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Time-efficient reformulation of the Lobatto III family of order eight

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ABSTRACT

Implicit block methods for solving initial value problems in ordinary differential equations are well-known among the contemporary scientific community, since they are cost-effective, self-starting, consistent, stable, and usually converge fast when applied to solve particularly stiff models. These characteristics of block methods are the primary reasons for the one-step optimized block method devised in the present research study with three off-grid points. Theoretical analysis, including the order of convergence, consistency, zero-stability, $\mathcal{A}$-stability, order stars, and the local truncation error, are considered. The obtained method may be categorized as the well-known Lobatto IIIA Runge–Kutta method. The superiority of the devised method over various existing approaches having similar features is proved via numerical simulations of stiff and nonlinear differential systems. Furthermore, a suitable reformulation of the devised method results in considerable savings in computation time, as revealed through the efficiency plots. This turns out in a strategy to reformulate Runge–Kutta type methods in order to get a better performance.

1. Introduction

Initial value problems of the form

$$y'(x) = f(x, y(x)),\ \ y(x_0) = y_0,\ x \in [x_0, X],\ y(x) \in \mathbb{R}^n,\ f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n \quad (1)$$

frequently appear in almost every field of science. This is evident from various models, based on ordinary differential equations, being proposed to comprehend transmission dynamics of the corona-virus pandemic [1], reaction-rate equations [2], exponential growth/decay [3], van der Pol oscillator [4], nonlinear corneal shape model [5], mechanical system with variable mass [6], double pendulum [7], and many more. The non-linearity and stiff nature of some models pose challenges for applied mathematicians to come up with effective strategies to obtain approximate solutions with acceptable accuracy within reasonable computational time. In the pursuit of such strategies, various numerical methods have been devised in the literature, including explicit/implicit Runge–Kutta methods, Adams–Bashforth/Moulton methods, multi-derivative methods, rational/nonlinear methods, and block methods. Due to its self-starting nature and overcoming the overlapping of piecewise solutions, block methods have been quite popular among the scientific community of numerical analysts. These methods, which contain main and additional formulas, are useful to obtain the approximate solution at more than one point at a time as observed in [8–12]. Several block methods have recently been devised in the literature, including one-, two-, and three-step block methods for solving first-order ordinary differential equations. Nonetheless, very few of these methods consider an adequate strategy for choosing the off-grid points used.

Keeping in view the frequent use and high demand for computationally efficient block methods, we attempt to devise a one-step block method using three off-grid points with interpolation and collocation techniques, while the resulting method is optimized under the first three terms of the local truncation error of the main formula. Although some of these optimized block methods have been proposed recently by some researchers [13,14], they are either computationally expensive, or have lower order of convergence, or they are good enough only for particular types of initial value problems.

The present research design is set as follows: the derivation of the new optimized one-step block method with three off-grid points is carried out in Section 2 wherein the optimization strategy is discussed in detail, and the reformulation of the proposed method including its implicit Runge–Kutta structure has been shown. The theoretical investigation of the method, including accuracy, consistency, zero-stability, convergence, linear stability, and order stars, is performed in Section 3 and its subsequent subsections. We have considered some challenging differential models taken from several areas of applied

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sciences, where the numerical results have been obtained under the proposed method and other methods with similar characteristics in Section 4. Final remarks with some future directions are stated in Section 5.

2. Derivation of the optimized block method

The one-step optimized block method with three off-grid points is derived in this section where the off-grid points are optimized through the local truncation error of the main formula. Let us consider the partition $x_0 < x_1 < \cdots < x_M = X$ on the integration interval $[x_0, X]$, with constant step-length $\Delta x = x_{k+1} - x_k$, $k = 0, 1, \ldots, M-1$, and assume that on a generic subinterval $[x_n, x_{n+1}]$ the true solution $y(x)$ of (1) can be approximated by a polynomial $L(x)$ in the following form

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

where $\gamma_j \in \mathbb{R}$ stand for real undetermined parameters.

Differentiation of Eq. (2) produces the following

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

Consider three off-grid points, $x_{n+r} = x_n + r\Delta x, x_{n+s} = x_n + s\Delta x, x_{n+u} = x_n + u\Delta x$ with $0 < r < s < u < 1$, to compute the approximate solution of the IVP (1) at the point x_{n+1}, assuming that $y_n = y(x_n)$. It is worth noting at this stage that the optimal values of these three off-grid points will be determined with the help of the local truncation error of the main formula. To start the procedure, consider the approximation in (2) determined at x_n, and its first-order derivative determined at the points $x_n, x_{n+r}, x_{n+s}, x_{n+u}, x_{n+1}$. By so doing, we obtain the following linear system of six equations in six real unknown parameters γ_j, $j = 0, 1, \ldots, 5$:

$$\begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 \\ 0 & 1 & 2x_n & 3x_n^2 & 4x_n^3 & 5x_n^4 \\ 0 & 1 & 2x_{n+r} & 3x_{n+r}^2 & 4x_{n+r}^3 & 5x_{n+r}^4 \\ 0 & 1 & 2x_{n+s} & 3x_{n+s}^2 & 4x_{n+s}^3 & 5x_{n+s}^4 \\ 0 & 1 & 2x_{n+u} & 3x_{n+u}^2 & 4x_{n+u}^3 & 5x_{n+u}^4 \\ 0 & 1 & 2x_{n+1} & 3x_{n+1}^2 & 4x_{n+1}^3 & 5x_{n+1}^4 \end{pmatrix} \begin{pmatrix} \gamma_0 \\ \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \gamma_4 \\ \gamma_5 \end{pmatrix} = \begin{pmatrix} y_n \\ f_n \\ f_{n+r} \\ f_{n+s} \\ f_{n+u} \\ f_{n+1} \end{pmatrix} \tag{4}$$

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

$$L(x_n + t\Delta x) = \gamma_0 y_n + \Delta x\left(\zeta_0 f_n + \zeta_r f_{n+r} + \zeta_s f_{n+s} + \zeta_u f_{n+u} + \zeta_1 f_{n+1}\right), \tag{5}$$

where

$$\begin{aligned}
\gamma_0 &= 1,\\
\zeta_0 &= \frac{t\begin{pmatrix} 20rst^2 - 30rstu - 15rt^3 + 20rt^2u - 15st^3 + 20st^2u + 12t^4 - 15t^3u \\ -30rst + 60rsu + 20rt^2 - 30rtu + 20st^2 - 30stu - 15t^3 + 20t^2u \end{pmatrix}}{60rsu},\\
\zeta_r &= -\frac{t^2(15st^2 - 20stu - 12t^3 + 15t^2u - 20st + 30su + 15t^2 - 20tu)}{60(r-1)(r-u)(r-s)r},\\
\zeta_s &= \frac{t^2(20rst - 15rt^2 - 15st^2 + 12t^3 - 30rs + 20rt + 20st - 15t^2)}{60(s-1)(s-u)(r-s)s},\\
\zeta_u &= \frac{t^2(20uvt - 15ut^2 - 15vt^2 + 12t^3 - 30uv + 20ut + 20vt - 15t^2)}{60(u-1)(s-u)(r-u)u},\\
\zeta_1 &= -\frac{t^2(20rst - 30rsu - 15rt^2 + 20rtu - 15st^2 + 20stu + 12t^3 - 15t^2u)}{60(u-1)(s-1)(r-1)}.
\end{aligned} \tag{6}$$

To get the one-step block method we evaluate $L(x_n + t\Delta x)$ at the collocation points x_{n+r}, x_{n+s}, x_{n+u}, and x_{n+1}, that is, we take $t = r, s, u, 1$ in (5). This results in the following four formulas:

$$\begin{aligned}
y_{n+r} = y_n + \frac{\Delta x}{60} &\times \Bigg(\frac{-3r^4 + 5r^3s + 5r^3u - 10r^2su + 5r^3 - 10r^2s - 10r^2u + 30rsu}{su} f_n \\
&- \frac{r(-12r^3 + 15r^2s + 15r^2u - 20rsu + 15r^2 - 20rs - 20ru + 30su)}{(r-1)(r-u)(r-s)} f_{n+r} \\
&+ \frac{r^2(-3r^3 - 5r^2u - 5r^2 + 10ru)}{(s-1)(s-u)(r-s)s} f_{n+s} \\
&+ \frac{r^2(-3r^3 + 5r^2s + 5r^2 - 10rs)}{(u-1)(s-u)(r-u)u} f_{n+u} \\
&- \frac{r^2(-3r^3 + 5r^2s + 5r^2u - 10rsu)}{(u-1)(s-1)(r-1)} f_{n+1} \Bigg),
\end{aligned} \tag{7}$$

$$\begin{aligned}
y_{n+s} = y_n + \frac{\Delta x}{60} \Bigg(&\frac{5rs^3 - 10rs^2u - 3s^4 + 5s^3u - 10rs^2 + 30rsu + 5s^3 - 10s^2u}{ru} f_n \\
&- \frac{s^2(3s^3 - 5s^2u - 5s^2 + 10su)}{(r-1)(r-u)(r-s)r} f_{n+r} \\
&+ \frac{s(15rs^2 - 20rsu - 12s^3 + 15s^2u - 20rs + 30ru + 15s^2 - 20su)}{(s-1)(s-u)(r-s)} f_{n+s} \\
&+ \frac{s^2(5rs^2 - 3s^3 - 10rs + 5s^2)}{(u-1)(s-u)(r-u)u} f_{n+u} - \frac{s^2(5rs^2 - 10rsu - 3s^3 + 5s^2u)}{(u-1)(s-1)(r-1)} f_{n+1} \Bigg),
\end{aligned} \tag{8}$$

$$\begin{aligned}
y_{n+u} = y_n + \frac{\Delta x}{60} \Bigg(&\frac{-10rsu^2 + 5ru^3 + 5su^3 - 3u^4 + 30rsu - 10ru^2 - 10su^2 + 5u^3}{rs} f_n \\
&- \frac{u^2(-5su^2 + 3u^3 + 10su - 5u^2)}{(r-1)(r-u)(r-s)r} f_{n+r} + \frac{u^2(-5ru^2 + 3u^3 + 10ru - 5u^2)}{(s-1)(s-u)(r-s)} f_{n+s} \\
&+ \frac{u(20rsu - 15ru^2 - 15su^2 + 12u^3 - 30rs + 20ru + 20su - 15u^2)}{(u-1)(s-u)(r-u)} f_{n+u} \\
&- \frac{u^2(-10rsu + 5ru^2 + 5su^2 - 3u^3)}{(u-1)(s-1)(r-1)} f_{n+1} \Bigg),
\end{aligned} \tag{9}$$

$$\begin{aligned}
y_{n+1} = y_n + \frac{\Delta x}{60} \Bigg(&\frac{30rsu - 10rs - 10ru - 10su + 5r + 5s + 5u - 3}{rsu} f_n \\
&- \frac{(10su - 5s - 5u + 3)}{(r-1)(r-u)(r-s)r} f_{n+r} + \frac{(10ru - 5r - 5u + 3)}{(s-1)(s-u)(r-s)s} f_{n+s} + \frac{(-10rs + 5r + 5s - 3)}{(u-1)(s-u)(r-u)u} f_{n+u} \\
&- \frac{(-30rsu + 20rs + 20ru + 20su - 15r - 15s - 15u + 12)}{(u-1)(s-1)(r-1)} f_{n+1} \Bigg),
\end{aligned} \tag{10}$$

where the y_{n+i} are approximations of the true solution $y(x_n + i\Delta x)$, and $f_{n+i} = f(x_{n+i}, y_{n+i})$, for $i = r, s, u, 1$. In the above-obtained approximations, three unknown parameters r, s, u, are concerned with the three off-grid points x_r, x_s, x_u. To get suitable values of these parameters, we will set the first three terms of the local truncation error (LTE) of the formula in (10) equal to zero. By so doing, optimal values of the parameters will be obtained, and 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 subinterval. Hence, via Taylor expansions, we consider the local truncation error of the formula given in (10), which is given by:

$$\begin{aligned}
\mathcal{L}(y(x_{n+1}); \Delta x) = &\left(\frac{1}{7200}((10u - 5)s - 5u + 3)r + \frac{1}{7200}(-5u + 3)s + \frac{1}{2400}u - \frac{1}{3600} \right) \\
&\times \Delta x^6 y^{(6)}(x_n) \\
&+ \left(\begin{aligned} &\frac{1}{302400}((70u - 35)s - 35u + 21)r^2 + \frac{1}{4320}((u - \tfrac{1}{2})s - \tfrac{u}{2} + \tfrac{3}{10})(s + u + 1)r \\ &+ \frac{1}{30240}(-35u + 21)s^2 + \frac{1}{302400}(-35u^2 - 14u + 21)s + \frac{u^2}{14400} + \frac{u}{14400} - \frac{1}{12600} \end{aligned} \right) \\
&\times \Delta x^7 y^{(7)}(x_n) \\
&+ \left(\begin{aligned} &\frac{1}{604800}((20u - 10)s - 10u + 6)r^3 + \frac{1}{30240}((u - \tfrac{1}{2})s - \tfrac{u}{2} + \tfrac{3}{10})(s + u + 1)r^2 \\ &+ \frac{1}{30240}((u - \tfrac{1}{2})s - \tfrac{u}{2} + \tfrac{3}{10})(s^2 + (u + 1)s + u^2 + u + 1)r - \frac{1}{604800}(-10u + 6)s^3 \\ &+ \frac{1}{604800}(-10u^2 - 4u + 6)s^2 + \frac{1}{604800}(-10u^3 - 4u^2 - 4u + 6)s \\ &+ \frac{u^3}{100800} + \frac{u^2}{100800} + \frac{u}{100800} - \frac{1}{67200} \end{aligned} \right)
\end{aligned}$$

$$\times \Delta x^8 y^{(8)}(x_n) + \mathcal{O}(\Delta x^9). \tag{11}$$

Using a standard strategy used in several other methods dealing with numerical solutions of partial differential equations [15–17], we set the coefficients of Δx^6, Δx^7, and Δx^8 equal to zero and obtain, after solving the resulting algebraic system, the following optimal values of the parameters:

$$r = \frac{1}{2} - \frac{\sqrt{21}}{14}, \quad s = \frac{1}{2}, \quad u = \frac{1}{2} + \frac{\sqrt{21}}{14}. \tag{12}$$

Substituting these values in the LTE, we obtain

$$\mathcal{L}(y(x_{n+1}); \Delta x) = -\frac{\left(\Delta x\right)^9 y^{(9)}(x_n)}{1422489600} + \mathcal{O}(\Delta x^{10}). \tag{13}$$

Thus, the obtained parameters yielded the following one-step optimized block method with three off-grid points (the pseudo-code for the method is provided in Appendix):

$$\begin{aligned}
y_{n+r} &= y_n + \frac{\Delta x}{4410 + 630\sqrt{21}} \begin{bmatrix} (45\sqrt{21}+288) f_n + (70\sqrt{21}+553) f_{n+r} \\ +(-80\sqrt{21}+208) f_{n+s} \\ +(-35\sqrt{21}+238) f_{n+u} - 27 f_{n+1} \end{bmatrix}, \\
y_{n+s} &= y_n + \Delta x \begin{bmatrix} \frac{13}{320} f_n + \left(\frac{7\sqrt{21}}{192} + \frac{49}{360}\right) f_{n+r} \\ + \frac{8}{45} f_{n+s} + \left(\frac{-7\sqrt{21}}{192} + \frac{49}{360}\right) f_{n+u} + \frac{3}{320} f_{n+1} \end{bmatrix}, \\
y_{n+u} &= y_n + \frac{\Delta x}{-4410 + 630\sqrt{21}} \begin{bmatrix} (-45\sqrt{21} - 288) f_n \\ +(-35\sqrt{21} - 238) f_{n+r} \\ +(-80\sqrt{21} - 208) f_{n+s} \\ +(70\sqrt{21} - 553) f_{n+u} + 27 f_{n+1} \end{bmatrix}, \\
y_{n+1} &= y_n + \Delta x \left[\frac{1}{20} f_n + \frac{49}{180} f_{n+r} + \frac{16}{45} f_{n+s} + \frac{49}{180} f_{n+u} + \frac{1}{20} f_{n+1}\right].
\end{aligned} \tag{14}$$

It is worth noting that the reformulation of the above proposed optimized block method produces substantial savings in the computational cost. The idea of reformulation is based on the strategy proposed by Ramos in [18]. The saving in the computational time comes from the fact that the number of occurrences of the values f_{n+i} is reduced, as shown below:

$$\begin{aligned}
\Delta x f_{n+r} &= \begin{bmatrix} \left(-\frac{3}{14}\sqrt{21} - \frac{81}{14}\right) y_n + \left(\frac{1}{2}\sqrt{21} + \frac{7}{2}\right) y_{n+r} \\ + \left(\frac{16}{21}\sqrt{21} - \frac{16}{7}\right) y_{n+s} + \left(-\frac{5}{6}\sqrt{21} + \frac{7}{2}\right) y_{n+u} \\ + \left(-\frac{3}{14}\sqrt{21} + \frac{15}{14}\right) y_{n+1} - \frac{3\Delta x}{7} f_n \end{bmatrix}, \\
\Delta x f_{n+s} &= \begin{bmatrix} \frac{9}{2} y_n + \left(-\frac{49}{48}\sqrt{21} - \frac{49}{16}\right) y_{n+r} + 2 y_{n+s} \\ + \left(\frac{49}{48}\sqrt{21} - \frac{49}{16}\right) y_{n+u} - \frac{3}{8} y_{n+1} + \frac{3\Delta x}{8} f_n \end{bmatrix}, \\
\Delta x f_{n+u} &= \begin{bmatrix} \left(-\frac{81}{14} + \frac{3}{14}\sqrt{21}\right) y_n + \left(\frac{7}{2} + \frac{5}{6}\sqrt{21}\right) y_{n+r} \\ + \left(-\frac{16}{7} - \frac{16}{21}\sqrt{21}\right) y_{n+s} + \left(\frac{7}{2} - \frac{1}{2}\sqrt{21}\right) y_{n+u} \\ + \left(\frac{15}{14} + \frac{3}{14}\sqrt{21}\right) y_{n+1} - \frac{3\Delta x}{7} f_n \end{bmatrix}, \\
\Delta x f_{n+1} &= \left[11 y_n - \frac{49}{3} y_{n+r} + \frac{32}{3} y_{n+s} - \frac{49}{3} y_{n+u} + 11 y_{n+1} + \Delta x f_n\right].
\end{aligned} \tag{15}$$

The above reformulation is later abbreviated as ROBM in the forthcoming sections. Moreover, the implicit Runge–Kutta structure of the optimized block method (14) is also presented by means of the usual Butcher tableau as follows (see Table 1):

It is worth mentioning, at this point, that the generalization of the devised approach to higher-order methods is possible with the choice of more than three off-grid points, however, the computational complexity may increase with an increase of the convergence order. Other possibilities for the improvement include two- and three-step block methods with increasing number of off-grid points.

3. Theoretical analysis

The theoretical characteristics for the one-step optimized block method with three off-grid points given in (14) or equivalently (15) are addressed in this section that contains order of accuracy, consistency, zero-stability, convergence, linear stability, and the theory of order stars.

3.1. Order of accuracy and consistency

The one-step optimized block method with three off-grid points given in (14) can be rewritten using the matrix notation as follows:

$$A_1 Y_{n+1} = A_0 Y_n + h(B_0 F_n + B_1 F_{n+1}), \tag{16}$$

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

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

$$B_0 = \begin{bmatrix} 0 & 0 & 0 & \frac{45\sqrt{21}+288}{630\sqrt{21}+4410} \\ 0 & 0 & 0 & \frac{13}{320} \\ 0 & 0 & 0 & \frac{45\sqrt{21}-288}{630\sqrt{21}-4410} \\ 0 & 0 & 0 & \frac{1}{20} \end{bmatrix}, \tag{17}$$

$$B_1 = \begin{bmatrix} \frac{70\sqrt{21}+553}{4410+630\sqrt{21}} & \frac{-80\sqrt{21}+208}{4410+630\sqrt{21}} & \frac{-35\sqrt{21}+238}{4410+630\sqrt{21}} & \frac{-27}{4410+630\sqrt{21}} \\ \frac{49}{360} + \frac{7\sqrt{21}}{192} & \frac{8}{45} & \frac{49}{360} - \frac{7\sqrt{21}}{192} & \frac{3}{320} \\ \frac{-35\sqrt{21}-238}{-4410+630\sqrt{21}} & \frac{-80\sqrt{21}-208}{-4410+630\sqrt{21}} & \frac{70\sqrt{21}-553}{-4410+630\sqrt{21}} & \frac{27}{-4410+630\sqrt{21}} \\ \frac{49}{180} & \frac{16}{45} & \frac{49}{180} & \frac{1}{20} \end{bmatrix}, \tag{18}$$

and

$$\begin{aligned}
Y_n &= (y_{n-1+r}, y_{n-1+s}, y_{n-1+u}, y_n)^T, \\
Y_{n+1} &= (y_{n+r}, y_{n+s}, y_{n+u}, y_{n+1})^T, \\
F_n &= (f_{n-1+r}, f_{n-1+s}, f_{n-1+u,} f_n)^T, \\
F_{n+1} &= (f_{n+r}, f_{n+s}, f_{n+u}, f_{n+1})^T.
\end{aligned} \tag{19}$$

The linear functional operator associated with the proposed block method (14) can be defined as:

$$\bar{\mathcal{L}}[J(x_n); \Delta x] = \sum_{k=0,r,s,u,1} \left[\bar{\gamma}_k J(x_n + k\Delta x) - \Delta x \bar{\eta}_k J'(x_n + k\Delta x)\right], \tag{20}$$

where $\bar{\gamma}_k$, and $\bar{\eta}_k$ are respectively the vector columns of the matrices A_1 and A_0. The expression $J(x)$ stands for an arbitrary test function

Table 1
The Butcher tableau for the implicit Runge-Kutta structure of the optimized block method given in Eq. (14).

0	0	0	0	0	0
$\frac{1}{2}-\frac{\sqrt{21}}{14}$	$\frac{288+45\sqrt{21}}{4410+630\sqrt{21}}$	$\frac{553+70\sqrt{21}}{4410+630\sqrt{21}}$	$\frac{208-80\sqrt{21}}{4410+630\sqrt{21}}$	$\frac{238-35\sqrt{21}}{4410+630\sqrt{21}}$	$\frac{-27}{4410+630\sqrt{21}}$
$\frac{1}{2}$	$\frac{13}{320}$	$\frac{49}{360}+\frac{7\sqrt{21}}{192}$	$\frac{8}{45}$	$\frac{49}{360}-\frac{7\sqrt{21}}{192}$	$\frac{3}{320}$
$\frac{1}{2}+\frac{\sqrt{21}}{14}$	$\frac{-288+45\sqrt{21}}{-4410+630\sqrt{21}}$	$\frac{-238-35\sqrt{21}}{-4410+630\sqrt{21}}$	$\frac{-208-80\sqrt{21}}{-4410+630\sqrt{21}}$	$\frac{-553+70\sqrt{21}}{-4410+630\sqrt{21}}$	$\frac{27}{-4410+630\sqrt{21}}$
1	$\frac{1}{20}$	$\frac{49}{180}$	$\frac{16}{45}$	$\frac{49}{180}$	$\frac{1}{20}$
1	$\frac{1}{20}$	$\frac{49}{180}$	$\frac{16}{45}$	$\frac{49}{180}$	$\frac{1}{20}$

taken to be sufficiently differentiable on the integration interval. The proposed optimized block method (14) and the corresponding linear difference operator are said to have at least order p if after expanding the terms $J(x_n+k\Delta x)$, and $J'(x_n+k\Delta x)$ in the Taylor's series about x_n, and collecting the coefficients of Δx, we get the following:

$$\bar{\mathcal{L}}[J(x_n);\Delta x]=\bar{P}_0J(x_n)+\bar{P}_1\Delta xJ'(x_n)+\bar{P}_2\Delta x^2J''(x_n)+\cdots+\bar{P}_i\Delta x^iJ^{(i)}(x_n)+\cdots \tag{21}$$

with $\bar{P}_0=\bar{P}_1=\cdots=\bar{P}_p=0$ and $\bar{P}_{p+1}\neq 0$. The coefficients $\bar{P}_i$ are vectors and $\bar{P}_{r+1}$ is said to be the vector of error constants. For the proposed optimized block method (14), we achieve $\bar{P}_0=\bar{P}_1=\cdots=\bar{P}_5=0$ whereas the vector of error constants is

$$\bar{P}_6=\left(-\frac{1}{987840}\frac{(\sqrt{21}+5)(\sqrt{21}-7)}{\sqrt{21}+7},\right.\\ \left.-\frac{1}{322560},\frac{(\sqrt{21}-5)(\sqrt{21}+7)}{987840\sqrt{21}-6914880},0\right)^T. \tag{22}$$

Hence, it has been proved from the above discussion that each of the formulas of the proposed optimized block method with three off-grid points given in (14) does possess at least a fifth order of accuracy. Using the equivalent formulation as Runge–Kutta method, we identify this method as the Lobatto IIIA method with 5 stages, which is known to have eight order. On this basis, the method (14) is considered to be consistent with the IVP (1).

3.2. Zero-stability and convergence

A significant requirement for a numerical method to be reliable is the requirement of zero-stability. Let the IVP in (1) be asymptotically stable, while the requirement is to show the stability of the proposed one-step optimized block method with three off-grid points given in (14). The concept of zero-stability relates to considering a homogeneous equation $y'=0$ and its discretized version, as written below:

$$A_0Y_{\lambda+1}-A_1Y_\lambda=0, \tag{23}$$

where A_0 and A_1 are the matrices shown earlier. Now, if the discrete algebraic Eq. (23) admits solutions which 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 the 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 should not exceed 1 [19]. The first characteristic polynomial of the proposed block method (14) is given by

$$\kappa(R)=R^3(R-1). \tag{24}$$

Hence, the proposed method with three off-grid points given in (14) is a zero-stable method. Being both zero-stable and consistent (as claimed by Jator in [20]), it results to be a convergent numerical method.

3.3. Linear stability analysis and order stars

Theorem 1. *The proposed one-step optimized block method with three off-grid points given in (14) is $\mathcal{A}-stable$.*

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-length $\Delta x\rightarrow 0$. In other cases, nonetheless, a different concept of stability is needed from a practical point of view, and that is related with a numerical method when it produces acceptable results for a particular value for the step-length $\Delta x>0$. Such behavior is called the linear stability behavior for the numerical method under consideration, and it requires to apply the method on a linear test problem, as the one introduced by Dahlquist [21] given by:

$$y'(x)=\mu y(x),\ \text{with}\ Re(\mu)<0. \tag{25}$$

It is required to determine the region within which the approximations obtained under the numerical method reproduce the behavior of the exact solution of the linear test problem given in (25). Having applied the proposed optimized block method in (14) to the linear test problem in (25), it turns out to get the recurrence equation:

$$Y_n=M(z)Y_{n-1}, \tag{26}$$

where $M(z)$ stands for the so-called stability matrix defined by

$$M(z)=(A_1-zB_1)^{-1}(A_0+zB_0),\ z=\mu\Delta x. \tag{27}$$

The eigenvalues of the stability matrix (27) determine the behavior of the approximate numerical solution. This is a commonly known stability property of a numerical method that uses the spectral radius also known as the maximum of the absolute values of the eigenvalues of $M(z)$. The region of absolute linear stability $\mathbb{A}$ is described by the following set as suggested in [22]:

$$\mathbb{A}=\{z\in\mathbb{C}:\rho[M(z)]<1\}, \tag{28}$$

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

$$\rho[M(z)]=\frac{z^4+20z^3+180z^2+840z+1680}{z^4-20z^3+180z^2-840z+1680}.\quad\square \tag{29}$$

The above stability function $\rho[M(z)]$ can be obtained if the proposed optimized block method (14) is applied to the linear test problem given in (25) while the same approach is used in several recent research works including [9–11] for the determination of such stability functions.

Remark 1. The graphical explanations given by Fig. 1 reveal that the whole left-half complex plane as denoted by $\mathbb{C}^-$ is included in the stability region of the optimized block method in (14). Such sort of $\mathcal{A}$–stability is further confirmed with the plot of order stars wherein it can be observed that the rational stability function given in (29) does not have any kind of pole in the region containing $\mathbb{C}^-$ as can be visualized

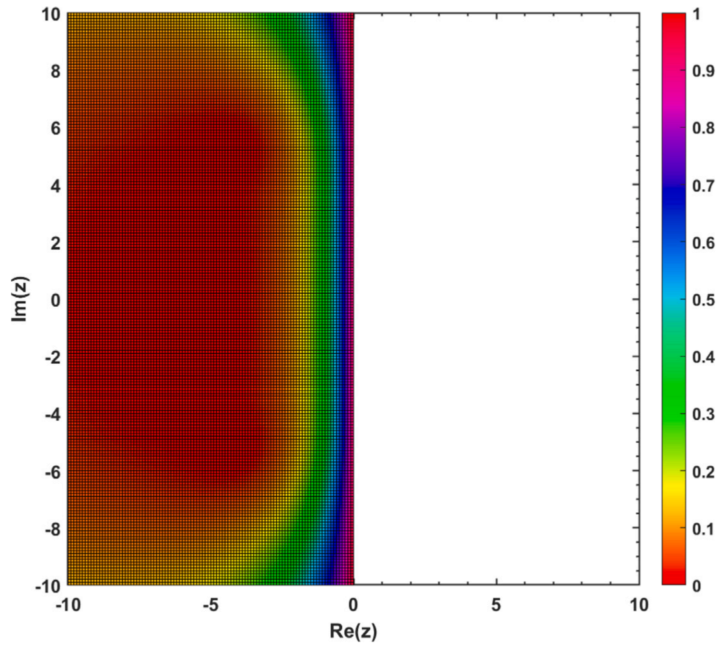

Fig. 1. Region of absolute stability of the proposed one-step optimized block method with three off-grid points given in (14).

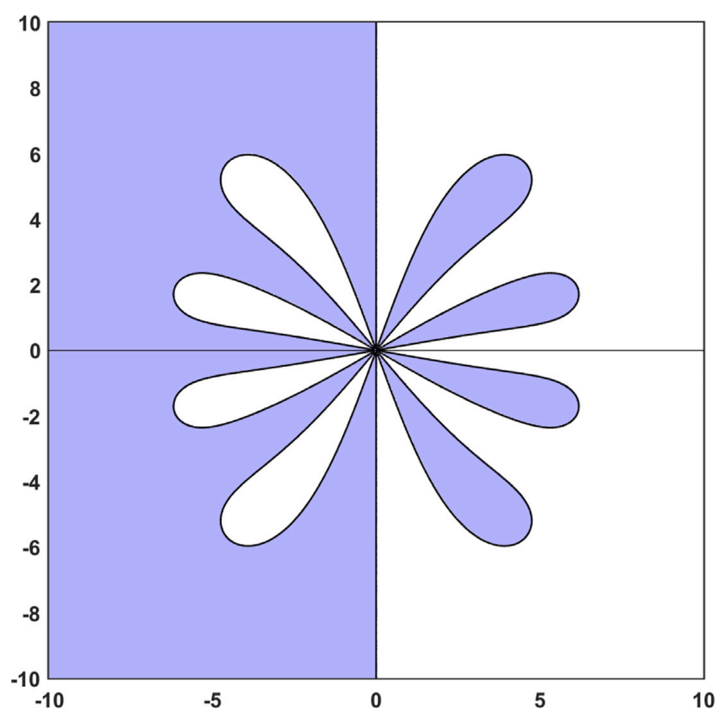

Fig. 2. The plot of order stars for the proposed one-step optimized block method with three off-grid points given in (14).

in Fig. 2 for the un-shaded region that appears on the left-half complex plane $\mathbb{C}^-$.

4. Numerical dynamics with results and discussion

This section shows the performance of the proposed one-step optimized block method given in (14) for solving different kinds of stiff problems. The method neither requires multiple initial conditions to start nor needs any predictor. While taking $n = 0$, the method (14) taken as a system is simultaneously solved with $y(x_0) = y_0$ known. We have employed the frequently used second-order convergent Newton–Raphson technique to obtain y_1 having solved the system. Next, the value y_2 is determined by considering y_1 from the previous block as the initial value, and the process continues until the end point x_M is reached. Since the proposed method is one-step and some of the methods used for comparisons are two-step methods, we have chosen the length of integration interval as a multiple of $2\Delta x$ (that is, $x_M - x_0 = k(2\Delta x)$, $k \in \mathbb{N}$). The FindRoot command from Mathematica 12.1 has been used to implement the Newton–Raphson method. It may be

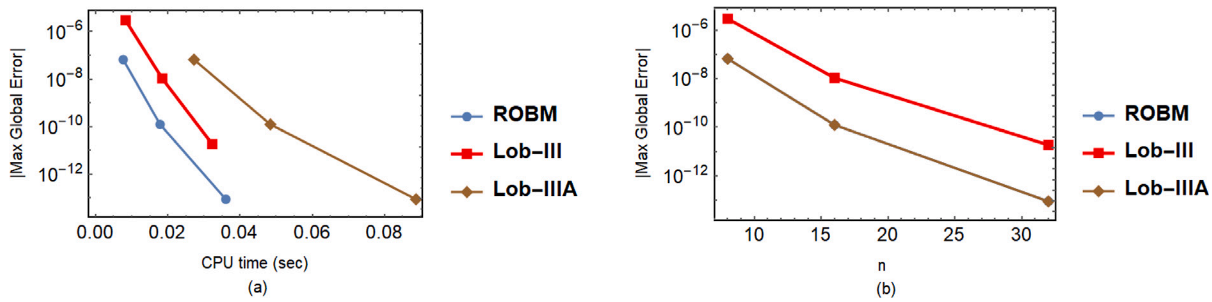

Fig. 3. Efficiency curves for the IVP in Problem 1 to observe the behavior of (a) absolute maximum global errors versus the CPU time (sec), and (b) absolute maximum global errors versus number of steps $n \in \{2^3, 2^4, 2^5\}$.

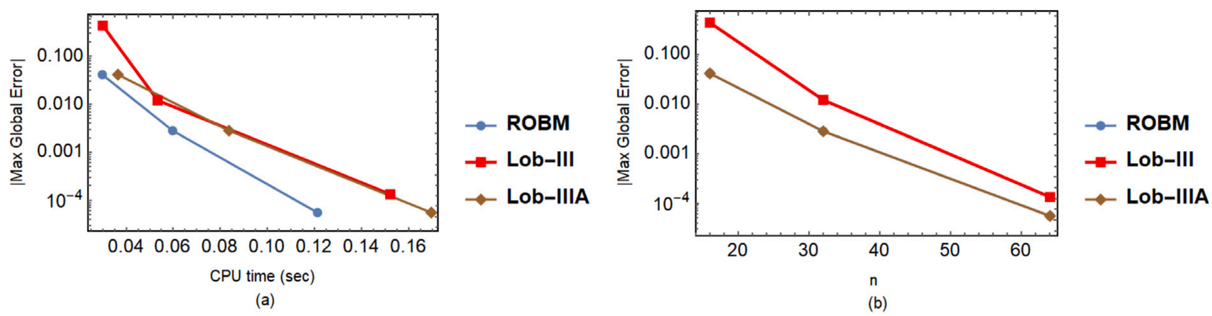

Fig. 4. Efficiency curves for the IVP in Problem 2 to observe the behavior of (a) absolute maximum global errors versus the CPU time (sec), and (b) absolute maximum global errors versus number of steps $n \in \{2^4, 2^5, 2^6\}$.

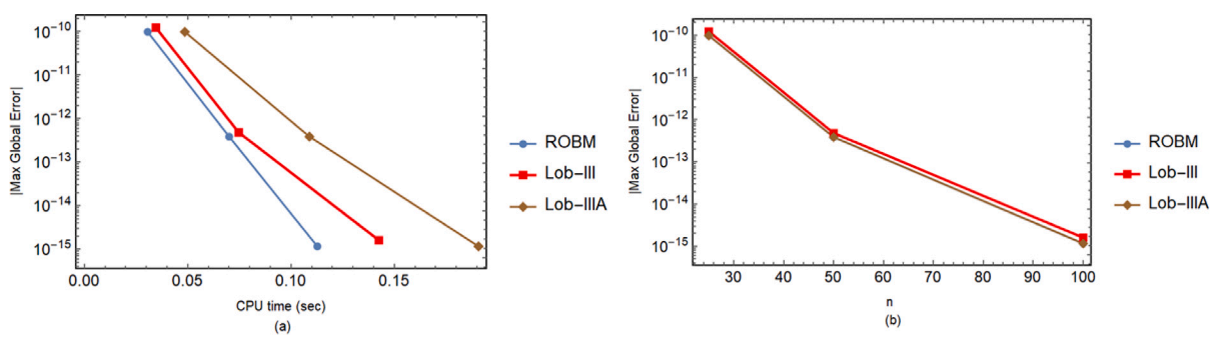

Fig. 5. Efficiency curves for the IVP in Problem 3 to observe the behavior of (a) absolute maximum global errors versus the CPU time (sec), and (b) absolute maximum global errors versus number of steps $n \in \{25, 50, 100\}$.

noted that all numerical computations are performed in Mathematica 12.1 on a personal computer running on Windows OS with Intel(R) Core(TM) i7-1065G7 CPU @ 1.30 GHz 1.50 GHz processor having 24.0 GB installed RAM. It may be noted that for comparison we have taken two methods of eighth-order with five stages from the Lobatto family of Runge–Kutta methods (Lobatto III & Lobatto IIIA) as given in [23, p 228].

Some numerical experiments are presented, being one scalar and the other higher dimensional systems. The tables collect the maximum absolute errors, ME; the error at the end point of the integration interval, LE; the average of absolute errors, AE; and the error with the L_2-norm, Norm, with the proposed ROBM and the Lob IIIA methods.

From the data given in Tables 2–6 one can see that the smaller values for the errors are obtained with the proposed ROBM and the Lob IIIA methods. The behavior shows that these methods are more robust from an accuracy viewpoint when compared with the Lob III method.

Furthermore, to better appreciate the performance of the methods, we have included two types of efficiency curves, the maximum absolute errors versus the computation time, and the maximum absolute errors versus the number of steps needed to solve the IVPs.

Since most of the errors in the reformulated method ROBM are very similar or coincide with the errors obtained with the Lob-IIIA, the corresponding curves in the right sides of Figs. 3–7 overlap. Nevertheless, the ROBM is found to be superior based on the computation time, as can be seen on the left sides of Figs. 3–7, where the ROBM method shows the best performance.

Problem 1. Consider the following nonlinear scalar IVP:

$$u'(x) = -10(u(x) - 1)^2, \ \ x \in [0, 1], \tag{30}$$

with the exact solution: $u(x) = 1 + \dfrac{1}{1 + 10x}$.

Problem 2. Consider the following two-dimensional stiff system [24]:

$$\begin{aligned} u'(x) &= 9u(x) + 24v(x) + 5\cos(x) - \frac{1}{3}\sin(x), \\ v'(x) &= -24u(x) - 51v(x) - 9\cos(x) + \frac{1}{3}\sin(x), \\ u(0) &= \frac{4}{3}, \ \ v(0) = \frac{2}{3}, \ \ x \in [0, 5], \end{aligned} \tag{31}$$

Table 2
Comparison of different methods based upon maximum error, last error, absolute error, Norm, number of function evaluations and CPU time (in seconds) of the IVP given in Problem 1, with increasing number of steps (n).

n	Methods	ME	LE	AE	Norm	CPU
8	ROBM	6.5886e−08	2.7583e−09	1.4937e−08	7.3957e−08	7.6444e−03
	Lob III	2.9253e−06	1.2256e−07	6.6346e−07	3.2842e−06	8.3177e−03
	Lob IIIA	6.5886e−08	2.7583e−09	1.4937e−08	7.3957e−08	2.7247e−02
16	ROBM	1.2411e−10	2.7300e−12	2.0468e−11	1.5161e−10	1.7860e−02
	Lob III	1.0611e−08	2.3517e−10	1.7579e−09	1.2992e−08	1.8445e−02
	Lob IIIA	1.2411e−10	2.7311e−12	2.0469e−11	1.5161e−10	4.8389e−02
32	ROBM	8.8152e−14	1.5543e−15	1.0598e−14	1.2509e−13	3.6056e−02
	Lob III	1.8383e−11	2.8733e−13	2.5333e−12	2.7002e−11	3.2293e−02
	Lob IIIA	8.8045e−14	1.3300e−15	1.1843e−14	1.2733e−13	8.8703e−02

Table 3
Comparison of different methods based upon maximum error, last error, absolute error, Norm, number of function evaluations and CPU time (in seconds) for the IVP given in Problem 2 with increasing number of steps (n).

n	Methods	ME	LE	AE	Norm	CPU
16	ROBM	4.1637e−02	2.6285e−11	2.5557e−03	4.1674e−02	2.9801e−02
	Lob III	4.3990e−01	1.9423e−06	4.6198e−02	4.8983e−01	3.0013e−02
	Lob IIIA	4.1637e−02	2.6285e−11	2.5557e−03	4.1674e−02	3.6468e−02
32	ROBM	2.8273e−03	4.1316e−13	8.6308e−05	2.8274e−03	5.9713e−02
	Lob III	1.2125e−02	2.0570e−10	3.7025e−04	1.2125e−02	5.3348e−02
	Lob IIIA	2.8273e−03	4.1314e−13	8.6308e−05	2.8274e−03	8.3677e−02
64	ROBM	5.5197e−05	2.7894e−15	9.3606e−07	5.5447e−05	1.2130e−01
	Lob III	1.3319e−04	9.2081e−13	2.2582e−06	1.3379e−04	1.5222e−01
	Lob IIIA	5.5197e−05	2.9005e−15	9.3606e−07	5.5447e−05	1.6969e−01

Table 4
Comparison of different methods based upon maximum error, last error, absolute error, norm, number of function evaluations and the CPU time (in seconds) for the IVP given in Problem 3 with increasing number of steps (n).

n	Methods	ME	LE	AE	Norm	CPU
25	ROBM	9.8311e−11	9.8311e−11	4.5166e−11	2.7629e−10	3.0632e−02
	Lob III	1.2242e−10	1.2242e−10	5.6544e−11	3.4602e−10	3.4620e−02
	Lob IIIA	9.8312e−11	9.8312e−11	4.5166e−11	2.7630e−10	4.8615e−02
50	ROBM	3.8558e−13	3.8558e−13	1.7603e−13	1.5086e−12	7.0071e−02
	Lob III	4.8139e−13	4.8139e−13	2.2011e−13	1.8853e−12	7.4709e−02
	Lob IIIA	3.8514e−13	3.8514e−13	1.7566e−13	1.5055e−12	1.0892e−01
100	ROBM	1.1657e−15	6.1062e−16	4.5961e−16	5.4273e−15	1.1275e−01
	Lob III	1.6098e−15	1.5543e−15	7.4747e−16	8.9700e−15	1.4253e−01
	Lob IIIA	1.8319e−15	1.8319e−15	8.0966e−16	9.6976e−15	1.9073e−01

Table 5
Comparison of different methods based upon maximum error, last error, absolute error, Norm, number of function evaluations and CPU time (in seconds) for the IVP given in Problem 4 with increasing number of steps (n).

n	Methods	ME	LE	AE	Norm	CPU
50	ROBM	9.9179e−17	5.4955e−17	2.9076e−17	3.2902e−16	3.9276e−01
	Lob III	4.4100e−13	4.4100e−13	7.4949e−14	1.0661e−12	4.6170e−01
	Lob IIIA	9.9179e−17	5.4955e−17	2.9076e−17	3.2902e−16	5.8544e−01
100	ROBM	6.9918e−19	2.1373e−19	1.8237e−19	3.0559e−18	7.4178e−01
	Lob III	3.4257e−15	3.3759e−15	5.8328e−16	1.2138e−14	9.4713e−01
	Lob IIIA	6.9918e−19	2.1373e−19	1.8237e−19	3.0559e−18	1.1981
200	ROBM	6.9905e−21	6.4473e−21	1.6457e−21	4.1973e−20	1.5106
	Lob III	2.3849e−17	2.3849e−17	3.0526e−18	9.4927e−17	1.8780
	Lob IIIA	6.9905e−21	6.4473e−21	1.6457e−21	4.1973e−20	2.3662

with the exact solution:

$$u(x) = 2\exp(-3x) - \exp(-39x) + \frac{1}{3}\cos(x),$$
$$v(x) = -\exp(-3x) + 2\exp(-39x) - \frac{1}{3}\cos(x). \tag{32}$$

Table 6
Comparison of different methods based upon maximum error, last error, absolute error, Norm, number of function evaluations and the CPU time (in seconds) for the IVP given in Problem 5 with increasing number of steps (n).

n	Methods	ME	LE	AE	Norm	CPU
250	ROBM	2.6723e-16	1.4470e-16	8.8132e-17	1.8686e-15	1.8558
	Lob-III	4.8774e-16	2.5393e-16	1.6318e-16	3.3741e-15	2.2759
	Lob-IIIA	2.6723e-16	1.4470e-16	8.8132e-17	1.8686e-15	3.407
500	ROBM	1.0442e-18	5.6526e-19	3.4443e-19	1.0315e-17	3.6604
	Lob-III	1.8976e-18	9.8728e-19	6.3584e-19	1.8573e-17	4.685
	Lob-IIIA	1.0442e-18	5.6526e-19	3.4443e-19	1.0315e-17	6.0419
1000	ROBM	4.0788e-21	2.2080e-21	1.3457e-21	5.6964e-20	8.0593
	Lob-III	7.3981e-21	3.8474e-21	2.4806e-21	1.0241e-19	8.2694
	Lob-IIIA	4.0788e-21	2.2080e-21	1.3457e-21	5.6964e-20	1.1508e+01

Problem 3. Consider another two-dimensional stiff system [25]:

$$\begin{aligned} u'(x) &= -u(x) - 10v(x), \\ v'(x) &= 10u(x) - v(x), \\ u(0) &= 1,\ v(0) = 0,\ \ x \in [0, 1], \end{aligned} \tag{33}$$

with the exact solution:

$$u(x) = \exp(-x)\cos(10x), \quad v(x) = \exp(-x)\sin(10x).$$

Problem 4. Consider the following three-dimensional system, which present a strong nonlinearity, taken from [26]:

$$\begin{aligned} u_1(x) &= -10^3(u_1(x)^3 u_2(x)^6 - \cos(x)^3\sin(x)^6) - \sin(x), \quad u_1(0) = 1, \\ u_2(x) &= -10^3(u_2(x)^5 u_3(x)^4 - \sin(x)^9) + \cos(x), \quad u_2(0) = 0, \\ u_3(x) &= -10^3(u_1(x)^2 u_3(x)^3 - \cos(x)^2\sin(x)^3) + \cos(x), \quad u_3(0) = 0, \\ &0 \le x \le 1, \end{aligned} \tag{34}$$

The exact solution is $u_1(x) = \cos(x), \quad u_2(x) = \sin(x) = u_3(x)$.

Problem 5. Consider the following nonlinear two-body system taken from [27]:

$$\begin{aligned} u_1''(x) &= \frac{-u_1(x)}{r^3}, \quad u_1(0) = 1, \quad u_1'(0) = 0, \\ u_2''(x) &= \frac{-u_2(x)}{r^3}, \quad u_2(0) = 0, \quad u_2'(0) = 1, \\ r &= \sqrt{u_1(x)^2 + u_2(x)^2}, \quad 0 \le x \le 1, \end{aligned} \tag{35}$$

The exact solution is $u_1(x) = \cos(x),\ u_2(x) = \sin(x)$.

5. Concluding remarks

A new one-step optimized block method has been developed with the help of interpolation and collocation techniques, and the resulting order of convergence is computed to be eight. Its theoretical analysis, carried out in the present study, proves the consistency, zero-stability, linear stability, theory of order stars, and convergence, which makes the method competent enough to numerically solve various nonlinear and stiff models that arise from the fields of applied sciences. Furthermore, its optimization is based on the local truncation errors obtained via the Taylor series for the three off-grid points of the method. The numerical experiments chosen from several fields have shown that the proposed block method performs better than other similar methods taken from literature. Not only this, but the reformulation of the obtained block method results in a substantial reduction in the computation time while solving the stiff models. Thus, the optimized block method proposed in the present study can be recommended for solving initial value problems in ordinary differential equations. In the future, an improvement in the order of convergence in the existing optimized block method will be attempted based on the quadrature approaches

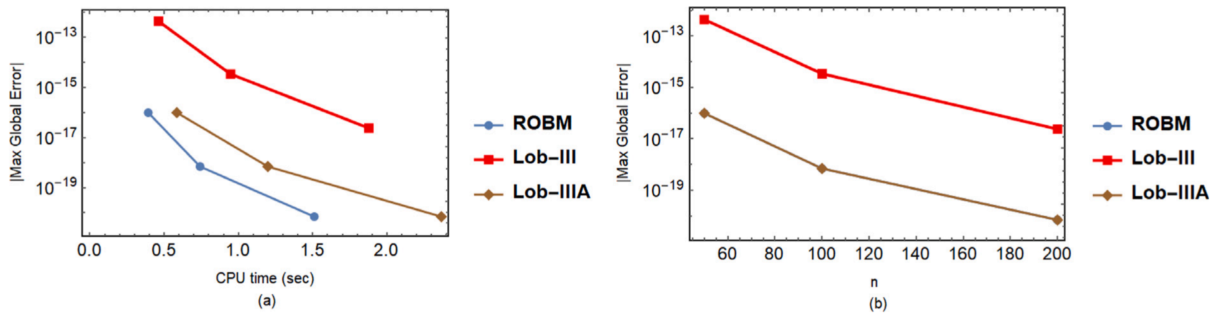

Fig. 6. Efficiency curves for the IVP in Problem 4 to observe the behavior of (a) absolute maximum global errors versus the CPU time (sec), and (b) absolute maximum global errors versus number of steps $n \in \{50, 100, 200\}$.

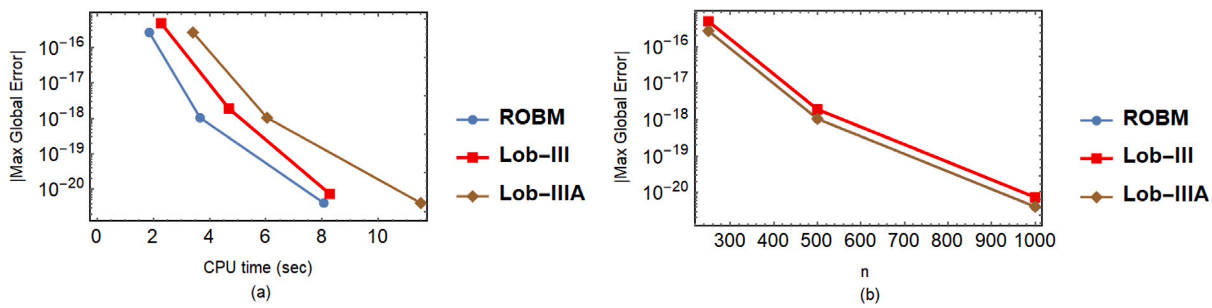

Fig. 7. Efficiency curves for the IVP in Problem 5 to observe the behavior of (a) absolute maximum global errors versus the CPU time (sec), and (b) absolute maximum global errors versus number of steps $n \in \{250, 500, 1000\}$.

discussed in [28–31], possibly including second-order derivatives for obtaining better numerical results with $\mathcal{L}$-stability features.

CRediT authorship contribution statement

Sania Qureshi: Conceived of the idea, and derived the proposed optimized block method, Writing and finalizing the article. **Higinio Ramos:** Numerical simulations, Writing and finalizing the article. **Amanullah Soomro:** Theoretical analysis, Writing and finalizing the article. **Evren Hincal:** Supervision of the entire work, Writing and finalizing the article.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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All authors approved the version of the manuscript to be published.

Ethics approval

We hereby affirm that the contents of this article are original. Furthermore, it has been neither published elsewhere fully or partially in any language nor submitted for publication (fully or partially) elsewhere simultaneously. It contains no matter that is scandalous, obscene, fraud, plagiarism, libelous, or otherwise contrary to law.

Consent to participate

Each author has approved of and agreed to submit the article.

Consent for publication

Each author agreed to publish the article.

Appendix

Algorithm 1: Pseudo-code for the proposed one-step optimized block method with three off-grid points.

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

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

1 Let $n = 0$, $\Delta x = \dfrac{X - x_0}{N}$
2 Let $x_n = x_0, y_n = y_{00}, y'_n = y'_{10}$
3 Let **sol** $= \{(x_n, y_n)\}$
4 Solve (14) to get y_{n+k}, y'_{n+k}, where $k = 0, r, s, u, 1$
5 Let **sol** $=$ **sol** $\cup \{(x_{n+k}, y_{n+k})\}_{k=0,r,s,u,1}$
6 Let $x_n = x_n + h, y_n = y_{n+1}, y'_n = y'_{n+1}$
7 Let $n = n + 1$
8 **if** $n = N$ **then**
9 | go to 13
10 **else**
11 | go to 4;
12 **end**
13 End

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