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A new continuous hybrid block method with one optimal intrastep point through interpolation and collocation

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Abstract

Implicit block approaches are used by a number of numerical analyzers to model mild, medium, and hard differential systems. Their excellent stability characteristics, self-starting nature, quick convergence, and large decrease in computing cost all contribute to their widespread application. With these numerical benefits in mind, a new one-step implicit block method with three intrastep grid points has been created. The major term of the local truncation error is minimized to determine which of these points is optimal. The reformulation of the suggested technique leads to a significant decrease in computing cost while maintaining the same consistency, zero-stability, $\mathcal{A}$-stability, and convergence. Several sorts of error are calculated, together with CPU time and efficiency plot, to determine which is superior. Differential models from the fields of heat transfer, population dynamics, and chemical engineering show that the suggested method does a better job than some of the current hybrid block and implicit Radau methods with similar properties.

MSC: 65L05; 65L07; 65L20

Keywords: $\mathcal{A}$-stability; Stiff systems; Order stars; Efficiency curves; Radau method

1 Introduction

Ordinary differential equations are widely used in the real world, so it is crucial to develop efficient and accurate numerical methods for solving them. Several numerical techniques are proposed in this regard in the existing literature. Many domains, such as chemistry, flame propagation, computational fluid dynamics, population dynamics, engineering, and mathematical biology, require approximate solutions to tough problems, but most of these methods fall short. For models to be stiff enough, they need numerical approaches that cost a lot to compute and have unbounded stability areas. Most of the traditional methods such as explicit Runge–Kutta [1], Lobatto family [2], multi-step Adams family [3–5], and higher-order multiderivative types [6, 7] are not used due to either a large amount of computational effort required (very small step-size $\Delta x \approx 0$) or finite stability region (conditional stability). The implicit block methods, on the other hand, are preferred since they are self-starting, computationally robust (cost-effective), highly accurate, fast convergent, and $\mathcal{A}$-stable (a favorable property for stiff models). Some of the major advantages of the block methods include their self-starting nature and ability to overcome the overlapping of solution pieces.

We consider an initial value problem

$$\frac{dy(x)}{dx} = f\bigl(x, y(x)\bigr), \quad y(x_0) = y_0, x \in [x_0, T], y(x) \in \mathbb{R}^n, f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n, \tag{1}$$

where $f(x, y(x))$ is assumed to be Lipschitz continuous and satisfies conditions for the existence and uniqueness of solutions [8] to the problem (1). Milne [9] is thought to be the inventor of the block methods who employed them to get starting values for the predictor–corrector-type numerical methods. One of the most important research works on the block methods can be seen in [10], proposed way back in 1969. Later, several classical works were reported in [11–15] whereas some recently developed implicit block methods include [16–25] and most of the references cited therein. Higher-order block methods including one-, two-, and three-step approaches are proposed in the literature with the $\mathcal{A}$-stability feature. Still, they are, to some extent, computationally expensive, while some lower-order block methods, although time-efficient, are not accurate enough for stiff systems. In the recent past, Ramos et al. [26] presented an idea for optimization of the intermediate collocation points for k-step hybrid block methods from leading terms of the local truncation errors. Motivated by this research study, several block methods were proposed, including [27–29]. For example, Singh et al. [30] proposed a fifth-order block method with three off-step points in a one-step block while optimizing two off-step points and fixing the third, wherein the resulting block method was observed to have $\mathcal{A}$-stability. Singh and Ramos [31] designed an optimized seventh-order two-step hybrid block method with two intrastep points for numerical integration of second-order differential systems considering both fixed and variable step-size approaches. Similarly, Ramos [32] presented, while using interpolation and collocation techniques, a fifth-order two-step hybrid block method for solving first-order initial value problems, wherein the method considers minimization of the local truncation errors to optimize the intermediate two off-step points. Several other researches on the block methods can be found in the available scientific literature. Other works are recently reported in [33–35] wherein the authors have proposed variable-order techniques, including Haar wavelet collocations, to solve differential equations.

Our new one-step hybrid block technique takes into account three intra-step points and is inspired by recent advancements in the block method field. Minimizing the local truncation error leads to an optimal solution. It is important to note that there is currently no recorded one-step block approach with three intra-step points, of which only one is optimal, in the scientific literature. In this study, we seek to create a new one-step method that, unlike numerous existing block methods, just requires one step to minimize the major term of the local truncation error (see the section of numerical results). Using interpolation and collocation, the suggested method derives a continuous approximation of a polynomial.

The present paper is structured as follows: The proposed implicit hybrid block method is derived in Sect. 2 whereas its theoretical analysis, containing error constant from the local truncation error, consistency, zero-stability, linear stability, and the theory of order stars, is described in Sect. 3. Several physical models are considered in Sect. 4 to test the performance of the proposed method, and the final concluding remarks are presented in Sect. 5.

2 Derivation of the proposed block method

This section presents details about derivation of the proposed one-step hybrid block method with three intrastep points $x_{n+u}, x_{n+v}, x_{n+w}$ $(0 < u < v < w < 1)$ where one point is optimized from the principal term of the local truncation error. The method will later be used to numerically solve several initial value problems as in (1), in both scalar and vector forms. Consider a polynomial approximation of the actual solution $y(x)$ of (1) at the grid points $x_0 < x_1 < \cdots < x_N = T$ over the integration interval $[x_0, T]$, with fixed step-size $\Delta x = x_{k+1} - x_k, k = 0, 1, \ldots, N-1$. Suppose the following approximate solution:

$$y(x) \approx L(x) = \sum_{j=0}^{5} \zeta_j x^j. \tag{2}$$

Differentiation of Eq. (2) produces

$$y'(x) \approx L'(x) = \sum_{j=1}^{5} j\zeta_j x^{j-1}, \tag{3}$$

where $\zeta_j \in \mathbb{R}$ denote real undetermined coefficients. Consider three intrastep points $x_{n+u} = x_n + u\Delta x, x_{n+v} = x_n + v\Delta x, x_{n+w} = x_n + w\Delta x$ with $0 < u < v < w < 1$ for finding approximate solution of (1) on $[x_n, x_{n+1}]$ at the points x_n and x_{n+1}. To carry out the process, consider the approximation in (2) computed at the point x_n, and its first-order derivative computed at the points $x_n, x_{n+u}, x_{n+v}, x_{n+w}, x_{n+1}$. This setup brings the following matrix form of a linear system containing six equations in six real unknown coefficients $\zeta_j, j = 0, 1, \ldots, 5$:

$$\begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 \\ 0 & 1 & 2x_n & 3x_n^2 & 4x_n^3 & 5x_n^4 \\ 0 & 1 & 2x_{n+u} & 3x_{n+u}^2 & 4x_{n+u}^3 & 5x_{n+u}^4 \\ 0 & 1 & 2x_{n+v} & 3x_{n+v}^2 & 4x_{n+v}^3 & 5x_{n+v}^4 \\ 0 & 1 & 2x_{n+w} & 3x_{n+w}^2 & 4x_{n+w}^3 & 5x_{n+w}^4 \\ 0 & 1 & 2x_{n+1} & 3x_{n+1}^2 & 4x_{n+1}^3 & 5x_{n+1}^4 \end{pmatrix} \begin{pmatrix} \zeta_0 \\ \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \zeta_4 \\ \zeta_5 \end{pmatrix} = \begin{pmatrix} y_n \\ f_n \\ f_{n+u} \\ f_{n+v} \\ f_{n+w} \\ f_{n+1} \end{pmatrix}. \tag{4}$$

Solving the above linear system gives values of the six unknown coefficients $\zeta_j, j = 0, 1, \ldots, 5$ which, for the sake of brevity, are not shown here. Putting these values in (2), while using the change of variable $x = x_n + t\Delta x$, we obtain

$$L(x_n + t\Delta x) = \zeta_0 y_n + \Delta x(\eta_0 f_n + \eta_u f_{n+u} + \eta_v f_{n+v} + \eta_w f_{n+w} + \eta_1 f_{n+1}), \tag{5}$$

where

$$\begin{aligned} \zeta_0 &= 1, \\ \eta_0 &= \frac{t\begin{pmatrix} 20uvt^2 - 30uvtw - 15ut^3 + 20ut^2w - 15vt^3 + 20vt^2w + \\ 12t^4 - 15t^3w - 30uvt + 60uvw + 20ut^2 - 30utw + 20vt^2 \end{pmatrix}}{60uvw}, \\ \eta_u &= -\frac{t^2(15vt^2 - 20vtw - 12t^3 + 15t^2w - 20vt + 30vw + 15t^2 - 20tw)}{60(u-1)(u-w)(u-v)u}, \\ \eta_v &= \frac{t^2(15ut^2 - 20utw - 12t^3 + 15t^2w - 20ut + 30uw + 15t^2 - 20tw)}{60(v-1)(v-w)(u-v)v}, \end{aligned} \tag{6}$$

$$\eta_w = \frac{t^2(20uvt - 15ut^2 - 15vt^2 + 12t^3 - 30uv + 20ut + 20vt - 15t^2)}{60(w-1)(v-w)(u-w)w},$$
$$\eta_1 = -\frac{t^2(20uvt - 30uvw - 15ut^2 + 20utw - 15vt^2 + 20vtw + 12t^3 - 15t^2w)}{60(w-1)(v-1)(u-1)}.$$

Now to get the required one-step hybrid block method, we evaluate $L(x_n + t\Delta x)$ at the collocation points $x_{n+u}, x_{n+v}, x_{n+w}$, and x_{n+1} where $t = u, v, w, 1$. By so doing, the following system of four equations with four unknowns is obtained:

$$\begin{aligned} y_{n+u} &= y_n \\ &\quad - \frac{\Delta x}{60}\left(\frac{-3u^4 + 5u^3v + 5u^3w - 10u^2vw + 5u^3 - 10u^2v - 10u^2w + 30uvw}{vw} f_n \right. \\ &\quad + \frac{u(12u^3 - 15u^2v - 15u^2w + 20uvw - 15u^2 + 20uv + 20uw - 30vw)}{(u-1)(u-w)(u-v)} f_{n+u} \\ &\quad - \frac{u^2(-3u^3 + 5u^2w + 5u^2 - 10uw)}{(v-1)(v-w)(u-v)v} f_{n+v} - \frac{u^2(-3u^3 + 5u^2v + 5u^2 - 10uv)}{(w-1)(v-w)(u-w)w} f_{n+w} \\ &\quad \left. - \frac{u^2(-3u^3 + 5u^2v + 5u^2w - 10uvw)}{(w-1)(v-1)(u-1)} f_{n+1}\right), \end{aligned} \tag{7}$$

$$\begin{aligned} y_{n+v} &= y_n \\ &\quad - \frac{\Delta x}{60}\left(\frac{5uv^3 - 10uv^2w - 3v^4 + 5v^3w - 10uv^2 + 30uvw + 5v^3 - 10v^2w}{uw} f_n \right. \\ &\quad + \frac{v^2(-3v^3 + 5v^2w + 5v^2 - 10vw)}{(u-1)(u-w)(u-v)u} f_{n+u} \\ &\quad - \frac{v(-15uv^2 + 20uvw + 12v^3 - 15v^2w + 20uv - 30uw - 15v^2 + 20vw)}{(v-1)(v-w)(u-v)} f_{n+v} \\ &\quad \left. + \frac{v^2(5uv^2 - 3v^3 - 10uv + 5v^2)}{(w-1)(v-w)(u-w)w} f_{n+w} - \frac{v^2(5uv^2 - 10uvw - 3v^3 + 5v^2w)}{(w-1)(v-1)(u-1)} f_{n+1}\right), \end{aligned} \tag{8}$$

$$\begin{aligned} y_{n+w} &= y_n \\ &\quad - \frac{\Delta x}{60}\left(\frac{-10uvw^2 + 5uw^3 + 5vw^3 - 3w^4 + 30uvw - 10uw^2 - 10vw^2 + 5w^3}{uv} f_n \right. \\ &\quad + \frac{w^2(5vw^2 - 3w^3 - 10vw + 5w^2)}{(u-1)(u-w)(u-v)u} f_{n+u} - \frac{w^2(5uw^2 - 3w^3 - 10uw + 5w^2)}{(v-1)(v-w)(u-v)v} f_{n+v} \\ &\quad + \frac{w(20uvw - 15uw^2 - 15vw^2 + 12w^3 - 30uv + 20uw + 20vw - 15w^2)}{(w-1)(v-w)(u-w)} f_{n+w} \\ &\quad \left. - \frac{w^2(-10uvw + 5uw^2 + 5vw^2 - 3w^3)}{(w-1)(v-1)(u-1)} f_{n+1}\right), \end{aligned} \tag{9}$$

$$\begin{aligned} y_{n+1} &= y_n \\ &\quad - \frac{\Delta x}{60}\left(\frac{30uvw - 10uv - 10uw - 10vw + 5u + 5v + 5w - 3}{uvw} f_n \right. \\ &\quad + \frac{-10vw + 5v + 5w - 3}{(u-1)(u-w)(u-v)u} f_{n+u} - \frac{-10uw + 5u + 5w - 3}{(v-1)(v-w)(u-v)v} f_{n+v} \\ &\quad + \frac{-10uv + 5u + 5v - 3}{(w-1)(v-w)(u-w)w} f_{n+w} \end{aligned} \tag{10}$$

$$-\frac{(-30uvw+20uv+20uw+20vw-15u-15v-15w+12)}{(w-1)(v-1)(u-1)}f_{n+1}\bigg),$$

where $y_{n+l} \simeq y(x_n + l\Delta x)$ are approximations of the exact solution, and $f_{n+l} = f(x_{n+l}, y_{n+l})$, for $l = u, v, w, 1$. The above approximations consist of the parameters u, v, w that are related to the intrastep points x_u, x_v, x_w. The suitable values of these parameters can be computed with the help of the principal term of the local truncation error in the main formula, that is, y_{n+1}. One of the parameters will be optimized by imposing a condition on the principal term to vanish. The reason to consider the principal term of the local truncation error in y_{n+1} to compute one of the optimized parameters is that at the end of the subinterval $[x_n, x_{n+1}]$, the value y_{n+1} is the only value required for advancing the integration on the next block. Thus, to achieve this, we have considered the following local truncation error obtained by expanding $y(x)$ in the Taylor series about x_n. So, the local truncation error in the formula given in (10) is given as follows:

$$\begin{aligned}
&\mathcal{L}\big(y(x_{n+1});\Delta x\big)\\
&\quad=\left(\frac{((10w-5)v-5w+3)u}{7200}+\frac{(-5w+3)v}{7200}+\frac{w}{2400}-\frac{1}{3600}\right)\Delta x^6 y^{(6)}(x_n)\\
&\qquad+\left(\frac{((70w-35)v-35w+21)u^2}{302{,}400}\right.\\
&\qquad+\frac{(v+w+1)((w-1/2)v-(1/2)w+3/10)u}{4320}+\frac{(-35w+21)v^2}{302{,}400}\\
&\qquad\left.+\frac{-35w^2-14w+21}{302{,}400}+\frac{w^2}{14{,}400}+\frac{w}{14{,}400}-\frac{1}{12{,}600}\right)\Delta x^7 y^{(7)}(x_n)\\
&\qquad+\mathcal{O}\big(\Delta x^8\big).
\end{aligned} \tag{11}$$

Equating the principal term (the coefficient of Δx^6) of the local truncation error in (11) to zero, we get the following single equation in three unknown parameters:

$$\frac{((10w-5)v-5w+3)u}{7200}+\frac{(-5w+3)v}{7200}+\frac{w}{2400}-\frac{1}{3600}=0. \tag{12}$$

The above equation (12) is expressed in terms of u and v as follows:

$$w=\frac{5uv-3v-3u+2}{10uv-5v-5u+3}. \tag{13}$$

Since there are more unknowns than equations, there exist infinitely many solutions for the parameters under consideration. Considering two of them (say, u, v) as free parameters, w is optimized. By so doing, the following set of parameters is determined, with w being the optimal one:

$$\left\{u=\frac{1}{4}, v=\frac{1}{2}, w=\frac{3}{4}\right\}. \tag{14}$$

Substituting these values into (11), the local truncation error of the main formula in (10) is computed as follows:

$$\mathcal{L}\big(y(x_{n+1});\Delta x\big)=-\frac{(\Delta x)^7 y^{(7)}(x_n)}{1{,}935{,}360}+\mathcal{O}\big(\Delta x^8\big). \tag{15}$$

Finally, substituting the values of the obtained parameters u, v, w into (7)–(10) yields the following required one-step hybrid block method with three intrastep points having at least fifth-order convergence while one of the intrastep points is optimized:

$$
\begin{aligned}
y_{n+\frac{1}{4}} &= y_n + \frac{\Delta x}{2880}[251f_n + 646f_{n+\frac{1}{4}} - 264f_{n+\frac{1}{2}} + 106f_{n+\frac{3}{4}} - 19f_{n+1}],\\
y_{n+\frac{1}{2}} &= y_n + \frac{\Delta x}{360}[29f_n + 124f_{n+\frac{1}{4}} + 24f_{n+\frac{1}{2}} + 4f_{n+\frac{3}{4}} - f_{n+1}],\\
y_{n+\frac{3}{4}} &= y_n + \frac{\Delta x}{320}[27f_n + 102f_{n+\frac{1}{4}} + 72f_{n+\frac{1}{2}} + 42f_{n+\frac{3}{4}} - 3f_{n+1}],\\
y_{n+1} &= y_n + \frac{\Delta x}{90}[7f_n + 32f_{n+\frac{1}{4}} + 12f_{n+\frac{1}{2}} + 32f_{n+\frac{3}{4}} + 7f_{n+1}].
\end{aligned}
\tag{16}
$$

The pseudocode for the above proposed method is presented in the algorithm of the Appendix. Moreover, it is easy to notice from the structure of the proposed block method (16) that the slope f occurs four times in each equation without considering f_n as it is just a numerical value. It becomes computationally expensive when f is complicated. This can, however, be overcome by minimizing the number of times f appears in each equation of the above formulae. To accomplish this, we simultaneously solve the set of equations (16) for $f_{n+u}, f_{n+v}, f_{n+w}$, and f_{n+1}. It results in an equivalent formulation of (16) reducing the occurrences of f to just one. This proves to be computationally cost-effective, particularly when f is not a simple differentiable function. The obtained reformulation is structured as follows:

$$
\begin{aligned}
\Delta x f_{n+\frac{1}{4}} &= -\frac{37}{12}y_n + \frac{2}{3}y_{n+\frac{1}{4}} + 3y_{n+\frac{1}{2}} - \frac{2}{3}y_{n+\frac{3}{4}} + \frac{1}{12}y_{n+1} - \frac{\Delta x}{4}f_n,\\
\Delta x f_{n+\frac{1}{2}} &= \frac{31}{18}y_n - \frac{16}{3}y_{n+\frac{1}{4}} + 2y_{n+\frac{1}{2}} + \frac{16}{9}y_{n+\frac{3}{4}} - \frac{1}{6}y_{n+1} + \frac{\Delta x}{6}f_n,\\
\Delta x f_{n+\frac{3}{4}} &= -\frac{29}{12}y_n + 6y_{n+\frac{1}{4}} - 9y_{n+\frac{1}{2}} + \frac{14}{3}y_{n+\frac{3}{4}} + \frac{3}{4}y_{n+1} - \frac{\Delta x}{4}f_n,\\
\Delta x f_{n+1} &= \frac{28}{3}y_n - \frac{64}{3}y_{n+\frac{1}{4}} + 24y_{n+\frac{1}{2}} - \frac{64}{3}y_{n+\frac{3}{4}} + \frac{28}{3}y_{n+1} + \Delta x f_n,
\end{aligned}
\tag{17}
$$

where the above reformulation of (16) is now abbreviated as RPOBM_5. The function f is required to be evaluated at four points in both formulations; the computational cost, however, is reduced (as evident in the numerical experiments) while using (17) for solving problems as in (1).

3 Theoretical analysis

In this section, we investigate theoretical properties for the proposed implicit hybrid block method given in (16), or equivalently (17), including accuracy, consistency, zero-stability, convergence, linear stability, and $\mathcal{A}$-acceptability.

3.1 Order of accuracy and consistency

The hybrid block method in (16) can be rewritten in the following convenient form:

$$
A_1 Y_{n+1} = A_0 Y_n + \Delta x(B_0 F_n + B_1 F_{n+1}),
\tag{18}
$$

where A_0, A_1, B_0, and B_1 are 4×4 matrices given by

$$A_0 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \qquad A_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{19}$$

$$B_0 = \begin{bmatrix} 0 & 0 & 0 & \frac{251}{2880} \\ 0 & 0 & 0 & \frac{29}{360} \\ 0 & 0 & 0 & \frac{27}{320} \\ 0 & 0 & 0 & \frac{7}{90} \end{bmatrix}, \qquad B_1 = \begin{bmatrix} \frac{646}{2880} & -\frac{264}{2880} & \frac{106}{2880} & -\frac{19}{2880} \\ \frac{124}{360} & \frac{24}{360} & \frac{4}{360} & -\frac{1}{360} \\ \frac{102}{320} & \frac{72}{320} & \frac{42}{320} & -\frac{3}{320} \\ \frac{32}{90} & \frac{12}{90} & \frac{32}{90} & \frac{7}{90} \end{bmatrix}, \tag{20}$$

and

$$\begin{aligned} Y_n &= (y_{n-1+u}, y_{n-1+v}, y_{n-1+w}, y_n)^T, \\ Y_{n+1} &= (y_{n+u}, y_{n+v}, y_{n+w}, y_{n+1})^T, \\ F_n &= (f_{n-1+u}, f_{n-1+v}, f_{n-1+w}, f_n)^T, \\ F_{n+1} &= (f_{n+u}, f_{n+v}, f_{n+w}, f_{n+1})^T. \end{aligned} \tag{21}$$

The linear functional operator $\bar{\mathcal{L}}$ associated with (16) can be defined as

$$\bar{\mathcal{L}}\big[z(x_n); \Delta x\big] = \sum_{k=0,u,v,w,1} \big[\bar{\zeta}_k z(x_n + k\Delta x) - \Delta x \bar{\eta}_k z'(x_n + k\Delta x)\big], \tag{22}$$

where $\bar{\zeta}_k$ and $\bar{\eta}_k$ are the column vectors of the matrices A_1 and A_0, respectively. The term $z(x)$ is an arbitrary test function that is considered sufficiently differentiable in the interval $[0, T]$. The block method (16) and the corresponding linear difference operator are said to be at least of order r if after expanding the functions $z(x_n + k\Delta x)$ and $z'(x_n + k\Delta x)$ in Taylor series about x_n, and collecting the coefficients of Δx, we obtain

$$\bar{\mathcal{L}}\big[z(x_n); \Delta x\big] = \bar{C}_0 z(x_n) + \bar{C}_1 \Delta x z'(x_n) + \bar{C}_2 \Delta x^2 z''(x_n) + \cdots + \bar{C}_r \Delta x^r z^{(r)}(x_n) + \cdots, \tag{23}$$

with $\bar{C}_0 = \bar{C}_1 = \cdots = \bar{C}_r = 0$ and $\bar{C}_{r+1} \neq 0$. The coefficients $\bar{C}_r$ are vectors and $\bar{C}_{r+1}$ is known as the vector of error constants. For the proposed hybrid block method (16), we obtain $\bar{C}_0 = \bar{C}_1 = \cdots = \bar{C}_5 = 0$ with the error constant given by

$$\bar{C}_6 = \left(\frac{3}{655{,}360}, \frac{1}{368{,}640}, \frac{3}{655{,}360}, 0 \right)^T. \tag{24}$$

Thus, it proves that the one-step implicit hybrid block method with three intrastep points, while one of them is optimally obtained, has at least fifth algebraic order of accuracy. In addition, the method (16) does not have an order less than 1; therefore, it is also consistent with the IVP (1) (see the work of Jator in [36]).

3.2 Zero-stability and convergence

An essential crude requirement for a numerical method to be of some use is the requirement called zero-stability. For example, let the IVP given in (1) be asymptotically stable, whereas the need is to prove the stability of the proposed numerical method (16). The notion of zero-stability relates to considering a homogeneous equation $y' = 0$ and its discretized counterpart as given by

$$A_0 Y_{n+1} - A_1 Y_n = 0, \tag{25}$$

where A_0 and A_1 are given in (19). Now, if the discrete algebraic equation (25) admits solutions that grow in time, then the proposed block method will not be zero-stable and cannot be used in practice. On the other hand, the proposed block method is said to be zero-stable if zeros R_i of the first characteristic polynomial $\kappa(R) = |zA_1 - A_0|$ fulfill $|R_i| \leq 1$ and for those zeros with $|R_i| = 1$ the multiplicity does not exceed 1 [5]. The first characteristic polynomial of the proposed block method (16) is given by

$$\kappa(R) = R^3(R-1). \tag{26}$$

Thus, the proposed block method (16) can be considered a zero-stable method. Being both zero-stable and consistent, it deserves to be called a convergent method (check the work of Henrici in [37]).

3.3 Linear stability analysis and order stars

Theorem 3.1 *The proposed one-step hybrid block method with one optimal intrastep point given in* (16) *satisfies every criterion to be $\mathcal{A}$-stable.*

Proof As far as the concept of zero stability is concerned, it is related to the behavior of the underlying numerical method as the step-size $\Delta x \to 0$. In other situations, however, a different concept of stability is needed from a practical point of view. It is concerned with a numerical method that produces good results for a particular value of $\Delta x > 0$. Such behavior is known as the linear stability behavior for the numerical method, and it requires applying the method on a linear test problem proposed by Dahlquist [38], namely

$$y'(x) = \sigma y(x), \quad \text{with } \operatorname{Re}(\sigma) < 0. \tag{27}$$

It is required to determine the region wherein the approximations obtained under the numerical method reproduce the behavior of the true solution of the test problem (27). After using the proposed block method (16) on the test problem in (27), the recurrence equation given below is obtained:

$$Y_n = H(z) Y_{n-1}, \tag{28}$$

where $H(z)$ denotes the stability matrix given by

$$H(z) = (A_1 - zB_1)^{-1}(A_0 + zB_0), \quad z = \sigma \Delta x. \tag{29}$$

The eigenvalues of the stability matrix (29) determine the behavior of the numerical solution. This is the commonly known stability property of the numerical method that uses the

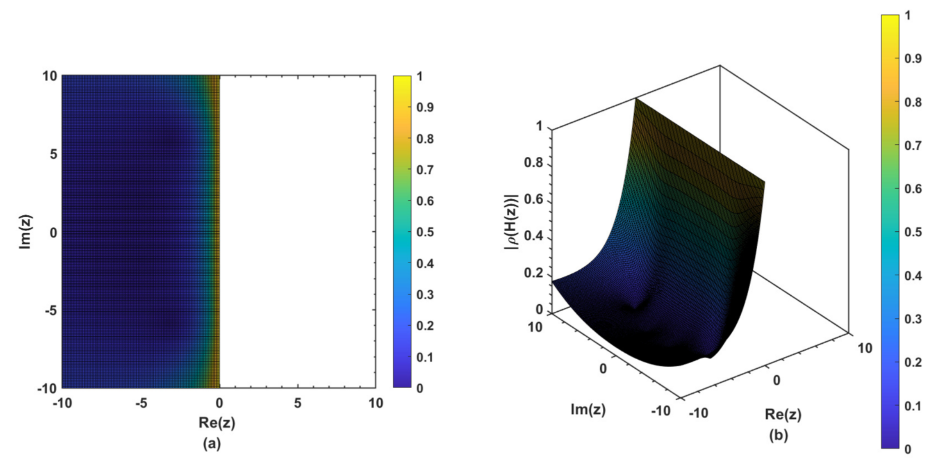

Figure 1 The stability region in 2D and 3D of the proposed one-step block method (16) with three intrastep points, including one optimal

spectral radius (supremum among the absolute values of the elements in the spectrum) of $H(z)$. The region of absolute linear stability $\mathbb{A}$ is defined by the set [39]

$$\mathbb{A} = \{z \in \mathbb{C} : |\rho[H(z)]| < 1\}, \tag{30}$$

and if $\mathbb{C}^- \subseteq \mathbb{A}$, the underlying numerical method is said to be $\mathcal{A}$-stable. The spectral radius is easily computed as the following rational function:

$$\rho[H(z)] = \frac{3z^4 + 50z^3 + 420z^2 + 1920z + 3840}{3z^4 - 50z^3 + 420z^2 - 1920z + 3840}, \tag{31}$$

which has modulus less than one in $\mathbb{C}^-$. This completes the proof for the $\mathcal{A}$-stability of the proposed block method given in (16). □

Remark 3.2 The graphical illustrations given by Fig. 1 show that the entire left-half complex plane $\mathbb{C}^-$ is included in the stability region of (16). This kind of $\mathcal{A}$- stability is further confirmed with the plot of order stars wherein the rational stability function (31) does not have any pole in $\mathbb{C}^-$ as can be seen in Fig. 2.

4 Numerical dynamics with results and discussion

The proposed one-step hybrid block method with three intrasteps, including one optimal point given in (16), is now employed, neither using any starting values nor any predictors, to determine the approximate solution of various single and systems of stiff ordinary differential equations. Keeping in mind that the initial value $y(x_0) = y_0$ is known, the system of equations in (16) is simultaneously solved for $n = 0$. The well-known quadratically convergent Newton's method is sufficient for solving the system to get the value $y(x_1) \cong y_1$. Later, taking y_1 from the previous block as the initial value, the value $y(x_2) \cong y_2$ is computed. This procedure continues until the computation of x_N (the last point). The entire length of the integration interval is chosen to be a multiple of $2\Delta x$ ($x_N - x_0 = \varepsilon(2\Delta x)$, $\varepsilon \in \mathbb{N}$), as we have selected, for comparison, some two-step methods. Newton's method under the Find

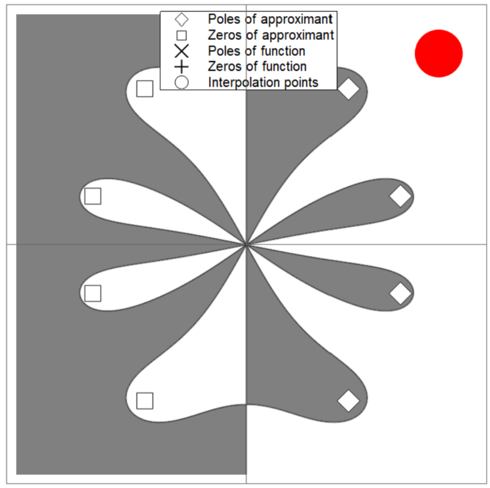

Figure 2 Order stars confirming $\mathcal{A}$-stability of the proposed one-step block method (16) with three intrastep points, including one optimal point

Root command in Mathematica 12.1 with 64-digit working precision arithmetic is used during the implementation of numerical simulations. All numerical simulations are carried out in Mathematica 12.1 on a personal computer running Windows OS with Intel(R) Core(TM) i7-1065G7 CPU @ 1.30 GHz and 1.50 GHz processor having 24.0 GB installed RAM.

Considering the potential of block methods to deal with stiff differential models, we have taken some well-known stiff applied problems that have appeared several times in the recent literature. These problems are solved with methods as given below:

- Proposed (POBM_5) one-step fifth-order hybrid block method with three intrastep grid points shown in (16).
- Reformulated proposed (RPOBM_5) one-step fifth-order hybrid block method with three intrastep points shown in (17).
- Block hybrid Simpson's method (BHSM_5) with two intrastep points for the stiff system that appeared in [40].
- Two-step sixth-order block method (Sahi_6) that appeared in [41].
- Fully-implicit RK-type fifth-order method, called Radau method (Radau I_5), that appeared in [1]. The Radau family is well-known for solving stiff differential systems.

Moreover, the performance of each method under consideration is measured on different types of error, including maximum global absolute errors ME = $(\max_{x\in[x_0,T]} |y(x_N) - y_N|)$, absolute error at final grid point LE = $(|y(x_N) - y_N|)$, average absolute error AE = $\frac{1}{N}(\sum_{i=1}^{N} |y(x_i) - y_i|)$, norm $(\sqrt{\sum_{i=1}^{N} |y(x_i) - y_i|^2})$, and the CPU time computed in seconds.

The problems under consideration are the most challenging IVPs in ODEs, including burning a ball for a match stick (flame propagation), Prothero–Robinson stiff problem, Kaps stiff system, and the nonlinear Blasius third-order ODE commonly encountered in fields like heat transfer and the computational fluid dynamics. The numerical simulations for each numerical experiment are shown in the Tables 1–5. Different absolute errors and CPU times are noted to compare the above-discussed methods.

It can be observed from these tables that the proposed block method (16) yields minor errors. In contrast, its reformulation also produces minor errors, reducing CPU times as

Table 1 Comparison of the methods under consideration on the basis of absolute errors and CPU time for the flame propagation model given in Problem 1 with different number of steps (n)

n	Method	ME	LE	AE	Norm	CPU time
64	POBM_5	1.232e–10	1.049e–12	1.645e–11	2.650e–10	3.739e–01
	RPOBM_5	1.232e–10	1.049e–12	1.645e–11	2.650e–10	2.898e–01
	BHSM_5	1.243e–08	1.905e–11	1.387e–09	2.329e–08	1.171e–01
	Sahi_6	1.155e–08	6.796e–11	1.568e–09	2.565e–08	1.733e–01
	Radau I_5	9.303e–09	3.043e–10	1.304e–09	2.048e–08	4.269e–01
128	POBM_5	1.967e–12	1.635e–14	2.590e–13	5.824e–12	5.682e–01
	RPOBM_5	1.967e–12	1.635e–14	2.590e–13	5.824e–12	4.026e–01
	BHSM_5	1.838e–10	2.934e–13	2.246e–11	5.244e–10	1.800e–01
	Sahi_6	2.239e–10	1.049e–12	2.381e–11	5.601e–10	2.579e–01
	Radau I_5	2.889e–10	9.259e–12	3.997e–11	8.842e–10	5.834e–01
256	POBM_5	3.067e–14	2.553e–16	4.058e–15	1.285e–13	3.051e+00
	RPOBM_5	3.067e–14	2.553e–16	4.058e–15	1.285e–13	9.716e–01
	BHSM_5	2.834e–12	4.568e–15	3.536e–13	1.166e–11	4.130e–01
	Sahi_6	3.621e–12	1.635e–14	3.701e–13	1.234e–11	6.724e–01
	Radau I_5	8.931e–12	2.857e–13	1.243e–12	3.866e–11	1.176e+00

an additional advantage over the proposed block method. When compared to other well-known methods from available literature, it is noted that the errors are more significant in magnitude; however, the CPU times are as promising as in the reformulated block method in some cases, particularly when the method has a simple form of coefficients such as that in [40]. The efficiency curves shown in Figs. 4 and 3 for the first and second numerical experiments, respectively, are obtained wherein the better performance of the proposed block method (16) and its reformulation given in (17) is seen in terms of absolute maximum global error and CPU times. Thus, the reformulated version of the proposed block method is proved to be the most time-efficient algorithm among considered to obtain an approximate solution of the IVP (1).

Problem 1 *Consider the following highly stiff IVP for the flame propagation taken from* [42]:

$$u_1'(x) = u_1^2(x) - u_1^3(x), \quad u_1(0) = \epsilon, x \in \left[0, \frac{2}{\epsilon}\right], \tag{32}$$

with the exact solution $u_1(x) = \frac{1}{\mathrm{ProductLog}[9\exp(-x+9)]+1}$, *where the function* ProductLog *is a special function whose details are available in the Wolfram language documentation.*

Problem 2 *We consider the well-known Prothero–Robinson model taken from* [43]:

$$u_1'(x) = \lambda\big(u_1(x) - f(x)\big) + f'(x), \quad u_1(0) = 0, x \in [0, 5], \tag{33}$$

with $\lambda = 10^{-7}, f(x) = \sin(x)$, *whose exact solution is* $u_1(x) = \sin(x)$.

Problem 3 *We consider the following stiff system of first-order ODEs taken from* [41]:

$$\begin{aligned} u_1'(x) &= -u_1(x) + 95v_1(x), \quad u_1(0) = 1, \\ v_1'(x) &= -u_1(x) - 97v_1(x), \quad v_1(0) = 1, \end{aligned} \tag{34}$$

Table 2 Comparison of the methods under consideration on the basis of absolute errors and CPU time for Problem 2 with different number of steps (*n*)

n	Method	ME	LE	AE	Norm	CPU time
256	POBM_5	2.868e–17	2.750e–17	1.882e–17	3.338e–16	8.907e–01
	RPOBM_5	2.868e–17	2.750e–17	1.882e–17	3.338e–16	7.023e–01
	SHM, 5	5.874e–15	5.633e–15	3.854e–15	6.836e–14	2.801e–01
	Sahi_6	7.802e–15	1.760e–15	3.156e–15	6.585e–14	5.546e–01
	Radau I_5	7.895e–14	2.829e–14	4.692e–14	8.608e–13	8.467e–01
512	POBM_5	4.482e–19	4.298e–19	2.942e–19	7.369e–18	2.018e+00
	RPOBM_5	4.482e–19	4.298e–19	2.942e–19	7.369e–18	1.485+00
	BHSM_5	9.178e–17	8.802e–17	6.025e–17	1.509e–15	5.645e–01
	Sahi	1.219e–16	2.750e–17	4.938e–17	1.455e–15	1.142e+00
	Radau I_5	2.467e–15	8.838e–16	1.468e–15	3.804e–14	1.562e+00
1024	POBM_5	7.003e–21	6.715e–21	4.598e–21	1.628e–19	4.491e+00
	RPOBM_5	7.003e–21	6.715e–21	4.598e–21	1.628e–19	3.378e+00
	BHSM_5	1.434e–18	1.375e–18	9.416e–19	3.334e–17	1.319e+00
	Sahi_6	1.905e–18	4.298e–19	7.721e–19	3.215e–17	2.008e+00
	Radau I_5	7.710e–17	2.762e–17	4.591e–17	1.681e-15	3.484e+00

Table 3 Comparison of the methods under consideration on the basis of absolute errors and CPU time for the stiff Problem 3 with different number of steps (*n*)

n	Method	ME_u	ME_v	LE_u	LE_v	CPU time
216	POBM_5	5.919e–07	5.919e–07	1.852e–17	1.949e–19	1.322e+00
	RPOBM_5	5.919e–07	5.919e–07	1.852e–17	1.949e–19	1.057e+00
	BHSM_5	1.917e–05	1.917e–05	6.320e–16	6.653e–18	7.299e–01
	Sahi_6	3.468e–05	3.468e–05	4.494e–14	4.730e–16	2.074e+00
	Radau I_5	3.468e–05	3.468e–05	1.185e–15	1.247e–17	1.270e+00
1296	POBM_5	1.232e–11	1.232e–11	3.969e–22	4.177e–24	7.689e+00
	RPOBM_5	1.232e–11	1.232e–11	3.969e–22	4.177e–24	6.723e+00
	BHSM_5	4.197e–10	4.197e–10	1.300e–20	1.426e–22	2.474e+00
	Sahi_6	3.821e–09	3.821e–09	5.763e–18	6.067e–20	7.311e+00
	Radau I_5	1.362e–09	1.362e–09	2.540e–20	2.674e–22	4.044e+00
7776	POBM_5	2.639e–16	2.639e–16	8.506e–27	8.954e–29	4.876e+01
	RPOBM_5	2.639e–16	2.639e–16	8.506e–27	8.954e–29	3.723e+01
	BHSM_5	9.010e–15	9.010e–15	2.903e–25	3.056e–27	1.450e+01
	Sahi_6	4.809e–13	4.809e–13	7.409e–22	7.798e–24	4.061e+01
	Radau I_5	3.811e–14	3.811e–14	5.444e–25	5.730e–27	2.482e+01

Table 4 Comparison of the methods under consideration on the basis of absolute errors and CPU time for Kaps Problem 4 with different number of steps (*n*)

n	Method	ME_u	ME_v	LE_u	LE_v	CPU time
128	POBM_5	5.214e–17	2.608e–19	7.487e–18	2.608e–19	9.962e–01
	RPOBM_5	5.214e–17	2.608e–19	7.487e–18	2.608e–19	7.935e–01
	BHSM_5	1.172e–17	9.559e–18	7.686e–18	9.554e–18	3.156e–01
	Sahi_6	9.182e–11	9.169e–14	9.3e–12	7.819e–15	8.553e–01
	Radau I_5	3.280e–15	4.168e–17	4.938e–16	1.668e–17	4.917e–01
256	POBM_5	8.034e–19	4.079e–21	1.137e–19	4.079e–21	2.691e+00
	RPOBM_5	8.034e–19	4.079e–21	1.137e–19	4.079e–21	2.029e+00
	BHSM_5	1.791e–19	1.494e–19	1.189e–19	1.493e–19	7.806e–01
	Sahi_6	3.111e–12	3.107e–15	4.179e–13	3.707e–16	1.977e+00
	Radau I_5	5.214e–17	6.584e–19	7.487e–18	2.608e–19	1.014e+00
512	POBM_5	1.236e–20	6.376e–23	1.748e–21	6.376e–23	4.106e+00
	RPOBM_5	1.236e–20	6.376e–23	1.748e–21	6.376e–23	3.685+00
	BHSM_5	2.727e–21	2.334e–21	1.835e–21	2.333e–21	1.348e+00
	Sahi_6	9.454e–14	9.442e–17	1.298e–14	1.150e–17	4.011e+00
	Radau I_5	8.034e–19	1.028e–20	1.137e–19	4.079e–21	2.772e+00

Table 5 Comparison of absolute errors at $x = 10$ for the Blasius equation of boundary layer flow given in Problem 5 with different number of steps (n)

n	Method	LE_u	LE_v	LE_w	CPU time
8	POBM_5	6.705e–05	1.051e–05	4.259e–11	8.084e–02
	RPOBM_5	6.705e–05	1.051e–05	4.259e–11	6.753e–02
	BHSM_5	5.437e–02	6.470e–03	2.294e–07	2.524e–02
	Sahi_6	1.847e–02	1.542e–03	3.599e–06	4.455e–02
	Radau_5	1.672e–03	1.640e–04	1.274e–06	7.56e–02
16	POBM_5	7.800e–07	1.288e–07	1.496e–11	2.958e–01
	RPOBM_5	7.800e–07	1.288e–07	1.496e–11	1.362e–01
	BHSM_5	1.933e–04	1.876e–05	1.839e–11	4.400e–02
	Sahi_6	6.705e–05	1.051e–05	4.259e–11	1.502e–01
	Radau_5	5.548e–05	5.016e–06	1.495e–11	1.758e–01
32	POBM_5	3.541e–07	3.004e–08	1.496e–11	2.680e–01
	RPOBM_5	3.541e–07	3.004e–08	1.496e–11	2.308e–01
	BHSM_5	4.330e–06	4.861e–07	1.496e–11	8.873e–02
	Sahi_6	7.800e–07	1.288e–07	1.496e–11	1.555e–01
	Radau_5	2.033e–06	1.761e–07	1.496e–11	2.727e–01

where $x \in [0, 2]$. The exact solution of the above system is

$$\begin{aligned} u_1(x) &= \frac{1}{47}\bigl[95\exp(-2x) - 48\exp(-96x)\bigr], \\ v_1(x) &= \frac{1}{47}\bigl[48\exp(-96x) - \exp(-2x)\bigr]. \end{aligned} \tag{35}$$

Problem 4 *We consider the stiff system of first-order ODEs known as the Kaps problem taken from* [31]:

$$\begin{aligned} u_1'(x) &= -1002u_1(x) + 1000v_1(x), \qquad u_1(0) = 1, \\ v_1'(x) &= u_1(x) - v_1(x)\bigl(1 + v_1(x)\bigr), \qquad v_1(0) = 1, \end{aligned} \tag{36}$$

where $x \in [0, 5]$. The exact solution of the above system is

$$\begin{aligned} u_1(x) &= \exp(-2x), \\ v_1(x) &= \exp(-x). \end{aligned} \tag{37}$$

Problem 5 *Consider the following nonlinear third-order ODE known as the Blasius equation of boundary layer flow taken from* [44]:

$$2\frac{d^3u_1(x)}{dv_1^3} + u_1(x)\frac{d^2u_1(x)}{dv^2} = 0, \quad u_1(0) = 0, u_1'(0) = 0, u_1''(0) = 1. \tag{38}$$

The above nonlinear equation can be rewritten as a system of three first-order ODEs as shown below:

$$\begin{aligned} u_1'(x) &= v_1(x), \quad u_1(0) = 0, \\ v_1'(x) &= w_1(x), \quad v_1(0) = 0, \\ w_1'(x) &= -\frac{1}{2}u_1(x)w_1(x), \quad w_1(0) = 1. \end{aligned} \tag{39}$$

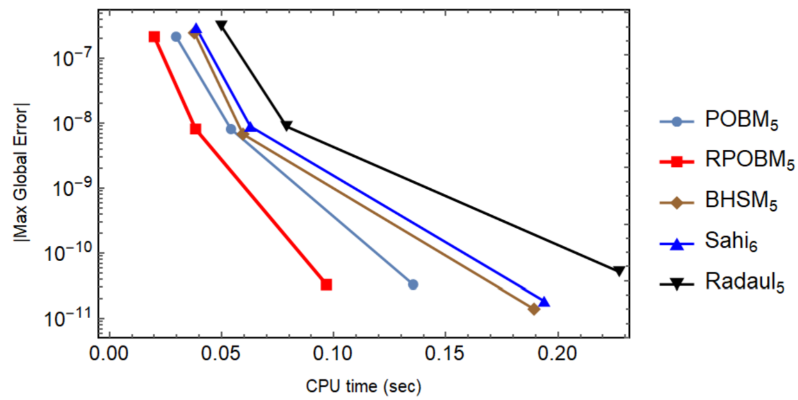

Figure 3 Efficiency curves of the maximum absolute global errors versus CPU times (s) for highly stiff IVP of the flame propagation given in the numerical experiment 1 with tolerance = 10^{-i}, $i = 7, 9, 11$

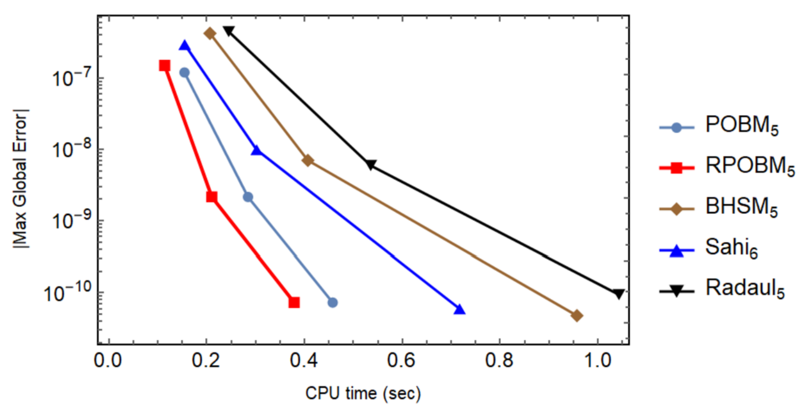

Figure 4 Efficiency curves of the maximum absolute global errors versus CPU times (s) for highly stiff IVP of the flame propagation given in the numerical experiment 1 with tolerance = 10^{-i}, $i = 7, 9, 11$

The reference solution of (38) *accurate to* 30 *dp is given at the final mesh point* $x = 10$ *as follows*:

$$\begin{pmatrix} u_1(x) \\ v_1(x) \\ w_1(x) \end{pmatrix}\Bigg|_{x=10} = \begin{pmatrix} 18.3691116226371336823274858370457809984710907345 82 \\ 2.0854091764379035978623786489081898250823577485323 \\ 1.9055567124740834810772164777626634323571010482536 \times 10^{-18} \end{pmatrix}.$$

5 Concluding remarks

This study presents a new one-step hybrid block approach with three intra-step points, including one optimally determined from the proposed method's local truncation error. The order of accuracy, consistency, zero-stability, convergence, $\mathcal{A}$-stability, and the theory of order stars are all thoroughly discussed. When the suggested technique was tried on certain tough models from applied sciences, the accuracy results were encouraging.

Furthermore, the inclusion of an efficiency plot comparing the errors of the proposed and existing numerical approaches in terms of computing cost for an increasing number of grid points supports reformulation of the suggested method. Future research will focus on the fully implicit block approach with three optimal intra-step points. This will lead to a technique that is truly optimal and is easy to rewrite in a computer. The field of fractional calculus [45–50] has additional opportunities to supplement the current study. The proposed hybrid block method can be changed so that it can be used to solve initial value problems of fractional order.

Appendix

Algorithm 1: Pseudocode for the optimal one-step $\mathcal{A}$-stable block method

Data: x_0, T (integration interval), N (number of steps), y_{00}, y_{10} (initial values), f.

Result: sol (discrete approximate solution of the IVP (1)).

Let $n = 0,\ \Delta x = \frac{T - x_0}{N}$.
Let $x_n = x_0, y_n = y_{00}, y'_n = y_{10}$.
Let **sol** $= \{(x_n, y_n)\}$.
Solve (16) to obtain y_{n+k}, y'_{n+k}, where $k = 0, u, v, w, 1$.
Let **sol** = **sol** $\cup \{(x_{n+k}, y_{n+k})\}_{k=0,u,v,w,1}$.
Let $x_n = x_n + \Delta x, y_n = y_{n+1}, y'_n = y'_{n+1}$.
Let $n = n + 1$,
if $n = N$ **then**
    go to 13
else
    go to 4;
end
End

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Ethics approval and consent to participate
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Consent to participate
Each author has approved of and agreed to submit the article.

Consent for publication
Each author agreed to publish the article.

Competing interests
The authors declare no competing interests.

Author contributions
The first, second and third authors have conceived the idea and derived the proposed optimized block method. The first and second author has supervised the entire work and guided, whereas the fourth author carried out a theoretical analysis of the proposed method. Finally, the fifth author performed numerical simulations. Each author equally contributed towards writing and finalizing the article.

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