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Research Article

Adaptive hybrid numerical schemes with singularity treatment for third order Lane–Emden-type equations

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Abstract

This paper introduces two hybrid algorithms with variable step sizes (PVSHM) designed for the efficient numerical solution of third-order initial value problems (IVPs) governed by Lane–Emden-type equations (LETEs). These equations frequently arise in various scientific and engineering fields, including astrophysics, fluid dynamics, and chemical engineering, where they serve as fundamental mathematical models for complex physical systems. The proposed methods utilize three internal interpolation points and employ specially designed starting formulas on the initial interval to properly handle the singular behavior at the origin. These formulations avoid the direct evaluation of the singular term while preserving the accuracy of the numerical scheme. To ensure both high accuracy and computational efficiency, the PVSHM operates within a variable step-size framework supported by an adaptive local error control strategy, which maintains truncation errors within predefined tolerances. Extensive numerical experiments validate the accuracy, stability, and computational effectiveness of the proposed algorithms, confirming their ability to efficiently solve a wide range of third-order LETE-based IVPs encountered in applied science and engineering contexts.

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1 Introduction

Singular initial value problems (SIVPs) governed by Lane–Emden-type equations (LETEs) are pivotal in various scientific and engineering disciplines, including astrophysics, fluid dynamics, and chemical engineering. These equations often exhibit singular behavior at the origin, posing significant challenges for numerical solutions. Traditional methods may struggle with such singularities, necessitating the development of advanced numerical techniques.

Recent advancements have introduced hybrid methods with variable step sizes to address these challenges effectively. For instance, a pair of optimized Nyström methods with variable step sizes was proposed, demonstrating improved accuracy and efficiency in solving SIVPs of Lane–Emden–Fowler type equations. Similarly, a variable step-size formulation of a pair of block methods was developed, effectively solving SIVP models of Lane–Emden–Fowler type equations [20, 21].

Building upon these developments, this paper introduces two novel hybrid algorithms with variable step sizes designed specifically for efficiently solving SIVPs governed by LETEs. The proposed methods utilize three internal interpolation points and employ modified formulations on the initial subinterval to accommodate the singular behavior near the origin. Rather than eliminating the singularity, these starting formulas avoid the direct evaluation of the singular term at the origin and ensure accurate numerical approximations. To ensure both high accuracy and computational efficiency, the pair of variable-step-size hybrid methods (PVSHM) operates within a variable step-size framework supported by an adaptive local error control strategy, maintaining truncation errors within predefined tolerances.

Extensive numerical experiments validate the accuracy, stability, and computational efficiency of the proposed algorithms. The results demonstrate their capability to effectively solve a wide range of third-order LETE-based initial value problems (IVPs) encountered in applied science and engineering contexts.

Apart from their role in characterizing fluid motion in engineering systems and describing the behavior of stellar or astrophysical structures, the LETEs offer a comprehensive mathematical framework for analyzing a wide spectrum of physical processes. Numerous studies [8, 25, 24] have extensively documented the versatility of LETEs in various branches of engineering, physics, and applied sciences. Motivated by these diverse and significant applications, the present work is devoted to developing an efficient numerical approach for determining the function $z : [0, T] \to \mathbb{R}$ that satisfies the following third-order Lane–Emden-type model problem:

$$\begin{aligned} &z'''(t) = l(t, z(t)) - k(t)z'(t) - \frac{\mu}{t} z''(t), \qquad t \in (0, T), \\ &z(0) = z_0, \qquad z'(0) = z_0', \qquad z''(0) = z_0'', \end{aligned} \tag{1}$$

where the parameters μ, z_0, z_0', z_0'', and $T > 0$ are known values and $k : [0,\ T] \to \mathbb{R}$ and $l : [0,\ T] \times \mathbb{R} \to \mathbb{R}$ are given continuous functions.

Given the broad range of real-world phenomena described by LETEs, the pursuit of analytical and numerical solutions has attracted significant attention from researchers in multiple scientific domains. The inherent nonlinearity and singularity at $t = 0$ further complicate the analytical treatment of these problems, making the derivation of closed-form solutions exceedingly difficult. As a result, numerical approaches have emerged as essential tools, enabling the reliable approximation of solutions and providing deeper insight into the complex behaviors governed by the singular structure of LETEs.

Among the various analytical approaches developed for solving differential equations such as the LETE presented in (1), a homotopy perturbation method has proven to be particularly effective. In this technique, a homotopy is formulated by introducing an auxiliary parameter that continuously deforms a simple problem into the original nonlinear one. The solution is then represented as a power series expansion in terms of the homotopy parameter. Substituting this expansion into the governing equation yields a sequence of recursive relations for the series coefficients, which can be solved iteratively to obtain progressively accurate approximations. Several other semi-analytical methods have also been employed to tackle (1) and its variants, including the Adomian decomposition method and the variational iteration method; detailed discussions can be found in [14, 32, 11, 2, 1, 15, 6, 17, 5].

The spline-based technique represents another numerical strategy for approximating the solutions of differential equations, including the LETE defined in (1). In this approach, the problem domain is divided into a set of subintervals, and the unknown solution is approximated within each subinterval using piecewise polynomial functions. The resulting system of algebraic equations is then solved, followed by an analysis of the convergence and stability of the approximation. The spline method offers several benefits, such as high accuracy and the capability to effectively manage nonuniformly spaced data. Nevertheless, its performance deteriorates when applied to stiff problems, and it often becomes computationally demanding for SIVPs because of the complexity associated with constructing spline functions and solving the corresponding algebraic systems.

Collocation techniques constitute another important category of numerical approaches employed for solving differential equations, including the third-order LETE presented in (1). In this framework, the computational domain is partitioned into discrete nodes, and the original differential equation is approximated by a system of algebraic equations enforced at selected collocation points. The approximate solution is represented through suitable basis functions, whose unknown coefficients are determined by satisfying the governing equation at these points. By solving the resulting algebraic system, an approximate numerical solution can be obtained. Collocation methods are capable of providing accurate results for a wide range of differential equations; however, their accuracy and stability are strongly dependent on the choice of collocation points and basis functions. Moreover, the convergence characteristics of these methods may differ depending on the nature of the problem and the particular collocation scheme adopted. Further details on spline-based and collocation techniques can be found in [10, 9, 13, 31, 3].

Several other numerical techniques have been developed to address LETEs and their related forms, including the finite difference method, Haar wavelet method, Chebyshev neural network approach, hybrid block algorithms, and various other computational schemes. Comprehensive discussions and comparative analyses of these approaches can be found in [27, 30, 12, 7, 18, 22, 16, 23, 4, 19, 26, 28]. However, most of these existing methods have been implemented using a constant step-size framework, which tends to be inefficient for problems characterized by rapid variations in the solution. Consequently, in order to maintain numerical stability and acceptable accuracy, many researchers have restricted their computations to small integration intervals, thereby limiting the overall efficiency of such methods.

In this study, a PVSHM is developed for the numerical solution of third-order LETEs. The proposed framework combines adaptive error control with a singularity treatment strategy at the origin, enabling accurate and efficient computations over wider integration intervals. The method is designed to improve computational efficiency while maintaining the desired level of accuracy for a broad class of LETE problems.

The main contributions of this work can be summarized as follows:

1. A new PVSHM is developed for the direct numerical solution of third-order LETEs without reducing the original problem to a system of lower-order equations.

2. Special starting formulas are constructed for the initial interval to accurately accommodate the singular behavior near the origin while avoiding the direct evaluation of the singular term.

3. An embedded lower-order technique (LOT) is incorporated for local error estimation, enabling adaptive step-size selection without requiring additional function evaluations.

4. A frozen Jacobian implementation is employed within the Newton iteration process, reducing the computational cost associated with repeated Jacobian evaluations and matrix factorizations.

5. Numerical experiments demonstrate that the proposed PVSHM achieves high accuracy with fewer integration steps and reduced computational effort compared with several existing methods reported in the literature.

The manuscript is organized as follows. Section 2 presents the proposed numerical method, while Sections 3 and 4 provide a comprehensive theoretical analysis along with a strategy for estimating the local truncation error. Section 5 addresses the implementation details of the method, and Section 6 illustrates its performance through numerical examples. Finally, Section 7 summarizes the main findings and conclusions of the study.

2 Development of the proposed PVSHM

The polynomial $Q(t)$, defined as

$$z(t) \approx Q(t) = \sum_{n=0}^{7} b_n t^n, \tag{2}$$

is employed to approximate the analytical solution $z(t)$ at the grid points t_n, $n = 0, 1, \dots, N$, such that $t_0 = 0$ and $t_N = T$ span the entire interval $[0, T]$. The selection of three internal interpolation points was motivated by the objective of constructing a high-order hybrid scheme while maintaining a manageable computational structure. Together with the interpolation and collocation conditions employed in the derivation, these points provide sufficient information to uniquely determine the coefficients of the seventh-degree polynomial approximation. This configuration leads to the eighth-order accuracy established later in the paper, while avoiding the substantial increase in algebraic complexity associated with additional internal points. Although higher-order approximations may be obtained by introducing more interpolation points, the resulting coefficient expressions and nonlinear systems become considerably more complicated, often with limited practical gains in efficiency. Therefore, the adopted configuration represents a balanced compromise between accuracy, stability, and computational cost.

The coefficients b_n in the polynomial can be determined by imposing collocation conditions at suitable points. To compute the unknown coefficients $b_0, b_1, \ldots, b_7$, three intermediate points $t_{n+p_1} = t_s + p_1 h$, $t_{n+p_2} = t_s + p_2 h$, and $t_{n+p_3} = t_s + p_3 h$ are considered within the interval $[t_n, t_{n+1}]$, where $h = t_{j+1} - t_j$ denotes the step size and $0 < p_1 < p_2 < p_3 < 1$. By evaluating the approximation in (2) and its derivatives at these specific points, a system of equations is established to determine the coefficients b_n:

$$\begin{array}{lll} Q(t_n) = z_n, & Q^{'}(t_n) = z_n^{'}, & Q^{''}(t_n) = z_n^{''}, \\ Q^{'''}(t_n) = f_n, & Q^{'''}(t_{n+p_1}) = f_{n+p_1}, & Q^{'''}(t_{n+p_2}) = f_{n+p_2}, \\ Q^{'''}(t_{n+p_3}) = f_{n+p_3}, & Q^{'''}(t_{n+1}) = f_{n+1}, & \end{array}$$

where z_{n+j}, z'_{n+j}, z''_{n+j}, and f_{n+j} with $j = 0,\ p_1, p_2, p_3,\ 1$ denote approximate values of $z\left(t_{n+j}\right)$, $z'\left(t_{n+j}\right)$, $z''\left(t_{n+j}\right)$ and $z'''\left(t_{n+j}\right)$, respectively.

To derive the polynomial approximation $Q(t)$, the coefficients b_n $(n = 0, \ldots, 7)$ in (2) are expressed in terms of a local variable substitution $t = t_n + xh$. This transformation yields the following polynomial representation:

$$\begin{aligned} Q(t_n + xh) &= a_0(x) z_n + h a_1(x) z_n' + h^2 a_2(x) z_n'' \\ &\quad + h^3 \big[\beta_0(x) f_n + \beta_{p_1}(x) f_{n+p_1} + \beta_{p_2}(x) f_{n+p_2} \\ &\quad + \beta_{p_3}(x) f_{n+p_3} + \beta_1(x) f_{n+1}\big]. \end{aligned} \tag{3}$$

The coefficients $a_0,\ a_1,\ a_2,\ \beta_0,\ \beta_{p_1},\ \beta_{p_2},\ \beta_{p_3}$ and β_1, which depend on p_1, p_2, and p_3, are continuous functions of x. These coefficients are determined by the values of b_n and the intermediate collocation points employed in the approximation. Once these coefficients are obtained, the next step is to substitute them into (3) and evaluate $Q(t)$, $Q^{'}(t)$, and $Q^{''}(t)$ at $t_{n+1} = t_n + h$. This procedure yields the approximations for $z(t_{n+1})$, $z^{'}(t_{n+1})$ and $z^{''}(t_{n+1})$. For brevity, and without loss of generality, assuming $n = 0$, the resulting approximations are expressed as follows:

$$\begin{aligned} z_1 &= z_0 + h z_0^{'} + \frac{h^2}{2} z_0^{''} + \frac{h^3}{1680} \left[3\left(99 f_{p_1} - 64 f_{p_2} + 36 f_{p_3}\right) + 72 f_0 - 5 f_1\right], \\ z_1^{'} &= z_0^{'} + h z_0^{''} + \frac{h^2}{120} \left[54 f_{p_1} - 32 f_{p_2} + 27 f_{p_3} + 11 f_0\right], \\ z_1^{''} &= z_0^{''} + \frac{h}{120} \left(81 f_{p_1} - 64 f_{p_2} + 81 f_{p_3} + 11 f_0 + 11 f_1\right), \end{aligned} \tag{4}$$

where $p_1 = \frac{1}{3}$, $p_2 = \frac{1}{2}$, and $p_3 = \frac{3}{4}$. For the proposed PVSHM to be implemented in block mode, the evaluation of $Q(t)$, $Q'(t)$, and $Q''(t)$ at the intermediate points t_{n+p_1}, t_{n+p_2}, and t_{n+p_3} is carried out. This evaluation yields nine additional formulas, which are then incorporated with the formulas provided in (4) to construct the proposed method.

It is important to note that the formulas presented above, as well as the additional derived relations, cannot be directly applied to solve the LETE in (1) due to the presence of a singularity at $t_0 = 0$. This singularity prevents the evaluation of $f_0 = f(t_0,\ z_0,\ z_0^{'}, z_0^{''})$, which is essential for the numerical solution of the LETE defined in (1). To overcome this issue and enhance accuracy near the origin, alternative formulas must be employed for the subinterval $[t_0, t_1]$. The construction of these modified formulas follows the same procedure used to derive (4), with the exception that the evaluation of f_0 is omitted. These specially designed formulas effectively eliminate the singularity at the origin and are expressed as follows:

$$\begin{aligned} z_1 &= z_0 + hz_0^{'} + \frac{h^2}{2} z_0^{''} + \frac{h^3}{240}\left(3\left(45f_{p_1} - 64f_{p_2} + 36f_{p_3}\right) - 11f_1\right), \\ z_1^{'} &= z_0^{'} + hz_0^{''} + \frac{h^2}{120}\left(153f_{p_1} - 208f_{p_2} + 126f_{p_3} - 11f_0\right), \\ z_1^{''} &= z_0^{''} + \frac{h}{2}\left(3f_{p_1} - 4f_{p_2} + 3f_{p_3}\right), \end{aligned} \tag{5}$$

where $p_1 = \frac{1}{3}$, $p_2 = \frac{1}{2}$, and $p_3 = \frac{2}{3}$. Additionally, the remaining formulas are obtained by evaluating $Q(t)$, $Q^{'}(t)$, and $Q^{''}(t)$ at the intermediate points t_{p_1}, t_{p_2}, and t_{p_3}. By combining the main formulas in (4) and (5) with these additional relations obtained from the evaluations of $Q(t)$, $Q^{'}(t)$, and $Q^{''}(t)$ at the intermediate points, a pair of hybrid methods is constructed.

3 Characteristics of the PVSHM

This section presents a detailed theoretical investigation of the proposed PVSHM method and examines its fundamental properties. The analysis focuses on determining the order of accuracy, assessing the stability characteristics, and deriving the local truncation error associated with the approximate solution.

3.1 Order of accuracy for the proposed PVSHM

To determine the order of accuracy of the proposed PVSHM, the set of equations presented in (4) is combined with nine additional relations. This combination yields the following expressions:

$$\overline{S}_1 z_n = h\overline{S}_2 z'_n + h^2\overline{S}_3 z''_n + h^3\overline{S}_4 F_n, \tag{6}$$

where $\overline{S}_1,\ \overline{S}_2,\ \overline{S}_3$, and $\overline{S}_4$ are coefficient matrices generated from (4) and additional formulas from the evaluation of $Q(t)$, $Q'(t)$, and $Q''(t)$ at the intermediate points t_{n+p_1}, t_{n+p_2}, t_{n+p_3} and

$$\begin{aligned}\mathbf{z}_n &= (z_n, z_{n+p_1}, z_{n+p_2}, z_{n+p_3}, z_{n+1})^T,\\ \mathbf{z}_n^{'} &= \left(z_n^{'}, z_{n+p_1}^{'}, z_{n+p_2}^{'}, z_{n+p_3}^{'}, z_{n+1}^{'}\right)^T,\\ \mathbf{z}_n^{''} &= \left(z_n^{''}, z_{n+p_1}^{''}, z_{n+p_2}^{''}, z_{n+p_3}^{''}, z_{n+1}^{''}\right)^T,\\ \mathbf{F}_n &= (f_n, f_{n+p_1}, f_{n+p_2}, f_{n+p_3}, f_{n+1})^T.\end{aligned}$$

Assuming $z(t)$ is sufficiently differentiable, the operator $\mathcal{L}$ associated with (4) can be represented as

$$\begin{aligned}&\mathcal{L}(z(t);\ h) \\ &= \sum_{j\in I}\left[\psi_j z(t+jh) - h\sigma_j z^{'}(t+jh) - h^2\gamma_j z^{''}(t+jh) - h^3 v_j z'''(t\ +\ jh)\right],\end{aligned} \tag{7}$$

where $\psi_j,\ \ \sigma_j,\ \gamma_j$, and v_j are vectors derived from the coefficient matrices $\bar{S}_1,\ \bar{S}_2,\ \bar{S}_3$ and $\bar{S}_4$, respectively. Assuming that $z(t)$ is sufficiently differentiable, the operator $\mathcal{L}$ can be expressed as a series expansion in powers of h using the following Taylor series:

$$\begin{aligned}\mathcal{L}\left(z(t);\ h\right) =& M_0 z(t) + M_1 h z^{'}(t) + M_2 h^2 z^{''}(t) + M_3 h^3 z^{'''(t)} + \cdots \\ &+ M_r h^r z^{r(t)} + \cdots,\end{aligned} \tag{8}$$

where M_r is given by

$$\begin{aligned}M_r =& \frac{1}{r!}\left[\sum_{j\in I} j^r\psi_j - r\sum_{j\in I} j^{r-1}\sigma_j\right.\\ &\left.-r(r-1)\sum_{j\in I} j^{r-2}\gamma_j - r(r-1)(t-2)\sum_{j\in I} j^{r-3}v_j\right],\end{aligned} \tag{9}$$

For $r = 0, 1, 2, \dots$ and $I = \{0,\ p_1,\ p_2,\ p_3, 1\}$, by applying the equations in (4) to (8) and (9), the order (p) of the main formulas and their corresponding local truncation errors $(\mathcal{L})$ can be expressed as follows:

$$P = 5, \qquad \mathcal{L}\left(z_{n+1}; h\right) = \frac{h^8}{362\ 880}\ z^{(8)}(t_n) + O(h^9),$$

$$P=5, \qquad \mathcal{L}\left(z^{'}_{n+1};h\right)=\frac{h^8}{181\ 440}\ z^{(7)}(t_n)+O(h^8),$$
$$P=6, \qquad \mathcal{L}\left(z^{''}_{n+1};h\right)=\frac{h^9}{1\ 088\ 640}\ z^{(7)}(t_n)+O(h^{10}). \tag{10}$$

Assessing the consistency of a numerical method requires a thorough examination of the order of its approximation formulas. Since the proposed method possesses an order higher than one, it is considered consistent and is capable of providing accurate approximations for the LETE in (1). It is important to note, however, that while consistency is a necessary condition for convergence, it does not by itself guarantee the convergence of a numerical method. Therefore, additional theoretical properties of the proposed PVSHM, such as zero-stability, must be carefully analyzed to ensure the method's convergence.

3.2 Zero-stability for the proposed PVSHM

As h tends to zero, the behavior of (6) is closely related to the zero-stability of the proposed method. This behavior can be represented more succinctly by the following equation:

$B_1^{(0)}\ \bar{\mathbf{Z}}_\mu - B_1^{(1)}\ \bar{\mathbf{Z}}_{\mu-1}=0$, where

$\bar{\mathbf{Z}}_\mu=\left(z_{n+1},z_{n+p_3},z_{n+p_2},z_{n+p_1}\right)^T$,

$\bar{\mathbf{Z}}_{\mu-1}=\left(z_n,z_{n+p_3-1},z_{n+p_2-1},z_{n+p_1-1}\right)^T$,

$$B_1^{(0)}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}, \qquad B_1^{(1)}=\begin{pmatrix}1&0&0&0\\1&0&0&0\\1&0&0&0\\1&0&0&0\end{pmatrix}.$$

It should be noted that the above simplified form is obtained by taking the limit as $h\to 0$, providing a reliable assessment of the proposed method's accuracy in approximating the true solution of the problem. For the PVSHM to be considered zero-stable, its primary characteristic polynomial $P(s)$ must satisfy specific root conditions. These conditions require that the roots s_j obey $|s_j|\le 1$, and any roots with $|s_j|=1$ must have multiplicities not exceeding two. For the proposed PVSHM, the characteristic polynomial is given by $P(s)=(s-1)s^3$, which satisfies all the criteria for zero-stability. Consequently, the PVSHM is both consistent and zero-stable, fulfilling the necessary conditions for convergence. Therefore, the proposed PVSHM is a convergent numerical method.

4 Strategy to estimate the local error

This section introduces a variable step-size formulation for the PVSHM, which offers several advantages. In particular, this approach allows the use of larger integration intervals during computation, thereby increasing computational efficiency. To ensure accurate and reliable solutions of the LETE in (1), the truncation error is maintained below a specified relative tolerance. By employing an embedding technique, the proposed method can be implemented in an adaptive mode, which requires the construction of an additional LOT. The LOT is essential for accurately estimating the local error of the PVSHM. Notably, the LOT is derived using the same function evaluations as the PVSHM, so no additional computational cost is incurred. For the accurate estimation of the local error of the proposed PVSHM, the following LOT is utilized:

$$z^*_{n+1} = 2z_n - 9z_{n+p_1} + 8z_{n+p_2} + h^3\left(\frac{f_n}{1728} + \frac{f_{n+p_1}}{32} + \frac{f_{n+p_2}}{216} + \frac{11f_{n+p_3}}{576}\right) \tag{11}$$

with $\mathcal{L}\left(z^*_{n+1}\right) = \frac{17h^7 z^{(7)}(t_n)}{11{,}197{,}440} + O(h^8)$.

This LOT involves the computation of z^*_{n+1} using a combination of $z_n,\ z_{n+p_1},\ z_{n+p_2}$ and the corresponding function evaluations $f_n,\ f_{n+p_1},\ f_{n+p_2}$, and f_{n+p_3}, providing an accurate estimate of the local error. Specifically, z^*_{n+1} is computed as

$$z^*_{n+1} = 2z_n - 9z_{n+p_1} + 8z_{n+p_2} + h^3(1728f_n + 32f_{n+p_1} + 216f_{n+p_2} + 576f_{n+p_3}).$$

The local error estimate, denoted by ERRES, is then defined as

$$\mathrm{ERRES} = \frac{\parallel z^*_{n+1} - z_{n+1} \parallel}{1+ \parallel z_{n+1} \parallel}.$$

This formulation allows for the adaptive selection of the step size in the proposed PVSHM, ensuring that the local truncation error remains within the desired tolerance.

The formula above measures the difference between the approximations z^*_{n+1} and z_{n+1}, which are obtained using the LOT in (11) and the PVSHM in (6), respectively. The computed approximation is considered acceptable if the absolute value of ERRES is less than or equal to the specified relative error tolerance (RET).

Conversely, if the absolute value of ERRES exceeds the RET, the computed result is rejected, and the step size must be adjusted to improve the accuracy of the approximation. This adjustment is performed using the following procedure:

The adaptive step size is updated according to the formula

$$h_{\text{var}} = \Upsilon \; h_{\text{old}}(\frac{\text{RET}}{\parallel \text{ERRES} \parallel})^{\frac{1}{p+3}},$$

where $\Upsilon = 0.85$ is a suitable adjustment factor, and p denotes the order of the LOT in (11). This adaptive strategy for modifying the step size is particularly important because different problems may require different levels of accuracy. By appropriately adjusting the step size, the LETE in (1) can be solved efficiently, achieving the desired accuracy while minimizing computational cost.

5 Implementation

To implement the PVSHM, the error estimation procedure presented in Section 4 is employed. This requires reformulating the formulas given in (4) and (5), along with the additional relations obtained by evaluating $Q(t)$, $Q^{'}(t)$, and $Q^{''}(t)$ at the intermediate points, into the form $F(\widetilde{\mathbf{Z}}) = 0$. Here, the vector $\widetilde{\mathbf{Z}}$ is used to represent the unknowns in this reformulation process,

$$\widetilde{\boldsymbol{Z}} = \; (z_{p_1}, \; z^{'}{}_{p_1}, z^{''}{}_{p_1}, \; z_{p_2}, \; z^{'}{}_{p_2}, z^{''}{}_{p_2}, \; z_{p_3}, \; z^{'}{}_{p_3}, z^{''}{}_{p_3}, \; z_1, \; z'{}_1, \; z''{}_1).$$

By representing the unknowns as described above, the computations for the PVSHM can be performed efficiently. The resulting nonlinear equations can be solved using Newton's method, which iteratively updates the approximation according to

$$\widetilde{\mathbf{Z}}^{(j+1)} = \widetilde{\mathbf{Z}}^{(j)} - (J_0)^{-1} F^{(j)},$$

where J_0 denotes the Jacobian matrix of $F(\widetilde{\mathbf{Z}})$ and the superscript (j) indicates the current iteration. Here, $\widetilde{\mathbf{Z}}^{(j)}$ represents the approximation at iteration j, and $F^{(j)}$ is a vector that depends on the current approximation. The frozen Jacobian matrix of F is denoted by J_0.

In the present implementation, a frozen Jacobian strategy is adopted, where the Jacobian matrix is evaluated once at the initial approximation and subsequently reused throughout the Newton iterations. This approach avoids the repeated computation and factorization of the Jacobian matrix at every iteration, thereby reducing the overall computational cost. Since the nonlinear systems generated by the PVSHM are solved using sufficiently accurate initial predictors, the Jacobian matrix typically varies only mildly between successive iterations. Consequently, the frozen Jacobian strategy provides an efficient compromise between computational efficiency and convergence performance.

To apply Newton's method for solving the nonlinear system, suitable initial values for the approximation must be provided. These initial values are obtained using the following Taylor series formulas:

$$z_{n+j} = z_n + (jh)z'_n + \frac{(jh)^2}{2} z''_n + \frac{(jh)^3}{6} f_n$$

$$z'_{n+j} = z'_n + (jh)z''_n + \frac{(jh)^2}{2} f_n$$

$$z''_{n+j} = z''_n + (jh)f_n,$$

for $n = 1, 2, \ldots, N-1$, and $j = p_1, p_2, p_3,\ 1$.

6 Numerical examples

This section presents numerical examples to validate the performance and demonstrate the efficacy of the proposed PVSHM in solving the LETE in (1). Additionally, the results obtained using PVSHM are compared with those from various numerical methods reported in the scientific literature. The maximum absolute error (Err) is used to assess the accuracy of the numerical solutions. This measure allows for direct comparison between the computed solution and both exact and existing reference solutions. The Err is defined as

$$\text{ERR} = \max_{j=0,1,\ldots,N} \parallel z(t_j) - z_j \parallel,$$

where $z(t_j)$ is the exact solution, while z_j represents a numerical approximation. Using this formula, one can quantitatively assess the accuracy of PVSHM and juxtapose its performance with that of other methods in the available literature.

To facilitate the presentation of results and enhance readability, several abbreviations are introduced. PVSHM denotes the newly proposed method. HBM refers to the hybrid block method. CBST stands for the cubic B-spline technique. KHST denotes the kernel Hilbert space technique. PBM represents the pair block method.

Several computational variables are also used throughout the numerical experiments. CT measures the computational time, in seconds, required to solve a given LETE problem. h_0 denotes the initial step size used in the numerical solution. NoS represents the total number of steps employed during computation, and RET specifies the relative error tolerance.

The benchmark results reported for CBST, KHST, HBM, and PBM were taken directly from the corresponding references cited in Tables 1–5. Consequently, the computational settings, implementation details, numerical precision, and hardware specifications associated with these methods are those reported in the original publications. The purpose of these comparisons is to provide a qualitative assessment of the accuracy and efficiency of the proposed PVSHM relative to existing approaches. Since implementation environments may differ among studies, the reported comparisons should be interpreted within this context.

Example 1. Consider the studied LETE, which is given by

$$z^{'''}(t) = -\frac{2}{t} + \frac{9(t^6+8)}{8z(t)^5}, \quad z(0)=1, \quad z^{'}(0)=0, \qquad z^{''}(0)=0, \quad t\in[0,t_N], \tag{12}$$

with the exact solution $z(t)=\sqrt{1+t^3}$. The results of applying different numerical methods to Numerical Example 1 are summarized in Table 1. These results highlight the effectiveness of PVSHM, CBST, and KHST in approximating the solution of Numerical Example 1. For the parameters RET $= 10^{-7}$ and $h_0 = 10^{-1}$, the proposed PVSHM achieves Err $= 8.9681\times 10^{-8}$ using only six steps, demonstrating its high efficiency. When the parameters are tightened to RET $= 10^{-11}$ and $h_0 = 10^{-3}$, PVSHM delivers an even more accurate result, with Err $= 5.5020\times 10^{-10}$ using 14 steps, emphasizing the method's superior convergence properties. In comparison, while the CBST and KHST methods also provide reasonable approximations, they exhibit larger Errs under both parameter sets. Specifically, the CBST method produces Errs of 1.0×10^{-7} and 5.1900×10^{-7} with 10 and 40 steps, respectively. Similarly, the KHST method yields Errs of 7.7839×10^{-6} and 4.3964×10^{-6} using 20 and 35 steps, respectively. These comparisons demonstrate that the PVSHM not only achieves higher accuracy but also requires fewer computational steps compared to other methods.

Table 1: Comparison of the results obtained for Numerical Example 1 over the interval $t\in[0,1]$.

Method	NoS	Err
$PVSHM$	6	8.9681×10^{-8}
$CBST$	10	5.2500×10^{-5}
$KHST$	20	7.7839×10^{-6}
$PVSHM$	14	5.5020×10^{-10}
$CBST$	40	5.1900×10^{-7}
$KHST$	35	4.3964×10^{-6}

The data presented in Table 1 clearly indicate that the PVSHM achieves the smallest Errs among the three compared methods for both sets of parameters. This demonstrates that the PVSHM consistently outperforms the CBST and KHST methods in terms of accuracy. The superior performance of PVSHM further highlights its robust convergence when applied to the LETE defined in (12). Additional evidence of this performance is provided in Figure 1, where the analytical and PVSHM solutions are depicted on the left, and the corresponding absolute errors are shown on the right. To generate these plots, the computations were performed using RET $= 10^{-12}$, an initial step size of $h_0 = 10^{-3}$, and the interval $t\in[0,50]$.

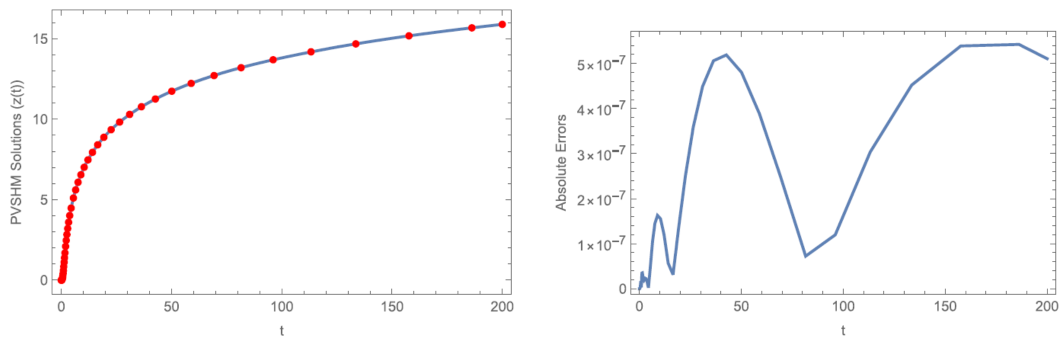

Figure 1: Absolute errors, analytical solution, and PVSHM approximation for Numerical Example 1 obtained with RET $= 10^{-12}$ and initial step size $h_0 = 10^{-3}$ over the interval $t \in [0, 50]$.

Example 2. Consider the LETE, which is given by

$$z'''(t) = 6(t^6 + 2t^3 + 10)e^{-3z(t)} + \frac{6}{t^2}z'(t) + \frac{6}{t}z''(t),$$
$$z(0) = 0, \quad z'(0) = 0, \quad z''(0) = 0, \quad t \in [0, t_N]. \tag{13}$$

The analytical solution to this LETE is

$$z(t) = \ln(1 + t^3).$$

Table 2 compares the Errs for Numerical Example 2 obtained using the PVSHM, CBST, and KHST methods. The results clearly indicate that the PVSHM consistently outperforms both the CBST and KHST methods in terms of accuracy. In the first set of parameters, with RET $= 10^{-7}$ and $h_0 = 10^{-2}$, the PVSHM requires only seven steps to achieve an error of 9.8681×10^{-8}. This error is significantly smaller than those obtained using the CBST and KHST methods, which yield errors of 5.1500×10^{-6} and 2.6839×10^{-6}, respectively, while requiring a larger NoS values (20 and 30). The smaller error achieved by the PVSHM with fewer steps demonstrates its superior efficiency and accuracy compared to the CBST and KHST methods.

In the subsequent set of parameters using RET $= 10^{-7}$ and $h_0 = 10^{-2}$ (as shown in Table 2), the PVSHM method further demonstrates its superior performance by achieving an error of 3.4020×10^{-9} with only 11 steps. In contrast, the CBST and KHST methods require 40 and 45 steps, respectively, and yield higher errors of 4.1800×10^{-7} and 1.2964×10^{-6}, indicating less accurate approximations compared to the PVSHM. Figure 2 provides a graphical comparison of these results: The absolute errors are shown on the right, while the analytical and PVSHM solutions are plotted on the left for Numerical Example 2. The computations for Figure 2 were performed over the interval $t \in [0, 200]$.

Table 2: Comparison of the results obtained for Numerical Example 2 over the interval $t \in [0, 1]$.

Method	NoS	Err
$PVSHM$	7	9.8681×10^{-8}
$CBST$	20	5.1500×10^{-6}
$KHST$	30	2.6839×10^{-6}
$PVSHM$	11	3.4020×10^{-9}
$CBST$	40	4.1800×10^{-7}
$KHST$	45	1.2964×10^{-6}

Example 3. Consider the LETE previously solved in [29], given by

$$\begin{aligned} &z'''(t) = -\frac{4}{t} z''(t) - z(t)^m, \\ &z(0) = 1, \quad z'(0) = 0, \quad z''(0) = 0, \quad t \in [0, t_N], \end{aligned} \tag{14}$$

where $m \geq 0$ is a constant. For $m = 0$, the exact solution of (14) is $z(t) = 1 - \frac{t^3}{30}$, and for $m \geq 1$, the exact solution is unknown.

For the computation of the error in Numerical Example 3 with $m = 5$, the NDSolve solution is employed as the reference solution. Numerical solutions are obtained using three different relative tolerances. Table 3 presents the results, clearly demonstrating that the PVSHM method outperforms the HBM in terms of accuracy. Furthermore, the effectiveness of the PVSHM method is illustrated in Figure 3, where the absolute error plots are displayed on the right, while the analytical solution (for $m = 0$) and the PVSHM solution are shown on the left for Numerical Example 3.

It is worth noting that the singular behavior of (14) is governed by the parameter μ, which directly controls the strength of the singular term $\left(\frac{\mu}{t} z''(t)\right)$. The proposed PVSHM employs specially designed starting formulas on the initial interval that avoid the direct evaluation of the singular term at the origin. Consequently, the effectiveness of the singularity treatment does not depend on a particular value of μ.

The numerical results obtained for Numerical Example 3 demonstrate that the proposed method remains stable and highly accurate in the presence of singular behavior. Moreover, since the starting formulas are derived independently of any specific value of the singularity parameter, the same treatment can be applied to a broader class of LETEs exhibiting different singularity strengths.

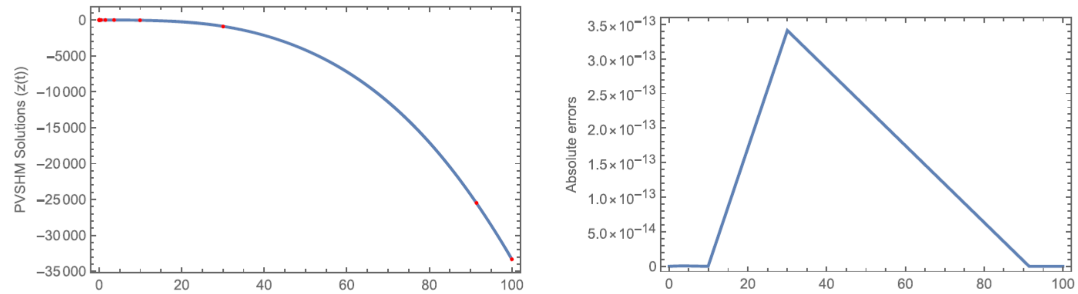

Figure 2: Comparison of the analytical solution and PVSHM approximation for Numerical Example 2, along with the corresponding absolute errors, computed using RET $= 10^{-8}$ and $h_0 = 10^{-3}$ over the interval $t \in [0, 200]$.

Table 3: Numerical comparison of the results for Numerical Example 3 over the interval $t \in [0, 10]$.

RET	Method	NoS	CT	Err
10^{-9}	PVSHM	74	0.0940	1.5269×10^{-6}
10^{-9}	HBM	111	0.1705	2.0191×10^{-6}
10^{-11}	PVSHM	143	0.1730	2.3768×10^{-8}
10^{-11}	HBM	201	0.2870	7.3995×10^{-8}
10^{-13}	PVSHM	275	0.3382	5.8712×10^{-10}
10^{-13}	HBM	375	0.4667	1.5499×10^{-9}

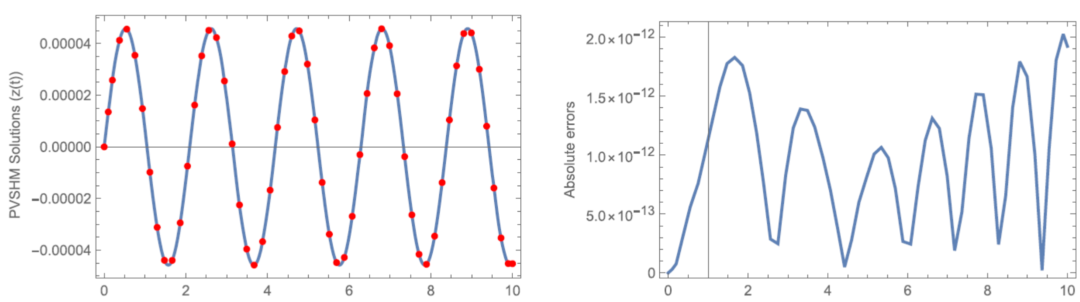

Figure 3: Comparison of the analytical solution and PVSHM approximation for Numerical Example 3, along with the corresponding absolute errors, computed for $m = 0$ using RET $= 10^{-10}$ and $h_0 = 10^{-2}$ over the interval $t \in [0, 100]$.

Example 4. Consider the following real-life problem in nonlinear science and engineering, specifically the self-adjoint LETE model, as discussed in [17]:

$$\varepsilon z'''(t) + \frac{1}{t} z''(t) + z(t) = 3\varepsilon \left[-27\varepsilon \cos(3t) - \frac{9\sin(3t)}{t} + \sin(3t) \right], \tag{15}$$

where the initial conditions for Numerical Example 4 are obtained from the exact solution $z(t) = 3\varepsilon \sin(3t)$.

The results presented in Table 4 clearly indicate that the PVSHM method outperforms the PBM method in terms of the NoS, computation time (CT), and Err for all tested tolerances ($10^{-8}, 10^{-10}$, and 10^{-12}). This superiority is consistently observed across all considered tolerances. For instance, at a tolerance of 10^{-8}, the PVSHM method required 16 steps with a computation time of 0.0170 s and achieved a maximum absolute error of 1.5268×10^{-9}, whereas the PBM method required 32 steps, a computation time of 0.0458 s, and yielded a maximum absolute error of 1.0190×10^{-9}.

Table 4: Numerical comparison of the results for Numerical Example 4 over the interval $t \in [0, 10]$.

RET	Method	NoS	CT	Err
10^{-8}	PVSHM	16	0.0170	1.5268×10^{-9}
10^{-8}	PBM	32	0.0458	1.0190×10^{-9}
10^{-10}	PVSHM	30	0.0440	1.3767×10^{-11}
10^{-10}	PBM	58	0.0974	5.3994×10^{-11}
10^{-12}	PVSHM	55	0.0678	2.8711×10^{-12}
10^{-12}	PBM	124	0.1298	3.5498×10^{-12}

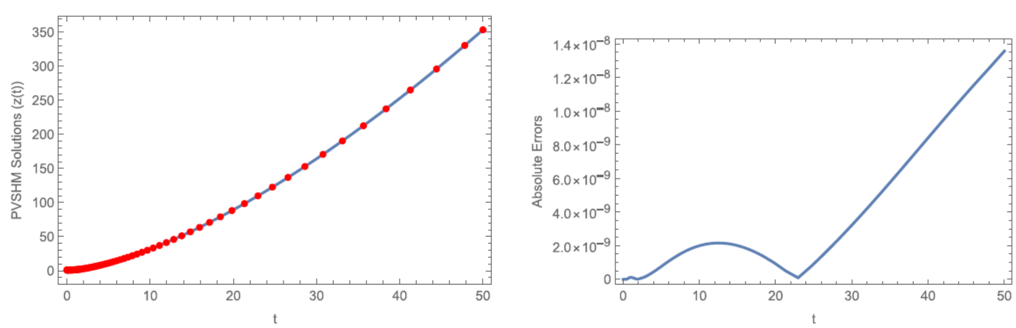

Figure 4: Comparison of the analytical solution and PVSHM approximation for (15), along with the corresponding absolute errors, computed using RET $= 10^{-12}$, $h_0 = 10^{-2}$, and $\varepsilon = 2^{16}$ over the interval $t \in [0, 10]$.

Furthermore, the superior performance of the PVSHM method is reinforced by the graphical representation shown in Figure 4. In this figure, the absolute errors are plotted on the right, while the analytical solution and the PVSHM approximation are displayed on the left for Numerical Example 4. Table 6 reports the efficiency-index comparison of the proposed PVSHM and the existing methods. For Numerical Examples 1 and 2, the efficiency index is computed using the

Table 5: Numerical comparison of the results for Numerical Example 5 over the interval $t \in [0, 10\pi]$.

RET	Method	NoS	CT	Err
10^{-9}	$PVSHM$	42	0.0941	2.5268×10^{-5}
10^{-9}	HBM	72	2.1704	1.0190×10^{-4}
10^{-10}	$PVSHM$	57	0.1720	6.3767×10^{-6}
10^{-10}	HBM	96	2.2860	1.3994×10^{-5}
10^{-11}	$PVSHM$	63	0.3372	1.8711×10^{-8}
10^{-11}	HBM	130	3.4657	5.5498×10^{-7}

number of integration steps, whereas for Numerical Examples 3–5 it is computed using the CT. Larger EI values indicate greater computational efficiency.

Table 6: Efficiency-index comparison of the proposed PVSHM and existing methods for the numerical examples considered in this study.

Example	Method	Error	NoS/CT	EI
Num. Ex. 1	PVSHM	8.9681×10^{-8}	NoS = 6	1.175
Num. Ex. 1	CBST	5.2500×10^{-5}	NoS = 10	0.428
Num. Ex. 1	KHST	7.7839×10^{-6}	NoS = 20	0.255
Num. Ex. 2	PVSHM	9.8681×10^{-8}	NoS = 7	1.001
Num. Ex. 2	CBST	5.1500×10^{-6}	NoS = 20	0.264
Num. Ex. 2	KHST	2.6839×10^{-6}	NoS = 30	0.186
Num. Ex. 3, 10^{-9}	PVSHM	1.5269×10^{-6}	CT = 0.0940	61.70
Num. Ex. 3, 10^{-9}	HBM	2.0191×10^{-6}	CT = 0.1705	33.55
Num. Ex. 4, 10^{-8}	PVSHM	1.5268×10^{-9}	CT = 0.0170	523.60
Num. Ex. 4, 10^{-8}	PBM	1.0190×10^{-9}	CT = 0.0458	196.10
Num. Ex. 5, 10^{-9}	PVSHM	2.5268×10^{-5}	CT = 0.0941	48.77
Num. Ex. 5, 10^{-9}	HBM	1.0190×10^{-4}	CT = 2.1704	18.40

Example 5. The final numerical example considers a system of LETEs from [21], given by

$$\begin{aligned}
&z_1''' + \frac{z_1''}{t} - \frac{z_1'}{t^2} - z_2^2\left(2z_1z_2z_1' + 3(z_1^2+1)z_2'\right) = 0,\\
&z_2''' + \frac{3z_2''}{t} - \frac{3z_2'}{t^2} - z_2^4\left(2z_1z_2z_1' + 5(z_1^2+3)z_2'\right) = 0,\\
&z_3''' - \frac{3(z_1' - tz_3'')}{t^2} - 4t^3z_2^7 - 7t^4z_2^6z_2' + 5z_2^4(z_3^2-6) = 0,\\
&z_2' + 2z_2^5(6z_2' + z_3z_3') = 0, \qquad t \in [0, t_N],
\end{aligned} \tag{16}$$

and the initial conditions are given by

$$z_1(0) = 1, \qquad z'_1(0) = 0, \qquad z''_1(0) = 1,$$

$$z_2(0) = 1, \qquad z'_2(0) = 0, \qquad z''_2(0) = -1,$$

$$z_3(0) = 1, \qquad z'_3(0) = 0, \qquad z''_3(0) = 1,$$

$$z'_n = (z'_n,\ z'_{n+p_1},\ z'_{n+p_2}, z'_{n+p_3},\ z'_{n+1})^T,$$

$$z''_n = (z''_n,\ z''_{n+p_1},\ z''_{n+p_2},\ z''_{n+p_3}, z''_{n+1}\ )^T,$$

$$F_n = (f_n,\ f_{n+p_1},\ f_{n+p_2},\ f_{n+p_3},\ f_{n+1})^T.$$

The analytical solution for this system is

$$z_1(t) = \sqrt{1+t^2}, \quad z_2(t) = \frac{1}{\sqrt{1+t^2}}, \quad z_3(t) = 1 - \frac{1}{\sqrt{1+t^2}}.$$

The results of Numerical Example 5 were compared using two numerical methods, PVSHM and HBM, over the time interval $t \in [0, 10\pi]$, as summarized in Table 5. The data clearly demonstrate that the PVSHM method consistently outperforms the HBM method across all tested RET levels of RETs. These results highlight the high accuracy of PVSHM, providing precise numerical solutions with minimal error. Combined with its efficiency in computational resources and execution time, the PVSHM method proves to be a reliable and effective approach for solving this system of LETEs.

6.1 Limitations and scope of applicability

Although the proposed PVSHM has demonstrated excellent accuracy and efficiency for the class of third-order LETEs considered in this study, several limitations should be noted. First, the method has been specifically developed for LETEs with singular behavior of the form considered in (1), and its performance for more general classes of singular differential equations has not been investigated. Second, the nonlinear systems arising from the discretization are solved using Newton iterations, and therefore the overall efficiency may depend on the quality of the initial approximation and the convergence behavior of the iterative solver. Third, while the proposed starting formulas effectively treat the singularity at the origin, additional modifications may be required for problems involving different singular structures or multiple singular points. Finally, the present work does not include a dedicated investigation of highly stiff problems, and therefore the performance of PVSHM for extremely stiff systems remains a topic for future research. These aspects provide promising directions for further development and extension of the proposed methodology. The present study focuses on the development, theoretical analysis, and numerical validation of a specific PVSHM configuration. Consequently, a systematic sensitivity analysis with respect to algorithmic parameters, such as the adaptive step-size control factor, the embedded LOT, and the number of internal interpolation points, has not been undertaken. Although the numerical results indicate stable and reliable performance for the parameter settings adopted in this work, a comprehensive investigation of parameter sensitivity may provide additional insight into the robustness and optimization of the method. Such an analysis constitutes an interesting direction for future research. The proposed PVSHM uses an adaptive step-size mechanism that automatically adjusts based on the local behavior of the solution. When the solution changes rapidly and the error increases, the step size is reduced to maintain accuracy. In smoother regions, larger steps are used to improve efficiency. This makes the method robust for problems with moderate gradients and varying scales.

However, the study does not specifically examine highly oscillatory or very stiff problems. In such cases, more advanced techniques such as stiffness-aware step-size control, implicit methods, or oscillation-preserving strategies may be needed. Therefore, the performance of PVSHM under extreme stiffness or strong oscillations remains an open topic for future research.

7 Conclusion

A PVSHM has been presented for solving third-order LETEs. The proposed formulation incorporates a singularity treatment near the origin and an adaptive error-control mechanism for step-size selection. Theoretical analysis confirms the consistency, zero-stability, and convergence of the method. Numerical experiments demonstrate that the proposed approach produces accurate solutions while requiring fewer computational steps than the methods considered for comparison. Although the present study focuses on third-order LETEs, the underlying ideas of the proposed PVSHM, including the adaptive step-size strategy, embedded error estimation mechanism, and specially designed treatment of singular behavior near the origin, are not restricted solely to this class of problems. The methodology has the potential to be extended to other singular ordinary differential equations arising in astrophysics, plasma physics, heat-transfer models in spherical geometries, nonlinear reaction–diffusion systems, and various engineering applications involving singular IVPs. Consequently, the proposed framework may serve as a useful basis for the development of efficient numerical solvers for a broader class of singular differential equations. These results indicate that PVSHM is a reliable numerical technique for a wide range of third-order LETE models.

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Conflicts of Interest

The author declares no conflicts of interest.

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