, N-1; \qquad A_{N,2N} = h\begin{bmatrix} -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{4}{5} & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}.$$

On the other hand, let U be a $6N \times (6N+2)$ matrix defined by

$$U = \begin{bmatrix} U_{1,1} & U_{1,2} & \ldots & U_{1,2N} \\ \vdots & \vdots & & \vdots \\ U_{2N,1} & U_{2N,2} & \ldots & U_{2N,2N} \end{bmatrix},$$

where the elements $U_{i,j}$ are 3×3 submatrices except for $U_{i,1}, U_{i,N+1}, i = 1, \ldots, 2N$, which have size 3×4. Those submatrices are given as follows

$$U_{1,1} = \begin{bmatrix} -\frac{24{,}917}{612{,}360} & -\frac{1861}{105{,}840} & \frac{6875}{857{,}304} & -\frac{6493}{1{,}224{,}720} \\ -\frac{36{,}524}{328{,}125} & -\frac{694{,}656}{3{,}828{,}125} & -\frac{164}{3675} & \frac{28{,}544}{1{,}640{,}625} \\ -\frac{461}{3360} & -\frac{1053}{3920} & -\frac{625}{4704} & \frac{13}{336} \end{bmatrix}; \qquad U_{i,i} = \begin{bmatrix} -\frac{1861}{105{,}840} & \frac{6875}{857{,}304} & -\frac{6493}{1{,}224{,}720} \\ -\frac{694{,}656}{3{,}828{,}125} & -\frac{164}{3675} & \frac{28{,}544}{1{,}640{,}625} \\ -\frac{1053}{3920} & -\frac{625}{4704} & \frac{13}{336} \end{bmatrix}, i = 2\ldots, N;$$

$$U_{i,i-1} = \begin{bmatrix} 0 & 0 & -\frac{24{,}917}{612{,}360} \\ 0 & 0 & -\frac{36{,}524}{328{,}125} \\ 0 & 0 & -\frac{461}{3360} \end{bmatrix}, i = 3, \ldots, N; \qquad U_{2,1} = \begin{bmatrix} 0 & 0 & 0 & -\frac{24{,}917}{612{,}360} \\ 0 & 0 & 0 & -\frac{36{,}524}{328{,}125} \\ 0 & 0 & 0 & -\frac{461}{3360} \end{bmatrix};$$

$$U_{N+1,1} = \begin{bmatrix} -\frac{8491}{46{,}656} & -\frac{859}{5040} & \frac{18{,}125}{326{,}592} & -\frac{2123}{58{,}320} \\ -\frac{1204}{9375} & -\frac{47{,}952}{109{,}375} & -\frac{8}{21} & \frac{6928}{46{,}875} \\ -\frac{25}{192} & -\frac{243}{560} & -\frac{625}{1344} & \frac{7}{240} \end{bmatrix}; \qquad U_{N+j,j} = \begin{bmatrix} -\frac{859}{5040} & \frac{18{,}125}{326{,}592} & -\frac{2123}{58{,}320} \\ -\frac{47{,}952}{109{,}375} & -\frac{8}{21} & \frac{6928}{46{,}875} \\ -\frac{243}{560} & -\frac{625}{1344} & \frac{7}{240} \end{bmatrix}, j = 2, \ldots, N;$$

$$U_{N+j,j-1} = \begin{bmatrix} 0 & 0 & -\frac{8491}{46{,}656} \\ 0 & 0 & -\frac{1204}{9375} \\ 0 & 0 & -\frac{25}{192} \end{bmatrix}, j = 3, \ldots, N; \qquad U_{N+2,1} = \begin{bmatrix} 0 & 0 & 0 & -\frac{8491}{46{,}656} \\ 0 & 0 & 0 & -\frac{1204}{9375} \\ 0 & 0 & 0 & -\frac{25}{192} \end{bmatrix};$$

$$U_{1,N+1} = h\begin{bmatrix} -\frac{151}{76{,}545} & 0 & 0 & \frac{67}{122{,}472} \\ -\frac{8432}{1{,}640{,}625} & 0 & 0 & -\frac{768}{546{,}875} \\ -\frac{1}{168} & 0 & 0 & -\frac{1}{280} \end{bmatrix}; \qquad U_{i,N+i} = h\begin{bmatrix} 0 & 0 & \frac{67}{122{,}472} \\ 0 & 0 & -\frac{768}{546{,}875} \\ 0 & 0 & -\frac{1}{280} \end{bmatrix}, i = 2\ldots, N;$$

$$U_{i,N+i-1} = h\begin{bmatrix} 0 & 0 & -\frac{151}{76{,}545} \\ 0 & 0 & -\frac{8432}{1{,}640{,}625} \\ 0 & 0 & -\frac{1}{168} \end{bmatrix}, i = 3, \ldots, N; \qquad U_{2,N+1} = h\begin{bmatrix} 0 & 0 & 0 & -\frac{151}{76{,}545} \\ 0 & 0 & 0 & -\frac{8432}{1{,}640{,}625} \\ 0 & 0 & 0 & -\frac{1}{168} \end{bmatrix};$$

$$U_{N+1,N+1} = h\begin{bmatrix} -\frac{611}{58,320} & 0 & 0 & \frac{109}{29,160} \\ -\frac{184}{46,875} & 0 & 0 & -\frac{608}{46,875} \\ -\frac{1}{240} & 0 & 0 & -\frac{1}{120} \end{bmatrix}; \qquad U_{N+i,N+i} = h\begin{bmatrix} 0 & 0 & \frac{109}{29,160} \\ 0 & 0 & -\frac{608}{46,875} \\ 0 & 0 & -\frac{1}{120} \end{bmatrix}, i = 2, \ldots, N;$$

$$U_{N+i,N+i-1} = h\begin{bmatrix} 0 & 0 & -\frac{611}{58,320} \\ 0 & 0 & -\frac{184}{46,875} \\ 0 & 0 & -\frac{1}{240} \end{bmatrix}, i = 3, \ldots, N; \qquad U_{N+2,N+1} = h\begin{bmatrix} 0 & 0 & 0 & -\frac{611}{58,320} \\ 0 & 0 & 0 & -\frac{184}{46,875} \\ 0 & 0 & 0 & -\frac{1}{240} \end{bmatrix},$$

where the remaining submatrices are null matrices.

I remark that all the submatrices $A_{i,j}$ and $U_{i,j}$ contain the coefficients of the proposed method in Equations (10) and (11) for $n = 0, 1, 2, \ldots, N-1$. I proceed to define the vectors of exact values as follows

$$\begin{aligned} Q &= \left(q(x_{c_1}), q(x_{c_2}), \ldots, q(x_{N-1+c_2}), q'(x_0), q'(x_{c_1}), \ldots, q'(x_N)\right)^\top, \\ F &= \big(f(x_0, q(x_0), q'(x_0)), f(x_{c_1}, q(x_{c_1}), q'(x_{c_1})), \ldots, f(x_N, q(x_N), q'(x_N)), \\ &\quad g(x_0, q(x_0), q'(x_0)), g(x_{c_1}, q(x_{c_1}), q'(x_{c_1})), \ldots, g(x_N, q(x_N), q'(x_N))\big)^\top. \end{aligned}$$

I also note that Q has $(3N-1)+(3N+1) = 6N$ components, while F has $(3N+1)+(3N+1) = 6N+2$ components.

By employing the notations mentioned above, the exact form of the system that gives the approximate values for the problem under consideration is defined by

$$A_{6N\times 6N} Q_{6N} + h^2 U_{6N\times(6N+2)} F_{6N+2} + C_{6N} = L(h)_{6N}, \tag{14}$$

where

$$C_{6N} = \left(-q_a, -q_a, -q_a, -q_a, 0, \ldots, 0, q_b, 0, \ldots, 0\right)^\top,$$

and

$$L(h)_{6N} = \begin{bmatrix} \frac{1697h^8 q^{(8)}(x_n)}{19,840,464,000} + \mathcal{O}(h^9) \\ \frac{32h^8 q^{(8)}(x_n)}{1,107,421,875} + \mathcal{O}(h^9) \\ -\frac{h^8 q^{(8)}(x_n)}{9,072,000} + \mathcal{O}(h^9) \\ \frac{1697h^8 q^{(8)}(x_1)}{19,840,464,000} + \mathcal{O}(h^9) \\ \vdots \\ -\frac{h^8 q^{(8)}(x_{N-1})}{9,072,000} + \mathcal{O}(h^9) \\ \frac{1861h^7 q^{(8)}(x_n)}{3,306,744,000} + \mathcal{O}(h^8) \\ -\frac{164h^7 q^{(8)}(x_n)}{221,484,375} + \mathcal{O}(h^8) \\ -\frac{h^7 q^{(8)}(x_n)}{1,512,000} + \mathcal{O}(h^8) \\ \frac{1861h^7 q^{(8)}(x_1)}{3,306,744,000} + \mathcal{O}(h^8) \\ \vdots \\ -\frac{h^7 q^{(8)}(x_{N-1})}{1,512,000} + \mathcal{O}(h^8) \end{bmatrix}.$$

Similarly, the system to obtain the approximate values of the problem under consideration is denoted by

$$A_{6N\times 6N} \bar{Q}_{6N} + h^2 U_{6N\times(6N+2)} \bar{F}_{6N+2} + C_{6N} = 0\,, \tag{15}$$

where $\bar{Q}_{6N}$ approximates the vector Q_{6N}, that is,

$$\bar{Q}_{6N} = \left(q_{c_1}, q_{c_2}, q_1, \ldots, q_{N-1+c_2}, q_0, q_{c_1}, \ldots, q_N\right)^\top,$$

and

$$\bar{F}_{6N+2} = \left(f_0, f_{c_1}, f_{c_2}, f_1, \ldots, f_N, g_0, g_{c_1}, g_{c_2}, g_1, \ldots, g_N\right)^\top.$$

On subtracting (15) from (14) and simplifying, I obtain

$$A_{6N\times 6N} E_{6N} + h^2 U_{6N\times(6N+2)} (F - \bar{F})_{6N+2} = L(h)_{6N}, \tag{16}$$

where $E_{6N} = Q_{6N} - \bar{Q}_{6N} = \left(e_{c_1}, \ldots, e_{N-1+c_2}, e'_0, e'_{c_1}, \ldots, e'_N\right)^\top$.

Using Mean-Value Theorem (see [31]), one can express for $i = 0(c_1)N$

$$f(x_i, q(x_i), q(x_i)) - f(x_i, q_i, q'_i) = (q(x_i) - q_i)\frac{\partial f}{\partial q}(\xi_i) + (q(x_i) - q'_i)\frac{\partial f}{\partial q}(\xi_i)$$
$$g(x_i, q(x_i), q(x_i)) - g(x_i, q_i, q'_i) = (q(x_i) - q_i)\frac{\partial g}{\partial q}(\eta_i) + (q(x_i) - q'_i)\frac{\partial g}{\partial q}(\eta_i)$$

where ξ_i and η_i are intermediate points on the line segment joining $(x_i, q(x_i), q(x_i))$ to (x_i, q_i, q'_i). Thus, I obtain

$$(F - \bar{F})_{6N+2} = \begin{pmatrix} \frac{\partial f}{\partial q}(\xi_0) & 0 & \ldots & 0 & \frac{\partial f}{\partial q}(\xi_0) & 0 & \ldots & 0 \\ 0 & \frac{\partial f}{\partial q}(\xi_{c_1}) & \ldots & 0 & 0 & \frac{\partial f}{\partial q}(\xi_{c_1}) & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \frac{\partial f}{\partial q}(\xi_N) & 0 & 0 & \ldots & \frac{\partial f}{\partial q}(\xi_N) \\ \frac{\partial g}{\partial q}(\eta_0) & 0 & \ldots & 0 & \frac{\partial g}{\partial q}(\eta_0) & 0 & \ldots & 0 \\ 0 & \frac{\partial g}{\partial y}(\eta_{c_1}) & \ldots & 0 & 0 & \frac{\partial g}{\partial q}(\eta_{c_1}) & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \frac{\partial g}{\partial q}(\eta_N) & 0 & 0 & \ldots & \frac{\partial g}{\partial q}(\eta_N) \end{pmatrix} \begin{pmatrix} e_0 \\ e_{c_1} \\ \vdots \\ e_N \\ e'_0 \\ e'_{c_1} \\ \vdots \\ e'_N \end{pmatrix}$$

$$= \begin{pmatrix} 0 & \ldots & 0 & \frac{\partial f}{\partial q}(\xi_0) & 0 & \ldots & 0 & 0 \\ \frac{\partial f}{\partial q}(\xi_{c_1}) & \ldots & 0 & 0 & \frac{\partial f}{\partial q}(\xi_{c_1}) & \ldots & 0 & 0 \\ \vdots & \ddots & 0 & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \ldots & \frac{\partial f}{\partial q}(\xi_{N-1+c_2}) & 0 & 0 & \ldots & \frac{\partial f}{\partial q}(\xi_{N-1+c_2}) & 0 \\ 0 & \ldots & 0 & 0 & 0 & \ldots & 0 & \frac{\partial f}{\partial q}(\xi_N) \\ 0 & \ldots & 0 & \frac{\partial g}{\partial q}(\eta_0) & 0 & \ldots & 0 & 0 \\ \frac{\partial g}{\partial q}(\eta_{c_1}) & \ldots & 0 & 0 & \frac{\partial g}{\partial q}(\eta_{c_1}) & \ldots & 0 & 0 \\ \vdots & \ddots & 0 & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \ldots & \frac{\partial g}{\partial q}(\eta_{N-1+c_2}) & 0 & 0 & \ldots & \frac{\partial g}{\partial q}(\eta_{N-1+c_2}) & 0 \\ 0 & \ldots & 0 & 0 & 0 & \ldots & 0 & \frac{\partial g}{\partial q}(\eta_N) \end{pmatrix} \begin{pmatrix} e_{c_1} \\ \vdots \\ e_{N-1+c_2} \\ e'_0 \\ e'_{c_1} \\ \vdots \\ e'_N \end{pmatrix}$$

$$= J_{(6N+2)\times 6N}\, E_{6N}\,.$$

The equation in (16) can be rewritten as follows

$$\left(A_{6N\times 6N} + h^2 U_{6N\times(6N+2)} J_{(6N+2)\times 6N}\right) E_{6N} = L(h)_{6N}, \tag{17}$$

and setting $M = D + h^2UJ$, I obtain

$$M_{6N\times 6N}E_{6N} = L(h)_{6N}. \tag{18}$$

I have that for sufficiently small values of $h > 0$, the equation in (18) may be rewritten as

$$E = \left(M^{-1}\right)L(h)\,. \tag{19}$$

I take into account the maximum norm in $\mathbb{R}$, $\|E\| = \max_i |e_i|$, and the associated matrix induced norm in $\mathbb{R}^{6N\times 6N}$. By expanding every term of M^{-1} in series around h, it can be proved that $\|M^{-1}\| = \mathcal{O}(h^{-1})$. For the details to prove that $\|M^{-1}\| = \mathcal{O}(h^{-1})$, see [24]. Then, by assuming that $q(x)$ has in $[a, b]$ bounded derivatives up to the required order, I deduce that:

$$\begin{aligned}\|E\| &\leq \|\left(M^{-1}\right)\|\,\|L(h)\| \\ &= \mathcal{O}(h^{-1})\,\mathcal{O}(h^7) \\ &\leq K h^6.\end{aligned}$$

From the above result, the proposed TDHBM is a six-order convergent method. □

4. Implementation and Numerical Experiments

Here, I discuss the computational details and apply the proposed TDHBM method for solving Equations (1)–(4).

Implementation

I denote the set of equations in Equations (10)–(13) by $F_n = 0$, taking into account the mixed boundary conditions in Equation (4) to formulate the algebraic system as follows

$$\begin{cases} m_1(q_0, q_0') - v_a = 0\,, \\ F_0 = 0\,, \\ F_1 = 0\,, \\ \quad \cdots \\ F_{N-1} = 0\,, \\ m_2(q_N, q_N') - v_b = 0, \end{cases} \tag{20}$$

In addition, the $6N + 2$ unknowns are denoted by

$$\mathbf{Q} = (q_0, q_0', q_{c_1}, q_{c_2}, q_1, q_1', q_{1+c_1}, q_{1+c_2}, q_2, q_2', \ldots, q_{N-1+c_1}, q_{N-1+c_2}, q_N, q_N')\,.$$

I solve the system $\mathbf{F} = 0$ using the following Newton iteration

$$\mathbf{Q}^{i+1} = \mathbf{Q}^i - \left(\mathbf{J}^i\right)^{-1}\mathbf{F}^i,$$

where the Jacobian matrix of $\mathbf{J}$ is denoted by $\mathbf{F}$. I take into consideration a stopping criterion with a maximum of 100 iterations and an error of less than 10^{-16} between two successive approximations.

I apply a homotopy-type procedure to obtain suitable starting values for Newton's method by considering a family of non-linear BVPs $H_j, j = 0, 1, 2, \ldots, r$, such that for $j = 0$,

the problem H_0 permits only the solution $q(x) = 0$, while for $j = r$, I obtain the original problem. In this manner, I obtain a family of BVPs represented by

$$H_j \equiv \begin{cases} q'' = f(x, q, q') - f(x, 0, 0) + \frac{j}{r} f(x, 0, 0), \\ m_1(q(a), q'(a)) = \frac{j}{r} v_a, \\ m_2(q(b), q'(b)) = \frac{j}{r} v_b, \end{cases} \tag{21}$$

for $j = 0, 1, \ldots, r$. For $j = r$, the nonlinear system related to the original problem is solved, taking the values obtained after solving the problem H_{r-1} as initial guesses.

5. Numerical Experiments

This section presents the numerical solutions for the problems of the form (1)–(4) using the proposed TDHBM method. The accuracy of the TDHBM is measured by utilising the maximum absolute error (MAE) and the rate of convergence (ROC) formulas:

$$\begin{aligned} MAE &= \max_{j=0,\ldots,N} \left\| q(x_j) - q_j \right\|_\infty, \\ ROC &= -\log_2 \left(\frac{MAE_h}{MAE_{2h}} \right), \end{aligned}$$

where $q(x_j)$ is the exact solution, and q_j is the computed result at each point x_j of the discrete grid.

Methods considered for numerical comparisons are indicated by:

- TDHBM: The third derivative one-step hybrid block method derived in this paper.
- TDFM: The third-derivative Falkner method of order six in [32].
- FDM: The finite difference method in [33].
- BSCM: The B-spline collocation method proposed in [34].
- DQCM: The differential quadrature collocation method in [35].

Some numerical experiments used to demonstrate the efficiency of the proposed TDHBM method are presented below:

5.1. Numerical Experiment 1

As a first numerical experiment, I consider the following isothermal packed-bed reactor BVP [33]

$$\frac{1}{M_{pe}} q''(x) + q'(x) - Rq^2(x) = \mu(x), \quad q'(0) = 0, \quad q(1) + \frac{1}{M_{pe}} q'(1) = 1, \quad x \in [0, 1], \tag{22}$$

where $\mu(x)$ is obtained on the basis that the exact solution of the isothermal packed-bed reactor BVP given in Equation (22) is

$$q(x) = \frac{M_{pe} e^{(x^2 - x^3)}}{(M_{pe} - 1)},$$

where M_{pe} denotes the axial Peclet number, and R stands for the reaction rate group.

The problem (22) is solved using the new TDHBM method with $R = \frac{1}{8}, M_{pe} = 8, r = 1$. Table 2 shows that the proposed method's numerical results are much closer to the exact solutions. In Table 3, one can see that the obtained *ROC* is consistent with the theoretical analysis of the proposed TDHBM method. Problem (22) is also solved by [33] using the same values of $R = \frac{1}{8}, M_{pe} = 8, r = 1$. It is worth noting that the reported MAE for the FDM with $h = \frac{1}{256}$ is 0.78390×10^{-5}, while for the TDHBM with $h = \frac{1}{4}$, the MAE is 6.73605×10^{-8}, confirming a better performance of the proposed TDHBM method. Moreover, Figure 1 shows the good results obtained with the TDHBM method when solving the isothermal packed-bed reactor BVP.

Table 2. Numerical results for Problem (22) with $h = 0.1$.

t	Exact	TDHBM	Absolute Error
0	1.1428571428421719	1.1428571428571428	1.49709×10^{-11}
0.1	1.1531892820395981	1.1531892820272776	1.23206×10^{-11}
0.2	1.1800200061659953	1.1800200060629924	1.03003×10^{-10}
0.3	1.2171735307427942	1.2171735305500633	1.92731×10^{-10}
0.4	1.2580103591061207	1.2580103588502614	2.55859×10^{-10}
0.5	1.2950268037779877	1.2950268035049444	2.73043×10^{-10}

Table 3. MAEs and order of convergence for Problem (22).

h	Method	MAE	ROC
$\frac{1}{4}$	TDHBM	6.73605×10^{-8}	
$\frac{1}{8}$	TDHBM	1.03770×10^{-9}	6.02
$\frac{1}{16}$	TDHBM	1.63760×10^{-11}	5.99
$\frac{1}{32}$	TDHBM	2.59570×10^{-13}	5.98

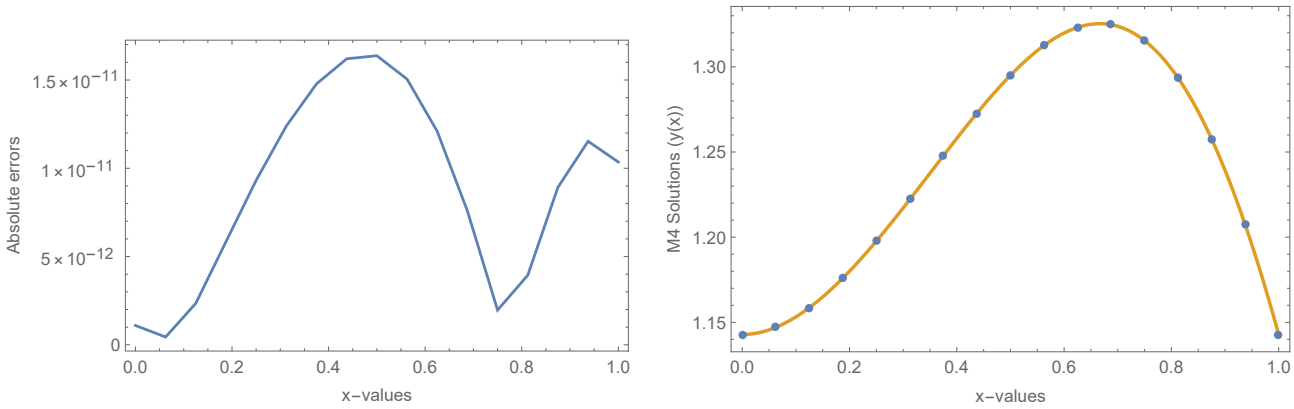

Figure 1. Plots of absolute errors (**left**), exact and TDHBM solutions (**right**) for Problem (22) with $r = 1, R = \frac{1}{8}, M_{pe} = 8, h = \frac{1}{16}$.

5.2. Numerical Experiment 2

In the next experiment, I consider

$$q''(x) = -\frac{1}{2}q(x)q'(x), \tag{23}$$

subject to

$$\{2q(0) - q'(0) = -1.44,\ q(4) + 0.5q'(4) = -6\},\ 0 \le x \le 4,$$

whose true solution is

$$q(x) = \frac{4}{x-5}.$$

The approximate solutions to Problem (23) are compared in Table 4. The data in Table 4 show that the results obtained with TDHBM are more accurate than the TDFM and BSCM methods. Additionally, Figure 2 compares the theoretical and approximative solutions for Problem (23) utilizing the homotopy-type approach with $r = 4$.

Table 4. Comparison of MAEs and order of convergence for Problem (23).

h	Method	*MAE*	*ROC*
$\frac{4}{20}$	TDHBM	2.12733×10^{-7}	
$\frac{4}{20}$	TDFM	1.87062×10^{-5}	
$\frac{4}{20}$	BSCM	2.64200×10^{-4}	
$\frac{4}{40}$	TDHBM	3.47122×10^{-9}	5.93745
$\frac{4}{40}$	TDFM	4.07756×10^{-7}	5.51967
$\frac{4}{40}$	BSCM	1.77700×10^{-5}	3.89411
$\frac{4}{80}$	TDHBM	5.50697×10^{-11}	5.97804
$\frac{4}{80}$	TDFM	7.49040×10^{-9}	5.76652
$\frac{4}{80}$	BSCM	1.12500×10^{-6}	3.98145

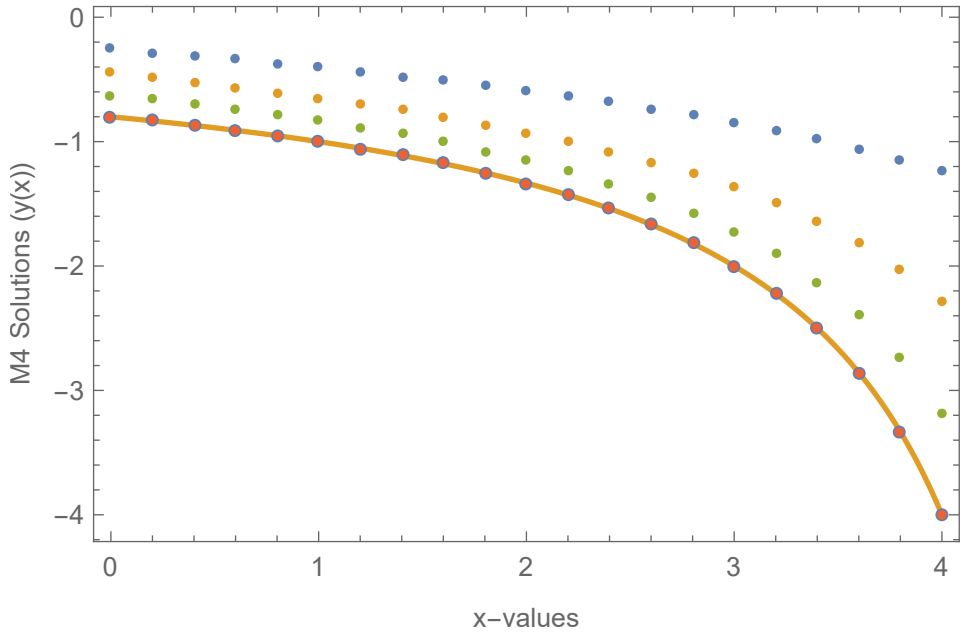

Figure 2. Exact and discrete solutions with the method TDHBM on Problem (23) with $h = \frac{4}{20}, r = 4$.

5.3. Numerical Experiment 3

In the next experiment, I consider a stiff second-order BVP with Dirichlet boundary conditions

$$q''(x) = \eta^2 q(x) - \frac{\pi(\eta^2 + 4\pi^2)\sin(2\pi x)}{\eta}, \tag{24}$$

subject to

$$q(0) = \frac{e^{-\eta} - 1}{e^{-\eta} + 1}, \quad q(1) = \frac{1 - e^{-\eta}}{e^{-\eta} + 1}$$

The exact solution is

$$q(x) = \frac{e^{\eta(x-1)} - e^{-\eta x}}{1 + e^{-\eta}} - \frac{\pi \sin(2\pi x)}{\eta}$$

Table 5 illustrates the comparison of the MAEs with $\eta = 50$ for different step sizes, indicating the better efficiency of the proposed approach.

Table 5. Comparison of MAEs and order of convergence for Problem (24).

h	Method	*MAE*	*ROC*
$\frac{1}{32}$	TDHBM	2.21413×10^{-6}	
$\frac{1}{32}$	TDFM	2.23714×10^{-4}	
$\frac{1}{64}$	TDHBM	3.23302×10^{-8}	6.09771
$\frac{1}{64}$	TDFM	4.40660×10^{-6}	5.66585
$\frac{1}{128}$	TDHBM	5.63709×10^{-10}	5.84179
$\frac{1}{128}$	TDFM	6.91612×10^{-8}	5.99356

5.4. Numerical Experiment 4

For the last numerical experiment, I consider

$$\begin{aligned} q_1''(x) + xq_1'(x) + \cos(\pi x)q_2'(x) &= f_1(x), \\ q_2''(x) + xq_1(x) + xq_2'(x) &= f_2(x), \end{aligned} \tag{25}$$

subject to

$$\begin{aligned} q_1(0) = q_1(1) = 0, \\ q_2(0) = q_2(1) = 0, \end{aligned}$$

where $0 \leq x \leq 1$ and

$$\begin{aligned} f_1(x) &= \sin(x) + (x^2 - x + 2)\cos(x) + (1 - 2x)\cos(\pi x), \\ f_2(x) &= -2 + x\sin(x) + (x^2 - x)\cos(x) + x(1 - 2x)^2. \end{aligned}$$

The analytical solution of Problem (25) is:

$$q_1(x) = (x - 1)\sin(x), \qquad q_2(x) = x - x^2.$$

From Table 6, one can see that the TDHBM is much more accurate than the technique utilised for comparison. Additionally, the plots in Figure 3 show that the numerical solution provided by the TDHBM method agrees with the analytical solution.

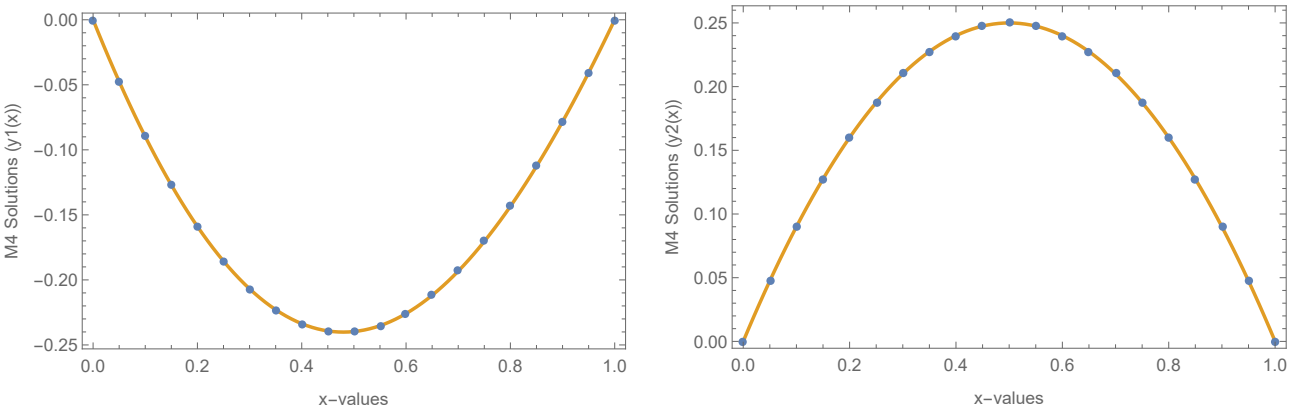

Figure 3. Exact and discrete solutions with the method TDHBM on Problem (25) with $h = \frac{1}{21}, r = 1$.

Table 6. Comparison of the MAE on Problem (25) with $r = 1$.

h	MAE with TDHBM	MAE with DQCM
$\frac{1}{21}$	8.743006×10^{-15}	5.5775×10^{-5}
$\frac{1}{41}$	1.11022×10^{-16}	1.3892×10^{-5}
$\frac{1}{61}$	5.55112×10^{-17}	6.0484×10^{-6}

6. Conclusions

This manuscript has proposed a third-derivative one-step hybrid block method (TDHBM) to solve second-order BVPs directly. The proposed method's numerical results demonstrate that it is suitable and efficient for solving the BVPs under consideration. In summary, I conclude thatthe TDHBM method suggested in this article is more accurate and effectively competitive than some of the existing numerical approaches for integrating the problem given in Equations (1)–(4).

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