

An Optimized Three-Off-Step Block Hybrid Method For Solving Singular Second Order Ordinary Differential Equations

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Abstract

In this article, a novel framework for constructing self-starting block methods for the numerical solution of second-order singular boundary value problems (SIBVPs). The approach integrates the shift operator applied to two distinct linear multistep formulas with an three optimized hybrid formulation developed within the initial sub-interval. The continuous coefficients of the linear multistep methods were systematically derived using the method of undetermined coefficients. The fundamental properties of the scheme are analyzed. The applicability of the schemes is demonstrated herein for the solution some SIBVP. Numerical results obtained through the implementation of the scheme are very much close to the theoretical solution and found favourably compared with various existing methods in the literature.

Keywords: A K-step pair of hybrid techniques (KSPHT) which include one-step 3-optimized hybrid point (1S3OP); One-block methods; shift operator, undetermined coefficients, singular Initial/Boundary value problems (SIBVP),

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I. Introduction

In this research, we consider an approximate solution of singular Initial/Boundary value problem (SIBVP) of Lane–Emden equations of the form:

$$y''(t) + \frac{\lambda}{t} y'(t) = G(t, y), \quad 0 \leq t \leq 1 \quad (1)$$

subject to the boundary conditions

$$\begin{aligned} y(0) = y_a, \quad y(1) = y_b, \\ \text{or} \\ y(0) = y_a, \quad y'(1) = y'_b, \\ \text{or} \\ y'(0) = y'_a, \quad y(1) = y_b, \end{aligned} \quad (2)$$

where $\lambda, y_a, y_b, y'_a, y'_b$, are real value, $G(t, y)$ 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 Pandey [1], Zhang [2].

Second-order singular boundary value problems arise in numerous domains of applied mathematics, physics, and engineering, including mathematical modelling, chemical kinetics, astrophysics, and catalytic diffusion processes [3]. Owing to their broad applicability, researchers in applied sciences and engineering have shown growing interest in developing more accurate and efficient techniques for solving equations of type (1).

However, obtaining analytical solutions to these problems is often extremely challenging. This difficulty stems from both the nonlinear nature of equation (1) and the presence of a singularity at $t=0$, commonly referred to as the singular point. As a result, numerical approaches have become essential tools for producing reliable solutions.

Several numerical methods have been proposed in the literature, including finite difference schemes in [4] and [5], spline-based techniques in [6] and [7], various approximation methods in [8] and [9], and high-order compact finite difference methods [10], among others.

In recent years, optimization-based approaches have gained substantial attention for the numerical solution of general second-order differential equations [12 -13]. In this study, we develop block methods constructed through two linear multistep formulas (LMFs) and their derivatives, formulated using a shift

operator. These are combined with three optimized hybrid ad-hoc schemes, applied exclusively on the first subinterval to address the singularity at $t=0$.

The aim of this work is to enhance the optimized ad-hoc formulation and improve the order of accuracy previously reported in [14]. As a result, we develop a K-step pair of hybrid techniques (KSPHT) that incorporates a one-step three-optimized hybrid point method (1S3OP). The proposed approach exhibits improved efficiency and accuracy when compared with the non-optimized ad-hoc method of Utalor et al. [15] and other existing numerical schemes.

The structure of this paper is as follows. Section 2 introduces the KSPHT method for solving singular boundary value problems (SBVPs). Section 3 discusses the analytical properties of the developed formulas. The implementation procedure is detailed in Section 4. Numerical experiments for several test problems, demonstrating the efficiency and reliability of the proposed approach, are presented in Section 5. Finally, Section 6 provides concluding remarks.

II. Construction Of The Method

We approximate the exact solution $y(t)$ of equation (1) over a uniform partition of the integration interval $[a, b]$ using a self-starting block method. The continuous coefficients $(\{\alpha_j(t)\}_{j=0}^k, \{\beta_i(t)\}_{i=0}^k \text{ and } \{\gamma_i(t)\}_{i=0}^k)$ of the underlying linear multistep formulas (LMFs) are obtained by enforcing the standard order conditions and applying the method of undetermined coefficients, following the procedures in [16 -18]. Details on the construction of the self-starting KSPHT block methods, including the development of the 2, 3, and 4 off-step non-optimized formulas used to circumvent the singularity, can be found in [15].

As a preliminary step, equation (1) is reformulated by transferring the singular behaviour into the function $f(t)$.

$$y''(t) = f(t, y(t), y'(t)) \text{ where } f(t, y(t), y'(t)) = G(t, y) - \left(\frac{\lambda}{t}\right)y'(t) \tag{3}$$

Because of the singularity at $t=0$, this main block method cannot be applied directly to the boundary value problem, as $f(t)$ cannot be evaluated at the singular point. To address this limitation, we construct a set of auxiliary multistep formulas designed specifically for the first subinterval. Consequently, the overall scheme consists of a main block method together with supplementary formulas that effectively circumvent the singularity.

MAIN FORMULAS ($k = 3$)

Consider the Linear Multi-step method(LMM) of the form

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

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

using the method of undetermined coefficients, we have the matrix equation:

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

For $k = 3$

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

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

and its derivative as

$$y'_{n+3} = \alpha_i y_{n+i} + \alpha'_i h y'_{n+i} + h (\beta_0 f_n + \beta_1 f_{n+1} + \beta_2 f_{n+2} + \beta_3 f_{n+3}) + h^2 (\gamma_0 G_n + \gamma_1 G_{n+1} + \gamma_2 G_{n+2} + \gamma_3 G_{n+3}) \tag{7}$$

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

Applying the theory in [15] on the method and its derivative, the coefficients of the resultant block method after the shift operator application in vector form are below

$$A_1 = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}, B_0 = \begin{bmatrix} 0 & 0 & 0 & 0.0096487 & 0 & 0 & 0 & 0.0023699 \\ 0 & 0 & 0 & 0.0218805 & 0 & 0 & 0 & 0.0053902 \\ 0 & 0 & 0 & 0.0300999 & 0 & 0 & 0 & 0.00705467 \\ 0 & 0 & 0 & 0.0352734 & 0 & 0 & 0 & 0.0084656 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$B_1 = \begin{bmatrix} 0.060615 & 0.336706 & 0.0930298 & 0 & 0.0359127 & 0.1290675 & -0.0138007 & 0 \\ 0.1324405 & 0.4657738 & 0.3799052 & 0 & 0.0800595 & 0.2532738 & -0.0424272 & 0 \\ 0.892063 & 0.965079 & 0.112757 & 0 & 0.196825 & -0.012698 & -0.0183422 & 0 \\ 0.6190476 & 0.9523810 & 0.3932981 & 0 & 0.1809524 & 0.1523810 & -0.0455026 & 0 \\ 0.0096487 & 0.060615 & 0.336706 & 0.0930298 & 0.0023699 & 0.0359127 & 0.1290675 & -0.0138007 \\ 0.0218805 & 0.1324405 & 0.4657738 & 0.3799052 & 0.0053902 & 0.0800595 & 0.2532738 & -0.0424272 \\ 0.0300999 & 0.892063 & 0.965079 & 0.112757 & 0.0070547 & 0.196825 & -0.012698 & -0.0183422 \\ 0.0352734 & 0.6190476 & 0.9523810 & 0.393298 & 0.0084656 & 0.1809524 & 0.1523810 & -0.0455026 \end{bmatrix} \tag{8}$$

Circumvent The Singularity (One-Step Method With Three Optimize Points)

By selecting various intermediate points through the method of undetermined coefficients, these three off-step points are determined by minimizing the local truncation error of the intermediate points in the main formula at the grid points. This approach helps to circumvent the singularity at the left end of the integration interval. As a result, we develop a set of multi-step formulas specifically tailored for the sub-interval where the value f_0 is unavailable.

Consider the Hybrid Linear Multi-step method (HLMM) of the form

$$y_{n+j} = y_{n+j-1} + y'_{n+j-1} + h^2 \left(\sum_{i=1}^3 \beta_i(t) f_{n+i} + \beta_{v_i}(t) f_{n+v_i} \right) \quad j = 1, \tag{9} \text{ given}$$

the matrix equation form as:

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

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

$i = 3$ so that $v_1 = r, v_2 = s, v_3 = w$, Where $j = t$ for $t = 1$, and $v_i = r, s, w$. Equation (10) is also solved by Mathematica software package method to obtain the value of the unknown parameters $\alpha_j, j = 0$ and $\beta_i(t), i = r, s, w, 1$, expressed as functions of t (whose expressions are not included), and can be written

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

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

$$\begin{aligned}
 y_{n+1} &= y_n + h^2 y'_n + h^2 \left(\frac{2-5s-5w+20sw}{60(-1+r)(r-s)(r-w)} f_{n+r} + \frac{2-5s-5w+20sw}{60(-1+r)(r-s)(r-w)} f_{n+s} \right. \\
 &\quad \left. + \frac{-2+5r+5s-20rs}{60(r-w)(s-w)(-1+w)} f_{n+w} - \frac{3-5r-5s+10rs-5w+10rw+10sw-30rsw}{60(-1+r)(-1+s)(-1+w)} f_{n+1} \right) \\
 y_{n+r} &= y_n + rhy'_n + h^2 \left(\frac{r^2(5r^2-3r^3-10rs+5r^2s-10rw+5r^2w+30sw-10rsw)}{60(-1+r)(r-s)(r-w)} f_{n+r} + \frac{r^2(-5r^2+2r^3+20rw-5r^2w)}{60(r-s)(-1+s)(s-w)} f_{n+s} \right. \\
 &\quad \left. + \frac{r^2(5r^2-2r^3-20rs+5r^2s)}{60(r-w)(s-w)(-1+w)} f_{n+w} - \frac{r^2(-2r^3+5r^2s+5r^2w-20rsw)}{60(-1+r)(-1+s)(-1+w)} f_{n+1} \right) \\
 y_{n+s} &= y_n + shy'_n + h^2 \left(\frac{s^2(-5s^2+2s^3+20sw+5s^2w)}{60(-1+r)(r-s)(r-w)} f_{n+r} + \frac{s^2(-10rs+5s^2+5rs^2-3s^3+30rw-10sw-10rsw+5s^2w)}{60(r-s)(-1+s)(s-w)} f_{n+s} \right. \\
 &\quad \left. + \frac{s(s^2(-20rs+5s^2+5rs^2-2s^3))}{60(r-w)(s-w)(-1+w)} f_{n+w} - \frac{s^2(5rs^2-2s^3-20rsw+5s^2w)}{60(-1+r)(-1+s)(-1+w)} f_{n+1} \right) \\
 y_{n+w} &= y_n + why'_n + h^2 \left(\frac{-w^2(20sw-5w^2-5sw^2+2w^3)}{60(-1+r)(r-s)(r-w)} f_{n+r} + \frac{w^2(20rw-5w^2-5ws^2+2w^3)}{60(r-s)(-1+s)(s-w)} f_{n+s} \right. \\
 &\quad \left. + \frac{w^2(-30rs+10rw+10sw+10rsw-5w^2-5rw^2+5sw^2+3w^3)}{60(r-w)(s-w)(-1+w)} f_{n+w} - \frac{w^2(-20rsw+5rw^2+5sw^2-2w^3)}{60(-1+r)(-1+s)(-1+w)} f_{n+1} \right) \tag{12}
 \end{aligned}$$

The first derivative of equation (11) with respect to t gives

$$L(t_n + zh) = \alpha_0 y_n + \alpha'_0 y'_n + h(\beta_r f_{n+r} + \beta_s f_{n+s} + \beta_w f_{n+w} + \beta_1 f_{n+1}) \tag{13}$$

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

$$\begin{aligned}
 y'_{n+1} &= y'_n + h \left(\frac{1-2s-2w+6sw}{12(-1+r)(r-s)(r-w)} f_{n+r} + \frac{1-2r-2w+6rw}{6(r-s)(12(r-s)(-1+s)(s-w))} f_{n+s} \right. \\
 &\quad \left. + \frac{-1-2r-2s+6rs}{12(r-w)(s-w)(-1+w)} f_{n+w} - \frac{3-4r-4s+6rs-4w+6rw+6sw-12rsw}{12(-1+r)(-1+s)(-1+w)} f_{n+1} \right) \\
 y'_{n+r} &= y'_n + h \left(\frac{r(4r^2-3r^3-6rs+4r^2s-6rw+4r^2w+12sw-6rsw)}{12(-1+r)(r-s)(r-w)} f_{n+r} + \frac{r(-2r^2+r^3+6rw-2r^2w)}{12(r-s)(-1+s)(s-w)} f_{n+s} \right. \\
 &\quad \left. + \frac{r(2r^2-r^3-6rs+2r^2s)}{12(r-w)(-1+w)(s-w)} f_{n+w} - \frac{r(-r^3+2r^2s+2r^2w-6rsw)}{6(-1+r)(12(-1+r)(-1+s)(-1+w))} f_{n+1} \right) \\
 y'_{n+s} &= y'_n + h \left(\frac{s(-2s^2+s^3+6sw-2s^2w)}{12(-1+r)(r-s)(r-w)} f_{n+r} + \frac{s(-6rs+4s^2+4rs^2-3s^3+12rw-6sw-6rsw+4s^2w)}{12(r-s)(-1+s)(s-w)} f_{n+s} \right. \\
 &\quad \left. + \frac{s(-6rs+2s^2+2rs^2-s^3)}{12(r-w)(-1+w)(s-w)} f_{n+w} - \frac{s(2rs^2-s^3-6rsw+2s^2w)}{12(r-s)(-1+s)(s-w)} f_{n+1} \right) \\
 y'_{n+w} &= y'_n + h \left(\frac{w(6sw-2w^2-2sw^2+w^3)}{12(-1+r)(r-s)(r-w)} f_{n+r} + \frac{w(6rw-2w^2-2rw^2+3w^3)}{12(r-s)(-1+s)(s-w)} f_{n+s} \right. \\
 &\quad \left. + \frac{s(w(-12rs+6rw+6sw+6rsw-4w^2-4rw^2-4sw^2+3w^3))}{12(r-w)(-1+w)(s-w)} f_{n+w} - \frac{w(-6rsw+2rw^2+2sw^2-w^3)}{12(-1+r)(-1+s)(-1+w)} f_{n+1} \right) \tag{14}
 \end{aligned}$$

In order to determine appropriate values for r, s, w , we choose to optimize the local truncation errors in the main formulae (12 and 14) respectively, which is obtained after expanding in Taylor series around t_n . Equating the principal term of this error to zero in each term, we obtain the system

$$\begin{cases}
 (-1 + s(2 - 5w) + 2w + r(2 - 5w + 5s(-1 + 4w))) = 0 \\
 -11 + 14w + 14w^2 - 7s^2(-2 + 5w) - 7s(-2 + 3w + 5w^2) + 7r^2(2 - 5w + 5s(-1 + 4w)) \\
 + 7r(2 - 3w - 5w^2 + 5s^2(-1 + 4w) + s(-3 + 10w + 20w^2)) = 0 \\
 -3 + s(5 - 10w) + 5w + 5r(1 - 2w + s(-2 + 6w)) = 0
 \end{cases} \tag{15}$$

and solving (15) for r, s and w , we get the value as

$$r = 0.0885880, s = 0.40946686 \text{ and } w = 0.7876595 \tag{16}$$

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

Considering the values in the block method results to be the following system of Eight equations

$$\begin{aligned}
 y_{n+r} &= y_n + 0.0885880 hy'_n + h^2 (0.00538268 f_{n+r} - 0.00242159 2 f_{n+s} + 0.00156464 56 f_{n+w} - 0.00060181 61 f_{n+1}) \\
 y_{n+s} &= y_n + 0.40946686 hy'_n + h^2 (0.06955830 f_{n+r} + 0.01612025 0 f_{n+s} - 0.00247876 66 f_{n+w} + 0.00063176 899 f_{n+1}) \\
 y_{n+w} &= y_n + 0.7876595 hy'_n + h^2 (0.15453781 f_{n+r} + 0.1448587 f_{n+s} + 0.01115013 56 f_{n+w} - 0.00034232 27 f_{n+1}) \\
 y_{n+1} &= y_n + hy'_n + h^2 (0.20093191 37 f_{n+r} + 0.22924110 64 f_{n+s} + 0.06982697 99 f_{n+w}) \\
 y'_{n+r} &= y'_n + h (0.1129995 f_{n+r} - 0.04030922 f_{n+s} + 0.02580237 7 f_{n+w} - 0.00990468 f_{n+1}) \\
 y'_{n+s} &= y'_n + h (0.23438399 6 f_{n+r} + 0.2068926 f_{n+s} - 0.04785712 8 f_{n+w} + 0.0160474 f_{n+1}) \\
 y'_{n+w} &= y'_n + h (0.21668178 f_{n+r} + 0.40612326 39 f_{n+s} + 0.18903651 8 f_{n+w} + 0.02418210 49 f_{n+1}) \\
 y'_{n+1} &= y'_n + h (0.2204622 f_{n+r} + 0.38819347 f_{n+s} + 0.32884432 f_{n+w} + 0.06250 f_{n+1})
 \end{aligned} \tag{17}$$

III. Analysis Of The Methods

Order and error Constants of the Methods

The linear difference operator L associated with the block (8) is defined

$$L[y(t); h] = A_1 h^\lambda Y_m^{(n)} - h^\lambda \sum_{i=0}^k A_0 Y_{m-i} + h^\mu \left(\sum_{i=1}^k B_1 F_m + B_0 F_{m-i} \right) \quad (26)$$

Expanding (8) using Taylor series, we obtained

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

where $C_q, q = 0, 1, 2, \dots$ are constants given in terms of α_j, β_j and λ_j

So that

$$L[y(t); h] = C_{p+2} h^{p+2} y^{(p+2)}(t) + O(h^{p+3}) \quad \text{with } p = 8$$

where $C_0 = C_1 = C_2 = \dots = C_{p+1} = 0$ and $C_{10} \neq 0 = C_{p+2}$.

In this case, p is the order and C_{p+2} is the error constant (Lambert [19]). The error constants $C_{p+2}^{T_j^{(\nu)}}$ for $j = 3$ and $\nu = 0, 1$ are given below

$$C_{p+2}^{T_j^{(\nu)}} = \left(\frac{89}{16934400}, \frac{1}{88200}, \frac{313}{25401600}, \frac{13}{793800} \right)^T$$

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 $z_s, s=1, \dots, n$ of the first characteristic polynomial $\bar{\rho}(z)$, defined by

$$\bar{\rho}(z) = \det[z \bar{A}_1 - A_0]$$

satisfies $|z_s| \leq 1$ and every root with $|z_s| = 1$ has multiplicity not exceeding two in the limit as $h \rightarrow 0$. 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 $y_m^{(n)} = (y_{n+1}, y_{n+2}, \dots, y_{n+k})^T$, $y_{m-i} = (y_{n-1}, y_{n-2}, \dots, y_n)^T$ and A_1, A_0 are constant matrices given by

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

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

$\therefore z = 0$

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

Definition -Let $y(t)$ be the theoretical of (1.1), and $\{y_j\}_{j=0, \dots, N}$ be the approximate solution at the grid points obtained by adopting proposed methods. The numerical method (KSPHT) is said to be a q^{th} -order convergence if for h sufficiently small, there exists a constant k independent of h , such that:

$$\max_{0 \leq j \leq N} \|y(t_j) - y_j\| \leq kh^q.$$

The following theorem is used to establish the convergence for the methods.

Theorem 3.3.2. According to Jator et al. [20] Let \bar{Y} be an approximation of the solution vector Y for the system obtained on a partition $\pi_N = \{a = t_0 < t_1 < t_2 < \dots < t_n = b\}$, and $E = Y - \bar{Y}$. Define

$$e_i = |y(t_i) - y_i|, h e_i^j = |h y^j(t_i) - h y_i^j|, \dots, h^\mu e_i^\mu = |h^\mu y^\mu(t_i) - h^\mu y_i^\mu| \text{ for } i=1, \dots, N$$

where the exact solution $y(t) \in C^n[a, b]$. Then the block method is a q -order convergent method. That is $\|E\|_\infty = O(h^q)$.

The convergence shall be proof by first expressing the main and additional formulas in matrix form adopting the following notations. Let A represent the $16N \times 16N$ matrix define by

$$A = \begin{pmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{2N,1} & A_{2N,2} & \cdots & A_{2N,2N} \end{pmatrix}$$

Where the elements $A_{i,j}$ are 8×8 submatrices ,except the $A_{1,N}$ $i=1, \dots, 2N$. The submatrices are given below;

$$A_{N,N} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}, \quad A_{i,i-1} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad i = 2, \dots, N$$

$$A_{2N-1,2N} = h \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad A_{i,i+1} = h \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad i = (N+1), \dots, N$$

$$A_{2N,2N} = h \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad A_{i,i} = h \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad i = (N+1), \dots, (2N-1)$$

$$A_{N,2N} = h \begin{pmatrix} -0.088588 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -0.409467 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -0.78766 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad A_{i,N+i} = h \begin{pmatrix} -0.088588 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -0.409467 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -0.78766 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad i = i, \dots, N-1$$

$A_{i,i} = I, i = 1, 2, \dots, N-1$, Where I is identity matrix ,for the rest of submatrices not included above it is $A_{i,j}$ are null matrices

On the other hand, let

$$U = \begin{pmatrix} U_{1,1} & U_{1,2} & \cdots & U_{1,2N} \\ \vdots & \vdots & \ddots & \vdots \\ U_{2N,1} & U_{2N,2} & \cdots & U_{2N,2N} \end{pmatrix}$$

Where the elements $U_{i,j}$, are 8×8 submatrices ,except the $U_{i,i}$, $U_{1,N+1}$ $i=1,\dots,2N$. The submatrices are given

$$U_{1,1} = \begin{pmatrix} 0 & 0.00538268 & -0.00242159 & 0.00156465 & -0.00060181 & 0 & 0 & 0 \\ 0 & 0.0695583 & 0.0161203 & -0.00247877 & 0.00063176 & 0 & 0 & 0 \\ 0 & 0.154538 & 0.144858 & 0.0111501 & -0.00034232 & 0 & 0 & 0 \\ 0 & 0.200932 & 0.229241 & 0.069827 & 0 & 0 & 0 & 0 \\ 0.0096487 & 0 & 0 & 0 & 0.060615 & 0.336706 & 0.0930298 & 0 \\ 0.0300999 & 0 & 0 & 0 & 0.892063 & 0.965079 & 0.112757 & 0 \\ 0 & 0 & 0 & 0 & 0.0096487 & 0.060615 & 0.336706 & 0.0930298 \\ 0 & 0 & 0 & 0 & 0.0300999 & 0.892063 & 0.965079 & 0.112757 \end{pmatrix}$$

$$U_{i,i} = \begin{pmatrix} 0.00538268 & -0.00242159 & 0.00156465 & -0.00060181 & 0 & 0 & 0 \\ 0.0695583 & 0.0161203 & -0.00247877 & 0.00063176 & 0 & 0 & 0 \\ 0.154538 & 0.144858 & 0.0111501 & -0.00034232 & 0 & 0 & 0 \\ 0.200932 & 0.229241 & 0.069827 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.060615 & 0.336706 & 0.0930298 & 0 \\ 0 & 0 & 0 & 0.892063 & 0.965079 & 0.112757 & 0 \\ 0 & 0 & 0 & 0.0096487 & 0.060615 & 0.336706 & 0.0930298 \\ 0 & 0 & 0 & 0.0300999 & 0.892063 & 0.965079 & 0.112757 \end{pmatrix} \quad i = 2, \dots, N$$

$$U_{N+1,1} = \begin{pmatrix} 0 & 0.112999 & -0.0403092 & 0.0258024 & -0.00990468 & 0 & 0 & 0 \\ 0 & 0.234384 & 0.206893 & -0.0478571 & 0.0160474 & 0 & 0 & 0 \\ 0 & 0.216682 & 0.406123 & 0.189037 & -0.0241821 & 0 & 0 & 0 \\ 0 & 0.220462 & 0.388193 & 0.328844 & 0.0625 & 0 & 0 & 0 \\ 0.0218805 & 0 & 0 & 0 & 0.1324405 & 0.4657738 & 0.3799052 & 0 \\ 0.0352734 & 0 & 0 & 0 & 0.6190476 & 0.9523810 & 0.393298 & 0 \\ 0 & 0 & 0 & 0 & 0.0218805 & 0.1324405 & 0.4657738 & 0.3799052 \\ 0 & 0 & 0 & 0 & 0.0352734 & 0.6190476 & 0.9523810 & 0.393298 \end{pmatrix}$$

$$U_{N+j,j} = \begin{pmatrix} 0 & 0.112999 & -0.0403092 & 0.0258024 & -0.00990468 & 0 & 0 & 0 \\ 0 & 0.234384 & 0.206893 & -0.0478571 & 0.0160474 & 0 & 0 & 0 \\ 0 & 0.216682 & 0.406123 & 0.189037 & -0.0241821 & 0 & 0 & 0 \\ 0 & 0.220462 & 0.388193 & 0.328844 & 0.0625 & 0 & 0 & 0 \\ 0.0218805 & 0 & 0 & 0 & 0.1324405 & 0.4657738 & 0.3799052 & 0 \\ 0.0352734 & 0 & 0 & 0 & 0.6190476 & 0.9523810 & 0.393298 & 0 \\ 0 & 0 & 0 & 0 & 0.0218805 & 0.1324405 & 0.4657738 & 0.3799052 \\ 0 & 0 & 0 & 0 & 0.0352734 & 0.6190476 & 0.9523810 & 0.393298 \end{pmatrix} \quad N = 2, \dots, N$$

$$U_{1,N+1} = \begin{pmatrix} 0_{4 \times 8} \\ 0.0023699 & 0 & 0 & 0 & 0.0359127 & -0.129067 & -0.0138007 \\ 0.00705467 & 0 & 0 & 0 & 0.196825 & -0.012698 & -0.018342 \end{pmatrix}$$

$$U_{i,N+i} = \begin{pmatrix} 0_{4 \times 8} \\ 0 & 0 & 0 & 0.0359127 & -0.129067 & -0.0138007 \\ 0 & 0 & 0 & 0.196825 & -0.012698 & -0.018342 \end{pmatrix} \quad i = 2, \dots, N$$

$$U_{2,N+1} = \begin{pmatrix} 0_{6 \times 8} \\ 0_{2 \times 7} & 0.0023699 \\ & 0.00705467 \end{pmatrix}, U_{i,N+i-1} = \begin{pmatrix} 0_{6 \times 8} \\ 0_{2 \times 7} & 0.0023699 \\ & 0.00705467 \end{pmatrix} \quad i = 3, \dots, N$$

$$U_{N+1,N+1} = \begin{pmatrix} 0_{4 \times 8} \\ 0.053902 & 0 & 0 & 0 & 0.0800595 & 0.2532738 & -0.424272 \\ 0.0084656 & 0 & 0 & 0 & 0.180952 & 0.1523810 & -0.045503 \end{pmatrix}$$

$$U_{N+i,N+i} = \begin{pmatrix} 0_{4 \times 8} \\ 0 & 0 & 0 & 0.0800595 & 0.2532738 & -0.424272 \\ 0 & 0 & 0 & 0.180952 & 0.1523810 & 0.045503 \end{pmatrix} \quad i = 2, \dots, N$$

$$U_{N+2,N+1} = \begin{pmatrix} 0_{6 \times 8} \\ 0_{2 \times 7} & 0.053902 \\ & 0.0084656 \end{pmatrix}, U_{N+i,N+i-1} = \begin{pmatrix} 0_{6 \times 8} \\ 0_{2 \times 7} & 0.053902 \\ & 0.0084656 \end{pmatrix} \quad i = 3, \dots, N$$

the rest of the submatrice, $U_{i,j}$ that are not included are all Null matrices, that is $U_{i,j} = 0$. All those submatrices $A_{i,j}$, and $U_{i,j}$, contain the coefficients of the formulars in KSPHT. We defined the following vectors corresponding to be exact and function values.

$$Y = (y(t_r), y(t_s), y(t_w), y(t_1), y(t_2), \dots, y(t_{N-1}), y'(t_0), y'(t_r), y'(t_s), \dots, y'(t_N))^T,$$

$$F = \left(f(t_0, y(t_0), y'(t_0)), f(t_r, y(t_s), y'(t_r)), \dots, f(t_N, y(t_N), y'(t_N)), \right. \\ \left. g(t_0, y(t_0), y'(t_0)), g(t_r, y(t_r), y'(t_r)), \dots, g(t_N, y(t_N), y'(t_N)) \right)^T$$

Where Y has $(8N-1)+(8N+1)=16N$ components and F has $(8N+1)+(8N+1)=16N+2$ components, because due to the boundary condition in problem, $y(t_0)$ and $y(t_N)$, are known value,

By using the above notations, the exact form of the system that provides the approximate values of the problem at hand is given by

$$A_{16N \times 16N} Y_{16N} + h^2 U_{16N \times (16N+2)} F_{(16N+2)} + C_{16N} = L(h)_{16N} \quad (28)$$

with

$$C_{16N} = (-y_a, -y_a, -y_a, -y_a, 0, \dots, y_b, 0, \dots, 0)^T$$

$$L(h)_{16N} = (a_1, a_2, a_3, a_4, \dots, a_{6N}, b_1, b_2, b_3, b_4, \dots, b_{6N})^T$$

Where is a vector containing the known values and represents the local truncation error of the proposed formulars. We also define E

$$E = Y - \bar{Y} = (e_1, e_2, \dots, e_N, he'_1, \dots, he'_N, h^2 e''_1, \dots, h^2 e''_N, \dots)^T \quad (29)\#$$

Where $\bar{Y} = (y_r, y_s, y_w, y_1, y_2, \dots, y_{N-1+r}, y'_0, y'_r, y'_s, \dots, y'_N)^T$

Which are the errors associated with the solution and the derivative.

Proof of Theorem 3.3.2

The proof follows from [20]. Let the exact form of the system of the problem be as given in (28), while the approximate form is defined as

$$A_{16N \times 16N} \bar{Y}_{16N} + h^2 U_{16N \times (16N+2)} \bar{F}_{(16N+2)} + C_{16N} = 0 \quad (30)** \quad \text{where}$$

\bar{Y}_{16N} approximates the vector Y_{16N} , that is,

$$\bar{Y}_{16N} = (y_r, y_s, y_s, y_1, y_2, \dots, y_{N-1}, y'_0, y'_r, y'_s, \dots, y'_N)^T,$$

$$\bar{F}_{12N+2} = (f_r, \dots, f_N, g_0, g_r, \dots, g_N)^T$$

Using (29), subtracting (30) from (28), gives

$$A_{16N \times 16N} E_{16N} + h^2 U_{16N \times (16N+2)} (F - \bar{F})_{(16N+2)} = L(h)_{16N} \quad (31)$$

where

$$E_{16N} = Y_{16N} - \bar{Y}_{16N} = (e_r, e_s, \dots, e_{N-1}, e'_0, e'_r, \dots, e'_N)^T \quad \text{By}$$

using the Mean- Value Theorem (Dym,(2007)), Since the problems is continuous in the close $[a,b]$ and differentiable we write for

$$f(t_i, y(t_i), y'(t_i)) - f(t_i, y_i, y'_i) = (y(t_i) - y_i) \frac{\partial f}{\partial y}(c_i) + (y'(t_i) - y'_i) \frac{\partial f}{\partial y'}(c_i),$$

$$g(t_i, y(t_i), y'(t_i)) - g(t_i, y_i, y'_i) = (y(t_i) - y_i) \frac{\partial g}{\partial y}(\bar{c}_i) + (y'(t_i) - y'_i) \frac{\partial g}{\partial y'}(\bar{c}_i)$$

where c_i and \bar{c}_i are intermediate points on the line segment joining $f(t_i, y(t_i), y'(t_i))$ to $f(t_i, y_i, y'_i)$

Thus,

$$\begin{aligned}
 F - \tilde{F} &= J_{16N \times (16N+2)} E_{16N} \\
 F - \tilde{F} &= \begin{pmatrix} \frac{\partial f}{\partial y}(c_0) & 0 & \dots & 0 & \frac{\partial f}{\partial y'}(c_1) & 0 & \dots & 0 \\ 0 & \frac{\partial f}{\partial y}(c_r) & \dots & 0 & 0 & \frac{\partial f}{\partial y'}(c_r) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{\partial f}{\partial y}(c_N) & 0 & 0 & \dots & \frac{\partial f'}{\partial y'}(c_N) \\ \frac{\partial g}{\partial y}(\bar{c}_0) & 0 & \dots & 0 & \frac{\partial g}{\partial y'}(\bar{c}_0) & 0 & \dots & 0 \\ 0 & \frac{\partial g}{\partial y}(\bar{c}_r) & \dots & 0 & 0 & \frac{\partial g}{\partial y'}(\bar{c}_r) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{\partial g}{\partial y}(\bar{c}_N) & 0 & 0 & \dots & \frac{\partial g}{\partial y'}(\bar{c}_N) \end{pmatrix} \begin{pmatrix} e_0 \\ e_{1/n} \\ \vdots \\ e_N \\ e'_0 \\ e'_{1/n} \\ \vdots \\ e'_N \end{pmatrix} \\
 &= \begin{pmatrix} 0 & \dots & 0 & \frac{\partial f}{\partial y'}(c_0) & 0 & \dots & 0 & 0 \\ \frac{\partial f}{\partial y}(c_0) & \dots & 0 & 0 & \frac{\partial f}{\partial y'}(c_r) & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \frac{\partial f}{\partial y}(c_{N-1+r}) & 0 & 0 & \dots & \frac{\partial f}{\partial y'}(c_{N-1+r}) & 0 \\ 0 & \dots & 0 & 0 & 0 & \dots & 0 & \frac{\partial f'}{\partial y'}(c_N) \\ 0 & \dots & 0 & \frac{\partial g}{\partial y'}(\bar{c}_0) & 0 & \dots & 0 & 0 \\ \frac{\partial g}{\partial y}(\bar{c}_0) & \dots & 0 & 0 & \frac{\partial g}{\partial y'}(\bar{c}_r) & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \frac{\partial g}{\partial y}(\bar{c}_{N-1+r}) & 0 & 0 & \dots & \frac{\partial g}{\partial y'}(\bar{c}_{N-1+r}) & 0 \\ 0 & \dots & 0 & 0 & 0 & \dots & 0 & \frac{\partial g}{\partial y'}(\bar{c}_N) \end{pmatrix} E_{16N}
 \end{aligned}$$

Where the second identity has been achieved through the fact that we know the exact problem conditions, that is Finally using the above result, the equation(31) may be written as

$$(A_{16N \times 16N} E_{16N} + h^2 U_{16N \times (16N+2)} J_{(16N+2) \times 16N}) E_{16N} = L(h)_{16N} \quad (32)$$

and dropping the dimension, let set

$$Z = A + h^2 UJ. \quad (33)$$

We get that

$$Z_{16N \times 16N} E_{16N} = L(h)_{16N}. \tag{34}$$

for some selected value of $h > 0$ matrix Z is invertible. Let $Z_N = Z_{12N \times 12N}$, for the matrix Z_N .

Where the submatrices have many zeros entries, it is confirmed that for $N=1$, the determinant is $|Z_N| = -h^{11}$, By mathematical induction, we know that $|Z_N| = -Nh^{N+6}$, thus $|Z_N|$ is invertible as long as $h > 0$.

Hence, equation(33) can be written as

$$|Z| = |A + h^2 UJ| = |A| |I - C|$$

where I is identity matrix of order $16N$, and $C = -h^2 UJZ^{-1}$.

As $|\lambda I - C| = \prod_{i=1}^{16} (\lambda - \lambda_i)$ is the characteristic polynomial of C , in order to have $|\lambda I - C| \neq 0$ for $\lambda = 1$

it is sufficient to choose h such that $h^2 \in \left\{ \frac{1}{\lambda_1} : \lambda_1 \text{ is an eigenvalue of } C \right\}$. For such value of h ,

Hence Z is invertible.

The equation (34) becomes

$$\begin{aligned} ZE &= L(h) \\ E &= (Z^{-1})L(h) \\ \|E\| &= \|(Z^{-1})L(h)\| \\ &\leq \|Z^{-1}\| \|L(h)\| \\ &\leq O(h^{-2}) O(h^{10}) \\ &\leq k(h^8) \end{aligned}$$

Therefore the method is 8-order convergent for KSPHT for 1S3HP.

IV. Implementation

The derived KSPHT, which incorporates the Add-co formula, is combined and implemented in block form. The solutions are computed over the interval divided into N blocks. The resulting formulas are expressed as $G(y) = 0$ with a set of unknown values to be determined, which are represented as

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

The nonlinear system is solved using the Newton iteration:

$$\text{change_in_y} = J_G \setminus -G;$$

$$y_new = \text{change_in_y} + (y_old);$$

$y_old = y_new;$

where J is the Jacobian matrix of G . Taylor series approximations are employed to generate the initial starting values for the iteration.

$$\begin{aligned} y_{n+j} &= y_n + jhy'_n + \frac{jh^2}{2} G_n \\ y'_{n+j} &= y'_n + (jh)G_n \end{aligned} \quad j = r, s, w, \dots, 1$$

V. Illustrations

In this section, numerical examples are presented to illustrate the efficiency of the proposed K -step pair of hybrid techniques (KSPHT), including the 1S3OP scheme (one step, three optimized points). The accuracy is measured by the absolute error $Erc = \|y(t_j) - y_j\|$

where $y(t_j)$ and y_j denote the exact and approximate solutions at the i -th node, respectively.

The following notations are used in the tables for clarity:

- 1S2OP – Block optimized Hybrid Methods [14]
- 1S3HP, 1S4HP – Construction of Block Hybrid Methods (non- optimization)[15]

- TWS – Taylor Wavelet Solution [22]
- AADM – Advanced Adomian Decomposition Method [25]
- MLMF – Modified Linear Multistep Formulas [26]

The results for the three test problems are presented both in tabular form and graphically, highlighting the performance and accuracy of the proposed methods.

Problem 1. Consider the following physical model SBVP problem of the isothermal gas sphere equilibrium, as described in [22] and [25]:

$$q''(t) + \frac{2}{t}q'(t) + q(t)^m = 0 \quad q'(0) = 0, \quad q(1) = \sqrt{\frac{3}{4}}$$

The equation arise in the study of stellar structure where $m=5$.

The exact solution is $q(t) = \sqrt{3/(3+t^2)}$.

Table 1. Comparison of absolute errors of Problem 1 obtained using KSPHT (1S3OP)

x	1S3OP	1S3HP[15]	1S4HP[15]	AADM[25]	TWS[22]	1S2OP[14]
0.1	3.02366e-10	5.294675e-9	3.62155e-10	1.65000e-6	6.46000 e- 6	2.3024615e-8
0.2	3.32341e-10	5.614592e-9	3.46792e-10	6.63000e-6	6.30000e- 6	2.2271241e-8
0.3	3.42722e-10	5.959704e-9	3.17325e-10	1.59000e-6	6.05000e- 6	2.0803594e-8
0.4	3.33343e-10	6.161494e-9	2.74391e-10	1.53000e-6	5.70000 e- 6	1.8716236e-8
0.5	3.05527e-10	6.062213e-9	2.21806e-10	1.44000e-6	5.30000 e- 6	1.6096693e-8
0.6	2.61814e-10	5.561083e-9	1.653e-10	1.34000e-6	4.84000 e- 6	1.3074469e-8
0.7	2.0559e-10	4.633646e-9	1.10888e-10	1.10000e-6	4.33000 e- 6	9.805192e-9
0.8	1.40673e-10	3.327415e-9	6.3487e-11	9.58000e-7	3.86000e- 6	6.44704e-9
0.9	7.0934e-11	1.741484e-9	2.616e-11	7.30000e-7	3.24000 e- 6	3.141175e-9
1	0	0	0	1.89000e-14	1.45000 e- 13	0

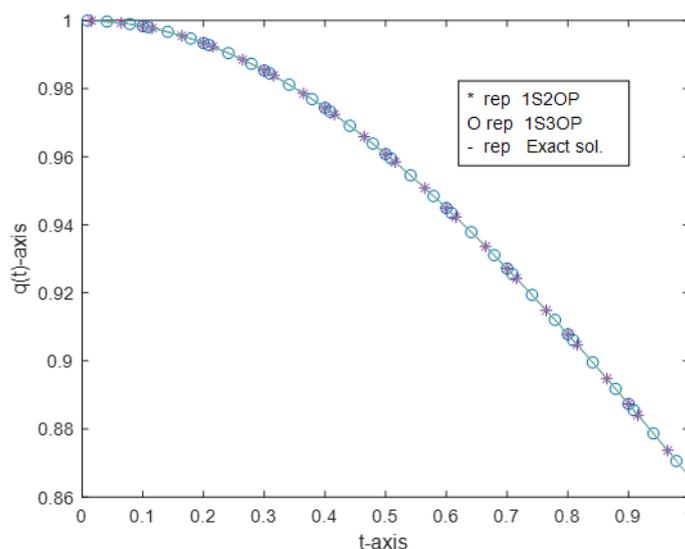


Figure 1. Plots of exact and KSPHT solution for Problem (1).

Problem 2.

The following model which corresponds to the reaction–diffusion process in a spherical permeable catalyst as reported in [8] and [15]

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

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

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

where θ represents the Thiele modulus. The value of θ is determined by the ratio of the reaction rate at the catalyst surface to the diffusion rate through the catalyst pores.

Table 2. Comparison of absolute errors of Problem 2

x	1S3OP	1S2OP[14]	1S3HP[15]	1S4HP[15]
0.1	6.35767e-10	1.16507398e-7	6.17621e-9	4.069691e-9
0.2	6.0224e-10	1.02523148e-7	6.861048e-9	3.8896e-10
0.3	6.05596e-10	9.3155702 e-8	7.966245e-9	2.9896e-10
0.4	6.32437e-10	8.5924964 e-8	9.473596e-9	2.671458e-9
0.5	6.71057e-10	7.8751406e-8	1.1316567e-8	5.88818e-10
0.6	7.06678e-10	6.9694737e-8	1.3291835e-8	7.4041e-10
0.7	7.15759e-10	5.7022468e-8	1.4898722e-8	5.092317e-9
0.8	6.57548e-10	3.9708057e-8	1.5045103e-8	2.062058e-9
0.9	4.60513e-10	1.8740297e-8	1.1513203e-8	1.513203e-9
1		0	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 2 displays the numerical outcomes for various values of θ and n . We observed that in Figure 2, the concentration profile increases when θ diminishes.

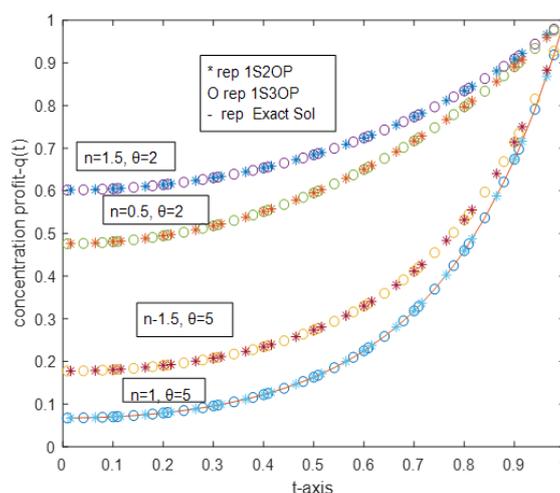


Figure 2. Plots of exact and KSPHT solution for Problem 2.

PROBLEM 3

Consider the nonlinear heat conduction model of the human head,

$$q''(t) + \frac{2}{t}q'(t) + e^{-q(t)} = 0 \quad q'(0) = 0 \quad \alpha q(1) + \beta q' = 0$$

Where $\alpha = 2$ and $\beta = 1$. The above nonlinear SBVP is discussed by Duggan R et al [] as a heat conduction model in the human head. However, The general analytical solution of problem is unknown (Umesh [25]).

Table 3. Comparison of KSPHT on Problem 3

x	1S3OP	1S2OP[14]	1S3HP[15]	1S4HP[15]	MLMF[26]	AADM[25]
0	0.27002964770543 5	0.27002966452995 2	0.27002964680 2432	0.2700296479 05256	0.27002964789 67	0.2700296466
0.1	0.26875690040863 0	0.26875691754786 2	0.26875689954 1846	0.2687569006 38243	0.26875690062 96	0.2687568993
0.2	0.26493281728639 7	0.26493283327299 1	0.26493281645 7765	0.2649328175 46941	0.26493281753 83	0.2649328162
0.3	0.25853978910605 8	0.25853980387077 4	0.25853978831 3346	0.2585397893 90099	0.25853978938 15	0.2585397881
0.4	0.24954817996214 5	0.24954819350670 6	0.24954817920 4708	0.2495481802 62417	-	0.2495481789
0.5	0.23791588728858 9	0.23791589962657 8	0.23791588656 7682	0.2379158875 97897	-	0.2379158863
0.6	0.22358770687868 9	0.22358771802593 2	0.22358770619 8023	0.2235877071 89813	-	0.2235877058
0.7	0.20649448272630	0.20649449269833	0.20649448209	0.2064944830	0.20649448302	0.2064944817

	0	7	2787	31891	38	
0.8	0.18655201388182 5	0.18655202269319 6	0.18655201330 6585	0.1865520141 74299	0.18655201416 67	0.1865520128
0.9	0.16365968131597 6	0.16365968898015 8	0.16365968081 5672	0.1636596815 87396	0.16365968158 04	0.1636596802
1	0.13769874637765 7	0.13769875290734 2	0.13769874597 6308	0.1376987466 19598	0.13769874661 36	0.1376987453

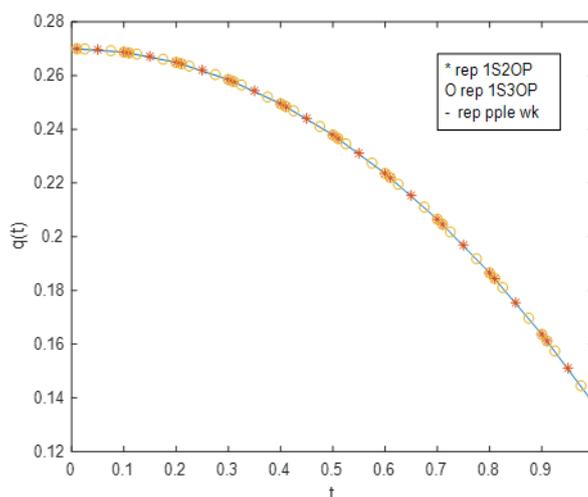


Figure 3. Plots of exact and KSPHT solution for Problem 3.

VI. Discussion Of Results

The results for the three test problems are summarized in Tables 1–3 and Figs. 1–3. For Problem 1, Tables 1 and fig 1 showed the KSPHT methods(1S3OP), demonstrated superior performance compared to 1S2OP in Utalor et al. (2025), 1S3HP,1S4HP in Utalor et al. (2025), Umesh (2021), and Gungum (2020), particularly in terms of accuracy at the points $t = 0(0.1)1.0$. For Problem 2, KSPHT(1S3OP) in Tables 2 again, outperformed the Block Hybrid Methods (Utalor et al., 2025), with graphical results in fig 2 is showing excellent agreement with the exact solution. The convergence of the methods improved as the number of off-step points increased. Tables 3 and Fig. 3 present the results for Problem 3, showing that the approximate solutions are in very good agreement, up to 8–9 decimal places, with results obtained using the Modified Linear Multistep Formulas (Olabode et al., 2024), the Advanced Adomian Decomposition Method (Umesh, 2021) and Block Hybrid Methods (Utalor et al., 2025). while the 1S4HP scheme showed better performance than 1S2OP and 1S3OP. It is observed from the all the Tables that the results obtained from the methods converged faster when the number of off step points were increased. Attempts to implement a 1S4OP scheme were limited by large, complex-valued matrices that complicated computation. Overall, the proposed methods demonstrate high accuracy, rapid convergence, and favorable comparison with existing techniques, highlighting their effectiveness for solving singular boundary value problems.

VII. Conclusion

This study has presented a novel strategy for constructing self-starting block methods for constructing self-starting block methods to solve second-order singular initial boundary value problems (SIBVPs). This approach employs a shift operator applied to two different linear multi-step formulas, which are then combined with three optimized hybrid sets of formulas developed for the first sub-interval. The continuous coefficients of the linear multi-step methods are derived based on the method of undetermined coefficients. The performance of the proposed methods was evaluated through three real-world model problems obtained from the literature. Numerical results demonstrate that the developed methods exhibit high accuracy and computational efficiency, yielding smaller errors compared to existing approaches. Furthermore, the incorporation of optimization techniques in selecting off-step points significantly enhances the accuracy, increase the order of the method and stability of the methods, establishing their superiority over non-optimized alternatives. Overall, the proposed framework offers a reliable and efficient tool for solving classes of second-order singular boundary value problems.

References

[1]. Pandey, R.K. On A Class Regular Singular Two Point Boundary Value Problems. J. Math. Anal. Appl. 1997, 208, 388–403.

- [2]. Zhang, Y. (1993). Existence Of Solutions Of A Kind Of Singular Boundary Value Problem. *Nonlinear Anal. Theory Methods Appl.* , 21(153–159).
- [3]. Thula, K.; Roul, P. (2018). A High-Order B-Spline Collocation Method For Solving Nonlinear Singular Boundary Value Problems Arising In Engineering And Applied Science. *Mediterr. J. Math.* 15, 176.
- [4]. Kumar, M. A. (2003). Difference Scheme Based On Non-Uniform Mesh For Singular Two-Point Boundary Value Problems. *Appl. Math. Comput.* , 136(281–288).
- [5]. Pandey, R.K. (1997). A Finite Difference Methods For A Class Of Singular Two Point Boundary Value Problems Arising In Physiology. *Int. J. Comput. Math.*, 65(131–140).
- [6]. Caglar, H.; Caglar, N.; Ozer, M. (2009). B-Spline Solution Of Non-Linear Singular Boundary Value Problems Arising In Physiology. *Chaos Solitons Fract.*, 39(1232–1237).
- [7]. Kadalbajoo, M.K.; Kumar, V. (2007). B-Spline Method For A Class Of Singular Two-Point Boundary Value Problems Using Optimal Grid. *Appl. Maths. Comput.* , 188(1856–1869).
- [8]. Allouche, H.; Tazdayte, A. (2017). Numerical Solution Of Singular Boundary Value Problems With Logarithmic Singularities By Padé Approximation And Collocation Methods. *J. Comput. Appl. Math.* , 311(324–341).
- [9]. Aydinlik, S.; Kiris, A. (2018). A High-Order Numerical Method For Solving Nonlinear Lane-Emden-Type Equations Arising In Astrophysics. *Astrophys. Space Sci.*, 363, 264.
- [10]. Malele, J.; Dlamini, P.; Simelane, S. (2023). Solving Lane–Emden Equations With Boundary Conditions Of Various Types Using High-Order Compact Finite Differences. *Appl. Math. Sci. Eng.* , 31, 2214303.
- [11]. H. Ramos, Z. Kalogiratu, Th. Monovasilis And T. E. Simos, (2015), An Optimized Two-Step Hybrid Block Method For Solving General Second Order Initial-Value Problems, *Numerical Algorithm*, Springer . DOI 10.1007/S11075-015- 0081-8.
- [12]. Asifa, T., Sania, Q., Amanullah , S., Evren , H., & Asif, A. (2022). A New Continuous Hybrid Block Method With One Optimal Intra Step Point Through Interpolation And Collocation Fixed Point . *Theory Algorithms Sci Eng* , 22.
- [13]. Rajat, S., Gurjinder, S., Higinio , R., & Kanwar , V. (2023). An Efficient Optimized Adaptive Step-Size Hybrid Block Method For Integrating $W'' = F(T,W,W')$ Directly. *Journal Of Computational And Applied Mathematics*, 114838, 420.
- [14]. Utalor, I. K., Oyowe, E. A., Okafor M. F., Ajie, I. J. (2025) Block Optimized Hybrid Methods For Integrating Singular Second Order Ordinary Differential Equations. *International Journal Of Research And Scientific Innovation (IJRSI) ISSN No. 2321-2705 | DOI: 10.51244/IJRSI*
- [15]. Utalor, I. K., Ajie, I. J., Durojaye, M.O, (2025). Construction Of Block Hybrid Methods For The Solution Of Singular Second Order Ordinary Differential Equation. *Asian Research Journal Of Mathematics*,21(5),23–37. <https://doi.org/10.9734/Arjom/2025/V21i5923>
- [16]. Ajie, I. J., Durojaye, M.O, Utalor, I. K., & Onumanyi, P. A. (2020). Construction Of A Family Of Stable One-Block Methods Using Linear Multi-Step Quadruple. *Journal Of Mathematics*, E-ISSN: 2278-5728
- [17]. Ajie, I. J., Utalor, I. K., & Onumanyi, P. A. (2019). A Family Of High Order One-Block Methods For The Solution Of Stiff Initial Value Problems. *Journal Of Advances In Mathematics And Computer Science*, 31(6), 1–14.
- [18]. Brugnano, L., Trigiante, D. (1998). *Solving Differential Problems By Multistep Initial And Boundary Value Methods*. Amsterdam: Gordon And Breach Science Publishers.
- [19]. Lambert J. D. (1973), *Computational Methods In Ordinary Differential Equations*, John Wiley And Sons, New York.
- [20]. S. N. Jator And V. Manathunga, Block Nystrom Type Integrator For Bratu’s Equation, *J. Comp. App. Math.* 327 341-349, 2018.
- [21]. Duggan R & Goodman A. (2017). Pointwise Bounds For A Nonlinear Heat Conduction Model Of The Human Head. *Bulletin Of Mathematical Biology, Springer Science And Business Media LLC*, 48(2), 229-236. DOI:10.1016/S0092-8240(86)80009-X
- [22]. Gungum, S. (2020). Taylor Wavelet Solution Of Linear And Non-Linear Lane-Emden Equations. *Appl. Numer. Math.*, 158, 44–53.
- [23]. Rajat, S., Gurjinder, S., Higinio , R., & Kanwar , V. (2023). An Efficient Optimized Adaptive Step-Size Hybrid Block Method For Integrating $W'' = F(T,W,W')$ Directly. *Journal Of Computational And Applied Mathematics*, 114838, 420.
- [24]. Rufai, M. A., And Ramos, H. (2021). Numerical Solution For Singular Boundary Value Problems Using A Pair Of Hybrid Nyström Techniques. *Axioms* 2021, 10, 202. *Axioms* , 10, 202.
- [25]. Umesh, Kumar, M. (2021). Numerical Solution Of Singular Boundary Value Problems Using Advanced Adomian Decomposition Method. *Eng. Comput.*, 37, 2853–2863.
- [26]. Olabode , B. T., Kayode , S. J., Odeniyan-Fakuade , F. H., & Momoh , A. L. (2024). Numerical Solution To Singular Boundary Value Problems (SBVPS) Using Modified Linear Multistep Formulas (LMF). *International Journal Of Mathematical Sciences And Optimization: Theory And Applications* 10(1), 34–52.