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Block Optimized Hybrid Methods for Integrating Singular Second Order Ordinary Differential Equations

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ABSTRACT

In this work, a block methods with characteristics of LMF are derived, analyzed and numerically applied to solve singular Initial/Boundary value problems. It was done by applying shift operator to two linear multi-step formula and combined with Optimize hybrid set of formula which are developed at the the first sub-interval to circumvent the singularity at the left end of the integration interval.The mathematical derivation of the proposed methods is based on method of undetermined coefficients where the coefficient in our Linear Multi-step Formulas (LMF) are determined. The fundamental properties of the proposed scheme are analyzed. Finally, the numerical implementation of the method are done on some singular I/B value problem which demonstrate the accuracy and validity of the suggested technique when compared to various strategies available in the current literature.

Keywords: One-block methods; shift operator, undetermined coefficients, Lane-Emden-type equation, singular Initial/Boundary value problems (SIBVP).

INTRODUCTION

The goal of this research paper was to find a reliable numerical approach for the solution of the singular Initial/Boundary value problem (SIBVP) of Lane–Emden equations of the form:

$$y''(t) + (d_1 + \frac{d_2}{t})y'(t) = G(t,y), 0 \le t \le 1 \quad (1)$$

subject to the boundary conditions

$$A_1 y(0) + K_1 y'(0) = S_1, A_2 y(1) + K_2 y'(1) = S_2 \quad (2)$$

where $d_1, d_2, A_1, A_2, k_1, k_2$are real constants, $G(t,y)$ is continuous real function. The Existence and uniqueness of the solution to the problem (1) subject to any boundary conditions have been rigorously determined by Zhang [24].

Second-order singular boundary value problems are commonly encountered in several areas of applied mathematics, physics and engineering, such as mathematical modeling, chemical kinetics, astrophysics, catalytic diffusion reactions [25] and among others. Researchers in various fields such as applied sciences and engineering have shown significant interest in solving equations (1) by trying to find better and efficient methods.The problem under consideration becomes one of the most complex problems to solved analytically, due to the nonlinear properties of (1) and the singularity arising at the point t = 0, called singular point.In order to overcome these challenges and obtain meaningful solutions, numerical methods have emerged as crucial tools, example of such methods include the finite difference methods proposed in Kumar [13] and Pandey [16], the spline methods discussed in Caglar et al.,[8], Kadalbajoo et al. [12], the approximation methods introduced in (Allouche et al. [5], and Aydinlik et al., [6], the high-order compact finite differences method in Malele et al.,[15] and among others.

In recent time, researchers has employ the use of the optimization technique by Ramos et al.,[17], Asifa et al., [1] and Rajat et al. [19] and non-optimization by Jator,[11] and Anake et al., [4] in solving general second order problem. .

The focus of this paper is block methods which posses good stability properties for solving differential equations. They are constructed using two different LMF with aid of shift operator, which are combined with optimized hybrid set of formula called ad-hoc method that is applied only to the first sub interval due to the singularity at t = 0. we aimed to obtain the optimization formulation ad-hoc developed in Utalor et al., [23] to further improve and check their performance. In this way, we obtain a scheme capable of solving the problem posed effectively.

The present work is outlined as follows. In Section 2, we present the KSPHT method for solving SBVPs. The characteristics of the developed formulas are analyzed in Section 3. In Section 4,shows the Implementation of the method.We present the numerical results of some Test problems to show the efficiency and reliability of the proposed technique in Section 5. Conclusions are outlined in Section 6.

CONSTRUCTION OF THE METHOD

We approximate the exact solution $y(t)$ of (1) in the partition $a = t_0 < t_1 < t_2 < ... < t_n = b$ of the integration interval $[a,b]$, with constant step size $h where h = t_{j+1} - t_j, j = 0,1,2,...,n-1$ by a self-starting block method. The continuous coefficients $(\{\alpha_j(t)\}_{j=0}^{k}, \{\beta_i(t)\}_{i=0}^{k} and \{\gamma_i(t)\}_{i=0}^{k})$ of the composing LMF are determined by imposing order condition on linear muti-step formula (L.M.F) and using the method of undetermined coefficients developed in Ajie et al.,[2, 3] and Brugnano et al., [7]. See [23] for how the the self-starting block methods (KSPHT) for the main method are obtained, and also the 2 off-steps of non- optimization formulas to circumvent the singularity.

First, reformulate the equation (1)

$$y''(t) = f(t,y(t),y'(t)) where f(t,y(t),y'(t)) = G(t,y) - (d_1 + \frac{d_2}{t})y'(t) \quad (3)$$

Thus, the singularity is transferred to the function f.This block method cannot be used directly for solving a BVP problem in (1) because it is not possible to evaluate $f_0 = f(t_0, y_0, y_o')$, since there is a singularity at $t_0 = 0$.To overcome this drawback, we develop a set of multi-step formulas to be applied at the first sub-interval

$$y_{n+j} = y_{n+j-1} + y'_{n+j-1} + h^2\left(\sum_{i=1} \beta_i(t) f_{n+i} + \beta_{v_i}(t) f_{n+v_i}\right) j = 1. \quad (4)$$

$[t_0, t_1]$ with the purpose of specifically avoiding the use of t_0. as a result of it, the method will have main formula and also the Formulas to Circumvent the Singularity.

MAIN FORMULAS ($k = 3$)

Let us consider the Linear Multi-step method(LMM) of the form

$$LMF_1: y_{n+j} = y_{n+j-1} + y'_{n+j-1} + h^2 \sum_{j=0}^{k} \beta_j^{(1)} f_{n+j} + h^3 \sum_{j=0}^{k} \gamma_j^{(1)} G_{n+j}, j = k and j - 1 = i$$

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$$LMF_2 : y_{n+j} = y_{n+j-2} + y'_{n+j-2} + h^2 \sum_{j=0}^{k} \beta_j^{(2)} f_{n+j} + h^3 \sum_{j=0}^{k} \gamma_j^{(2)} G_{n+j}, j = k and j - 2 = i \quad (5)$$

using definition of order, This leads to the following matrix equation:

$$\begin{pmatrix} 1 & 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ i & 1 & 0 & \dots & 0 & 0 & \dots & 0 \\ \frac{i^2}{2!} & i & 1 & \dots & 1 & 0 & \dots & 0 \\ \frac{i^3}{3!} & \frac{i^2}{2!} & 0 & \dots & k & 1 & \dots & 1 \\ . & . & . & \dots & . & . & \dots & . \\ . & . & . & \dots & . & . & \dots & . \\ . & . & . & \dots & . & . & \dots & . \\ \frac{i^q}{q!} & \frac{i^{q-1}}{q-1!} & 0 & \dots & \frac{k^{q-2}}{q-2!} & 0 & \dots & \frac{k^{q-3}}{q-3!} \end{pmatrix} \begin{pmatrix} \alpha_i \\ \alpha'_i \\ \beta_0 \\ . \\ . \\ . \\ \beta_k \\ \gamma_0 \\ . \\ . \\ . \\ \gamma_k \end{pmatrix} = \begin{pmatrix} 1 \\ j \\ \frac{j^2}{2!} \\ \frac{j^3}{3!} \\ . \\ . \\ . \\ \frac{j^q}{q!} \end{pmatrix} \quad (6)$$

For $\boldsymbol{k = 3}$

In equation (6) when $j = t$, is solved by Mathematica software package method to obtain the value of the continuous coefficient $\boldsymbol{\alpha_i(t), \beta_i(t)},$

$$y_{n+3} = \alpha_i y_{n+i} + \alpha'_i h y'_{n+i} + h^2(\beta_0 f_n + \beta_1 f_{n+1} + \beta_2 f_{n+2} + \beta_3 f_{n+3}) + h^3(\gamma_0 G_n + \gamma_1 G_{n+1} + \gamma_2 G_{n+2} + \gamma_3 G_{n+3})$$

and its derivative as

$$y'_{n+3} = \alpha_i y_{n+i} + \alpha'_i h y'_{n+i} + h(\beta_0 f_n + \beta_1 f_{n+1} + \beta_2 f_{n+2} + \beta_3 f_{n+3}) + h^2(\gamma_0 G_n + \gamma_1 G_{n+1} + \gamma_2 G_{n+2} + \gamma_3 G_{n+3})$$

(7) Evaluating (7) at the points *t=3* gives the method and its derivative.

Applying the theory in Utalor et al., [23] on the method and its derivative , the coefficients of the resultant block method after the shift operator application in vector form are below

$$A_1 = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}, B_0 = \begin{bmatrix} 0 & 0 & 0 & \frac{1313}{136080} & 0 & 0 & 0 & \frac{43}{18144} \\ 0 & 0 & 0 & \frac{397}{18144} & 0 & 0 & 0 & \frac{163}{30240} \\ 0 & 0 & 0 & \frac{256}{8505} & 0 & 0 & 0 & \frac{4}{567} \\ 0 & 0 & 0 & \frac{20}{567} & 0 & 0 & 0 & \frac{8}{945} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$B_1 = \begin{bmatrix} \frac{611}{10080} & \frac{1697}{5040} & \frac{3617}{38880} & 0 & \frac{181}{5040} & \frac{1301}{10080} & \frac{-313}{22680} & 0 \\ \frac{89}{672} & \frac{313}{672} & \frac{6893}{18144} & 0 & \frac{269}{3360} & \frac{851}{3360} & \frac{-1283}{30240} & 0 \\ \frac{281}{315} & \frac{304}{315} & \frac{137}{1215} & 0 & \frac{62}{315} & \frac{-4}{315} & \frac{-52}{2835} & 0 \\ \frac{13}{21} & \frac{20}{21} & \frac{223}{567} & 0 & \frac{19}{105} & \frac{16}{105} & \frac{-43}{945} & 0 \\ \frac{1313}{136080} & \frac{611}{10080} & \frac{1697}{5040} & \frac{3617}{38880} & \frac{43}{18144} & \frac{181}{5040} & \frac{1301}{10080} & \frac{-313}{22680} \\ \frac{397}{18144} & \frac{89}{672} & \frac{313}{672} & \frac{6893}{18144} & \frac{163}{30240} & \frac{269}{3360} & \frac{851}{3360} & \frac{-1283}{30240} \\ \frac{256}{8505} & \frac{281}{315} & \frac{304}{315} & \frac{137}{1215} & \frac{4}{567} & \frac{62}{315} & \frac{-4}{315} & \frac{-52}{2835} \\ \frac{20}{567} & \frac{13}{21} & \frac{20}{21} & \frac{223}{567} & \frac{8}{945} & \frac{19}{105} & \frac{16}{105} & \frac{-43}{945} \end{bmatrix}$$

(8)

OPTIMIZATION FORMULAS TO CIRCUMVENT THE SINGULARITY (ONE-STEP METHOD WITH TWO OPTIMIZE POINTS

Considering different intermediate points using undetermined coefficient .This off-step point are gotten by minimization of Local Truncation Error of the intermediate points of the main formula at the grid points, as to circumvent the singularity at the left end of the integration interval, as a result we will developed a set of multi-step formulas specially designed for the sub-interval $[t_0,t_1]$, where the value f_0 is absent,

Let us consider the Hybrid Linear Multi-step method(HLMM) of the form

$y_{n+j} = y_{n+j-1} + y'_{n+j-1} + h^2\left(\sum_{i=1} \beta_i(t) f_{n+i} + \beta_{v_i}(t) f_{n+v_i}\right) j = 1,$(9) This leads to the following matrix equation:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 1 & 1 & \cdots & 1 \\ 0 & 0 & r_1 & s_2 & w_3 & \cdots & 1 \\ 0 & 0 & r_1^2 & s_2^2 & w_3^2 & \cdots & 1 \\ 0 & 0 & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & r_1^q & s_2^q & w_3^q & \cdots & 1 \end{pmatrix} \begin{pmatrix} \alpha_0(t) \\ \alpha'_0(t) \\ \beta_{r_1}(t) \\ \beta_{s_2}(t) \\ \beta_{w_3}(t) \\ \vdots \\ \beta_1(t) \end{pmatrix} = \begin{pmatrix} 1 \\ j \\ \frac{j^2}{2!} \\ \vdots \\ \frac{j^q}{q!} \end{pmatrix} \quad (10)$$

Applying equation (9), two two different intermediate points are introduced,

$i = 2 so that v_1 = r, v_2 = s$, Where $j = t for t = 1, and v_i = r,s$. Equation (10) is solved by Mathematica software package method to obtain the value of the unknown parameters $\alpha_j, j = 0 and \beta_i(t), i = r,s,1$, expressed as functions of *t* (whose expressions are not included), and can be written as

$$L(t_n + zh) = \alpha_0 y_n + \alpha'_0 h y'_n + h^2(\beta_r f_{n+r} + \beta_s f_{n+s} + \beta_1 f_{n+1}) (11)$$

Evaluating (11) at the points $t = 1, t = r and t = s$ *gives the continuous form of the method,* which implied that

$$y_{n+1} = y_n + hy'_n + h^2\left(-\frac{1-4s}{12(-1+r)(r-s)} f_{n+r} + \frac{1-4r}{12(r-s)(-1+s)} f_{n+s} + \frac{1-2r-2s+6rs}{12(-1+r)(-1+s)} f_{n+1}\right)$$

$$y_{n+r} = y_n + rhy_n' + h^2\left(-\frac{r^2(2r-r^2-6s+2rs)}{12(-1+r)(r-s)}f_{n+r} + \frac{r^2(-4r+r^2)}{12(r-s)(-1+s)}f_{n+s} + \frac{r^2(-r^2+4rs)}{12(-1+r)(-1+s)}f_{n+1}\right)$$

$$y_{n+s} = y_n + shy_n' + h^2\left(-\frac{s^2(-4s+s^2)}{12(-1+r)(r-s)}f_{n+r} + \frac{s^2(-6r+2s+2rs-s^2)}{12(r-s)(-1+s)}f_{n+s} + \frac{s^2(4rs-s^2)}{12(-1+r)(-1+s)}f_{n+1}\right)(12)$$

The first derivative of equation (9) with respect to t gives

$$L(t_n + zh) = \alpha_0 y_n + \alpha_0' y_n' + h(\beta_r f_{n+r} + \beta_s f_{n+s} + \beta_1 f_{n+1})(13)$$

Evaluating (13) at the points $t = 1, t = r and t = s$ *gives the addition method,* which implied that

$$y_{n+1}' = y_n' + h\left(-\frac{1-3s}{6(-1+r)(r-s)}f_{n+r} + \frac{1-3r}{6(r-s)(-1+s)}f_{n+s} + \frac{2-3r-3s+6rs}{6(-1+r)(-1+s)}f_{n+1}\right)$$

$$y_{n+r}' = y_n' + h\left(-\frac{r(3r-2r^2-6s+3rs)}{6(-1+r)(r-s)}f_{n+r} + \frac{r(-3r+r^2)}{6(r-s)(-1+s)}f_{n+s} + \frac{r(-r^2+3rs)}{6(-1+r)(-1+s)}f_{n+1}\right)$$

$$y_{n+s}' = y_n' + h\left(-\frac{s(-3s+s^2)}{6(-1+r)(r-s)}f_{n+r} + \frac{s(-6r+3s+3rs-2s^2)}{6(r-s)(-1+s)}f_{n+s} + \frac{s(3rs-s^2)}{6(-1+r)(-1+s)}f_{n+1}\right)(14)$$

In order to determine appropriate values for r,s, we choose to optimize the local truncation errors in the main formulae (13 and 14) respectively. which is obtained after expanding in Taylor series around t_n, which results in

$$L(y(t_{n+1});h) = -\frac{(2-5s+5r(-1+4s))y^{(5)}(t_n))h^5}{360} + 0(h^6)$$

$$L(hy'(t_{n+1});h) = -\frac{(1-2s+r(-2+6s))y^{(5)}(t_n))h^5}{72} + 0(h^6) \quad (15)$$

Equating the principal term of this error to zero in each term in (15) , that is the coefficients of h^5 in the above formulae, we obtain the system

$$\begin{cases}(2-5s+5r(-1+4s)) = 0 \\ (1-2s+r(-2+6s)) = 0(16)\end{cases}$$

and solving (16) for *r and s* ,we get the value as

$$\mathrm{r} = 0.644949, and s = 0.155051 \quad (17)$$

and thus, there is a unique solution with the constraints $0 < r < s < 1$.

Note that we have six unknowns $(y_{n+j}, y_{n+j}', j = r,s,1)$, to get a one-step hybrid block method for solving the SBVP problem, we need to complete the above formulas. For that we consider the evaluation at y_r, y_s and its derivative. Considering the values in the block method results to be the following system of six equations

$$y_{n+r} = y_n + 0.155051hy_n' + h^2(0.0163763f_{n+r} - 0.00686652f_{n+s} + 0.00251066f_{n+1})$$

$$y_{n+s} = y_n + 0.644949hy_n' + h^2(0.1812f_{n+r} + 0.0286237f_{n+s} - 0.00184399f_{n+1})$$

$$y_{n+1} = y_n + hy_n' + h^2(0.318041f_{n+r} + 0.181959f_{n+s})$$

$$y_{n+r}' = y_n' + h(0.196815f_{n+r} - 0.0655354f_{n+s} + 0.023771f_{n+1})$$

$$y'_{n+s} = y'_n + h\left(0.394424 f_{n+r} + 0.292073 f_{n+s} - 0.0415488 f_{n+1}\right)$$
$$y'_{n+1} = y'_n + h\left(0.376403 f_{n+r} + 0.512486 f_{n+s} + 0.111111 f_{n+1}\right)$$
(18)

ANALYSIS OF THE METHODS

Order and error Constants of the Methods [14]

The linear difference operator L associated with the block (8) is defined $L\left[y(t);h\right] = A_1 h^{\lambda} Y_m^{(n)} - h^{\lambda}\sum_{i=0}^{k} A_0 Y_{m-i} + h^{\mu}\left(\sum_{i=1}^{k} B_1 F_m + B_0 F_{m-i}\right)$(26)

Expanding (8) using Taylor series ,we obtained

$$L\left[y(t);h\right] = C_0 y(t) + C_1 h y'(t) + C_2 h^2 y''(t) + \ldots + C_q h^q y^{(q)}(t) + \ldots (27)$$

$$where C_q, q = 0,1,2,\ldots are cons\tan t s given in terms of \alpha_j, \beta_j and \lambda_j$$

So that

$$L\left[y(t);h\right] = C_{p+2} h^{p+2} y^{(p+2)}(t) + 0(h^{p+3}) with p = 8$$
$$where C_0 = C_1 = C_2 = \ldots = C_{P+1} = 0 and C_{10} \neq 0 = C_{p+2}.$$

Here p is the order and C_{p+2} is the error constant (Lambert, 1973). The following table shows the error constant

Table 1. Error constants of the composing LMFs

formulae	C_{p+2}	formulae	C_{p+2}
LMF_1	$\frac{89}{16934400}$	$DLMF_1$	$\frac{313}{25401600}$
LMF_2	$\frac{1}{88200}$	$DLMF_2$	$\frac{13}{793800}$

where the formulae LMF, represent $y^{(r)}{}_{n+j}, r = 0,1 and j = 3$, it follows that for all the formulae, the order $p = 8$

Since the order of the formulas is greater than one, they are consistent. For the ad- hoc formulas used for the first step, it is easy to see that they are also consistent

Zero Stability

Definition 1:The implicit block method (8) is said to be zero stable if the roots z_s, s = 1,…,n of the first characteristic polynomial $\bar{\rho}(z)$, defined by

$$\overline{\rho}(z) = det\left[z\overline{A_1} - A_0\right]$$

satisfies $/z_s/\leq 1$ and every root with $/z_s/= 1$ has multiplicity not exceeding two in the limit as $h \to 0$ [14, 25]. Using the definitions, the method in (8) may be rewritten in a more appropriate vector form to study zero-stability as

$$A_1 y_m^{(n)} - A_0 y_{m-1} = 0 where y_m^{(n)} = (y_{n+1}, y_{n+2}, \ldots, y_{n+k})^T, y_{m-i} = (y_{n-1}, y_{n-2}, \ldots, y_n)^T$$
$$and A_1, A_0 are cons\tan d matrrice given by$$

$$wehave\bar{\rho}(z) = det\left[z\begin{pmatrix}0&1&1&0\\1&0&1&0\\0&0&1&1\\0&1&0&1\end{pmatrix} - \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}\right]$$

$$= -2z^4 = 0$$
$$\therefore z = 0$$

The same procedure are done for the ad-hoc formulas used for the first step,(whose expressions are not included), its was proofed to be zero stable and have higher order more than the the non- optimization formula due to the optimize strategy done.

Convergence

Theorem (1): Consistency and zero stability are sufficient condition for linear multistep method to be convergent [14]. Since the method (8) is consistent and zero stable, it implies the method is convergent for all point .

Implementation

The derive KSPHT which include the ad-co formula are combined and applied as block form. The solutions are considered in the interval$[t_{n,} t_{n+k}], n = 0,1,2,\ldots,N-K$ where N is the number of blocks. The formulas are written as G(y) = 0 with the following unknown values to be obtained and the unknowns are expressed as

$$\bar{y} = \{y_{j+r}, y_{j+s,y}, \ldots, y'_{j+r}, y'_{j+s}, \ldots\}_{j=0,1,\ldots,N-1} \cup \{y_j\}_{j=1,\ldots,N-1} \cup \{y'_j\}_{j=0,\ldots,N}$$

The resulting system is solved using Newton-Raphson iteration given as

change_in_y = $J_G \backslash - G$;

y_new = change_in_y+(y_old);

y_old = y_new;

where **J** is the Jacobian matrix of G. The following Taylor's approximations are considered as starting values

$$y_{n+j} = y_n + jhy'_n + \frac{jh^2}{2} G_n$$
$$y'_{n+j} = y'_n + (jh)G_n j = r,s,\ldots,1$$

NUMERICAL ILLUSTRATIONS

Numerical examples are presented in this section to show the efficiency of the developed methods, K-step pair of hybrid techniques (KSPHT) which include 1S2OP(one step, Two optimized points). The accuracy is measured by using the following formulas: $Erc = \left\| y(t_j) - y_j \right\|$, where Erc denotes the absolute error at the considered node, $y(t_j)$ and $y_j$are exact and approximate solutions of the problems, respectively.

The following notations are used in the tables when presenting the results:

Block Hybrid Methods which include non-optimazition of (KSPHT) 1S2HP , [23]. TWS-Taylor wavelet solution [10], AADM - Advanced Adomian decomposition method, [22], MLMF - Modified Linear Multistep Formulas [18]. The computed results for the three problems using the methods proposed are presented in tables and graphically.

Problem 1.

Consider the following physical model SBVP problem of the isothermal gas sphere equilibrium, as described in Gumgum, and Umesh et al., [10, 22]:

$$q''(t) + \frac{2}{t}q'(t) + q(t)^m = 0q'(0) = 0, q(1) = \frac{\sqrt{3}}{2} \tag{4.1.2}$$

The equation arise in the study of stellar structure where m=5. It exact solution is $q(t) = \sqrt{3/(3+t^2)}$. The example is solved within the interval [0, 1] over ten (10) iterations and the results are compared both with the other numerical results and the exact solution to show the efficiency and validity of the method.

Table 2. Comparison of absolute errors of Problem 1 obtained using KSPHT (1S2OP)

x	Exact	1S2OP	1S2HP	AADM	TWS
0.1	0.998337488459583	2.3024615e-8	7.78932376e-7	1.65000e-6	6.46000 e- 6
0.2	0.993399267798783	2.2271241e-8	7.5386121e-7	6.63000e-6	6.30000e- 6
0.3	0.985329278164293	2.0803594e-8	7.07239719e-7	1.59000e-6	6.05000e- 6
0.4	0.974354703692446	1.8716236e-8	6.3830484e-7	1.53000e-6	5.70000 e- 6
0.5	0.960768922830523	1.6096693e-8	5.49157323e-7	1.44000-6	5.30000 e- 6
0.6	0.944911182523068	1.3074469e-8	4.44458267e-7	1.34000e-6	4.84000 e- 6
0.7	0.927145540823120	9.805192e-9	3.30551613e-7	1.10000e-6	4.33000 e- 6
0.8	0.907841299003204	6.44704e-9	2.14367027e-7	9.58000e-7	3.86000e- 6
0.9	0.887356509416114	3.141175e-9	1.02404574e-7	7.30000e-7	3.24000 e- 6
1	0.866025403784439	0	0	1.8900e-14	1.45000e- 13

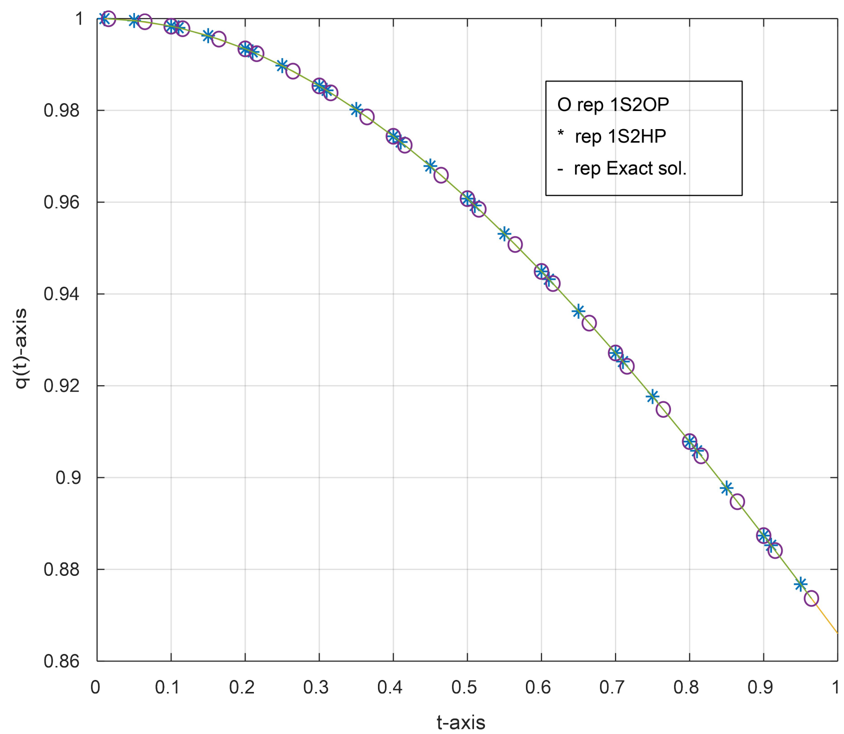

Figure 1. Plots of exact and KSPHT solution for Problem (1). It show good agreement between the numerical and exact solutions.

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PROBLEM 2

Consider the nonlinear heat conduction model of the human head, $q''(t) + \frac{2}{t}q'(t) + e^{-q(t)} = 0 q^{'}(0) = 0 \alpha q(1) + \beta q^{'} = 0$

Where $\alpha = 2 and \beta = 1$. The above nonlinear SBVP is discussed by Duggan R and Goodman A [19] as a heat conduction model in the human head. However, The general analytical solution of problem is unknown [22].

Table 3. Comparison of KSPHT and the exact solution on Problem 2

x	1S2OP	1S2HP	MLMF	AADM
0	0.270029664529952	0.270029706093745	0.2700296478967	0.2700296466
0.1	0.268756917547862	0.268756958875822	0.2687569006296	0.2687568993
0.2	0.264932833272991	0.264932875883028	0.2649328175383	0.2649328162
0.3	0.258539803870774	0.258539847740317	0.2585397893815	0.2585397881
0.4	0.249548193506706	0.249548238415984	-	0.2495481789
0.5	0.237915899626578	0.237915945201108	-	0.2379158863
0.6	0.223587718025932	0.223587763723984	-	0.2235877058
0.7	0.206494492698337	0.206494537783022	0.2064944830238	0.2064944817
0.8	0.186552022693196	0.186552066192176	0.1865520141667	0.1865520128
0.9	0.163659688980158	0.163659729631207	0.1636596815804	0.1636596802
1	0.137698752907342	0.137698789086042	0.1376987466136	0.1376987453

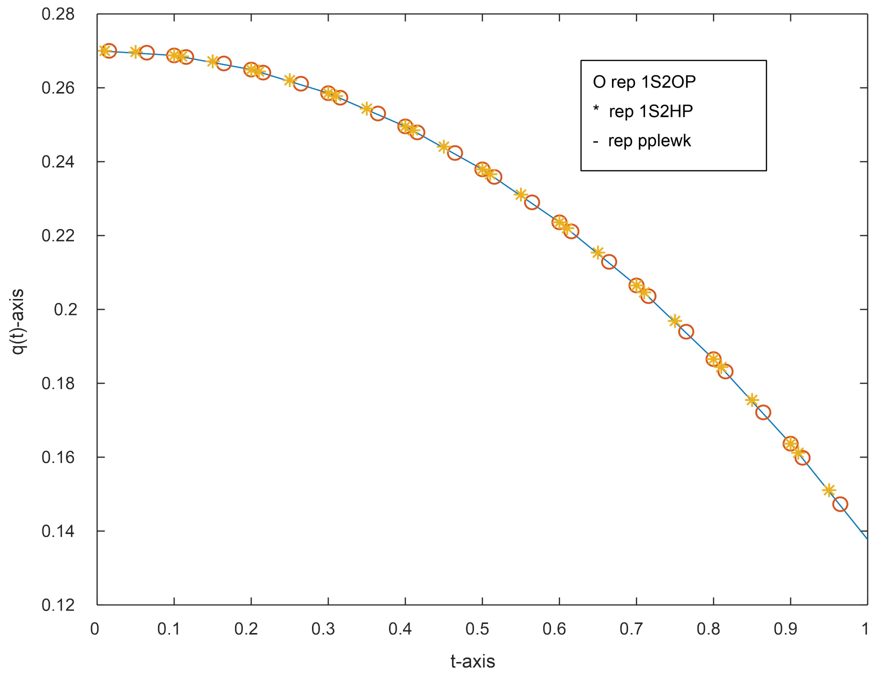

Figure 2. Plots of exact and KSPHT solution for Problem 2.

Problem 3.

The following model which corresponds to the reaction–diffusion process in a spherical permeable catalyst as reported in Allouche [5], Utalor et al. [23]

$$q''(t) + \frac{2}{t}q'(t) - \theta^2 q(t)^n = 0 q^{'}(0) = 0, q(1) = 1$$

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its analytical solution for $n = 1$, is given by

$$q(t) = \frac{sinh(t\theta)}{t\, sinh(\theta)} where n = 1 \theta = 5$$

whereθrepresents the Thiele modulus. The value of$\theta$is determined by

$$\varphi = \frac{\text{ratio of the reaction rate at the catalyst surface}}{\text{the diffusion rate through the catalyst pores.}}.$$

Table 4. Comparison of absolute errors of Problem 3 using KSPHT (1S2OP) within [0,1] over ten (10) iterations

x	Exact	1S2OP	1S2HP
0.1	0.070225439227791	1.16507398e-7	3.36833567e-7
0.2	0.079188028691280	1.02523148e-7	3.67734455e-7
0.3	0.095650823305130	9.3155702 e-8	4.19915345e-7
0.4	0.122193513582708	8.5924964 e-8	4.92803425e-7
0.5	0.163071231929978	7.8751406e-8	5.83054692e-7
0.6	0.225009916448920	6.9694737e-8	6.80232762e-7
0.7	0.318481161564393	5.7022468e-8	7.58832348e-7
0.8	0.459715910279232	3.9708057e-8	7.63576405e-7
0.9	0.673870380204315	1.8740297e-8	5.82698005e-7
1	1	0	0

To analyze the impact of the Thiele modulus (θ) on the concentration profile (y(x)),

we also considered other values of θ and n. Figure 3 displays the numerical outcomes for various values of θ and n. We observed that in Figure 3, the concentration profile increases when θ diminishes.

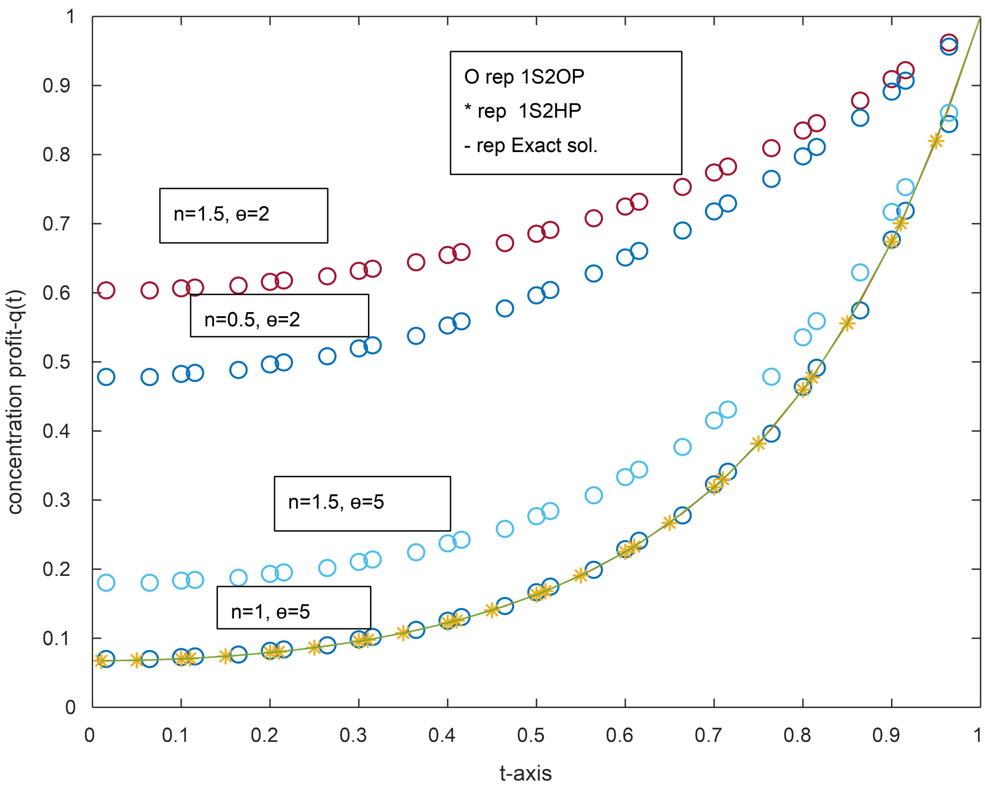

Figure 3. Plots of exact and KSPHT solution for Problem 3.

DISCUSSION OF RESULTS

The results obtained from the three test problems are summarized in Tables 2–4 and Figures 1–3. In **Table 2**, the solution of *Problem 1* obtained using the proposed methods (KSPHT), which include **1S2OP**, at the points x = 0(0.1)1.0, is compared with the results of **Utalor et al. (2025)**, **Umesh et al. (2021)**, and **Gumgum (2020)**. Overall, the KSPHT method based on the optimization technique demonstrates superior performance compared to other existing methods, as shown in column three of Table 2. **Table 3** and **Figure 2** present the comparison of approximate solutions for *Problem 2*. The proposed results show very good agreement—up to seven to eight decimal places—with those obtained using the Modified Linear Multistep Formulas (Olabode et al., 2024), the Advanced Adomian Decomposition Method (Umesh et al., 2021), and the Block Hybrid Methods (Utalor et al., 2025). For *Problem 3*, the results displayed in **Table 4** and **Figure 3** indicate that the proposed methods (KSPHT), particularly the **1S2OP** variant, outperform the Block Hybrid Methods of **Utalor et al. (2025)**. Figures 1 and 3 further show that the numerical solutions are in close agreement with the exact solutions. In general, the proposed methods compare favorably with existing approaches in the literature, demonstrating improved accuracy and efficiency despite differences in formulation.

CONCLUSION

A new approach for constructing self-starting block methods for solving second-order singular boundary value problems (SIBVPs) has been presented. The strategy involves applying a shift operator to two distinct linear multistep formulas and combined with an optimized hybrid set of formulas developed over the first sub-interval. The continuous coefficients of the linear multistep methods were obtained using the method of undetermined coefficients. To demonstrate the effectiveness of the proposed methods, three real-world model problems from the literature were solved. The numerical results show that the proposed methods produce highly accurate solutions with smaller errors when compared to existing techniques. Furthermore, the results indicate that the optimized selection of off-step points yields superior performance compared to non-optimized approaches, confirming the efficiency and robustness of the developed methods.

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