

An Optimized Two-Step Hybrid Block Method Formulated in Variable Step-Size Mode for Integrating $y'' = f(x, y, y')$ Numerically

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Abstract. An optimized two-step hybrid block method is presented for integrating general second order initial value problems numerically. The method considers two intrastep points which are selected adequately in order to optimize the local truncation errors of the main formulas for the solution and the first derivative at the final point of the block. The new proposed method is consistent, zero-stable and has seventh algebraic order of convergence. To illustrate the performance of the method, some numerical experiments are presented for solving this kind of problems, in comparison with methods of similar characteristics in the literature.

AMS subject classifications: 65Lxx, 65L99

Key words: Ordinary differential equations, second-order initial value problems, hybrid block method, optimization strategy, variable step-size.

1. Introduction

It is well-known that the formulation of many physical phenomena in mathematical language results in second order differential equations. For instance, the mass movement under the action of a force, problems of orbital dynamics, circuit theory, control theory, chemical kinetics, or in general, any problem involving second Newton's law.

The present article is concerned with approximating on a given interval the solution of a general second order initial value problem (I.V.P) of the form

$$y''(x) = f(x, y(x), y'(x)), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0. \quad (1.1)$$

An equation of the form (1.1) can be integrated by reformulating it as a system of two first order ODEs and then applying one the methods available for solving such systems.

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It seems less costly to develop numerical methods in order to integrate (1.1) directly. In this regard, many authors have proposed different methods for integrating the problem (1.1) directly (see for references, Hairer and Wanner [6], Chawla and Sharma [3], and Vigo-Aguiar and Ramos [1] among others). Among those procedures, block methods have been developed in order to obtain the numerical solution at more than one point at a time. One can see one of the pioneering works on block methods in [25]. Some advantages of block methods include (i) overcoming the overlapping of pieces of solutions and (ii) that they are self starting, thus avoiding the use of other methods to get starting values. Some useful references are [1-29].

In this article, we develop a two-step hybrid block method with two intra-step points using interpolation and collocation procedures with a constant step-size. Further, we will formulate the new proposed method in a variable step-size mode in order to make it more efficient from a practical point of view.

The article is organized as follows: Section 2 is concerned with development of the block method. Main characteristics of the block method are presented in Section 3. A formulation in variable step-size mode of the block method is considered in Section 4 using an embedded-type approach. To illustrate the performance of the proposed method, some numerical experiments are presented in Section 5 which show the efficiency of the new method when it is compared with other methods proposed in the scientific literature. Finally, some conclusions are presented in Section 6.

2. Development of the method

We present here the derivation of the block method with a constant step-size, and then a variable step-size formulation will be considered. To derive the block method, consider a polynomial approximation of the true solution $y(x)$ of (1.1) at the grid points $a = x_0 < x_1 < \dots < x_N = b$ of the integration interval, with constant step-size $h = x_{j+1} - x_j$, $j = 0, 1, \dots, N - 1$. Let

$$y(x) \simeq p(x) = \sum_{n=0}^8 a_n x^n \quad (2.1)$$

from which we get

$$y'(x) \simeq p'(x) = \sum_{n=1}^8 a_n n x^{n-1}, \quad (2.2a)$$

$$y''(x) \simeq p''(x) = \sum_{n=2}^8 a_n n(n-1) x^{n-2}, \quad (2.2b)$$

$$y'''(x) \simeq p'''(x) = \sum_{n=3}^8 a_n n(n-1)(n-2) x^{n-3}, \quad (2.2c)$$

where $a_n \in \mathbb{R}$ are real unknown coefficients to be determined. Consider two intra-step points $x_r = x_n + rh$, $x_s = x_n + sh$ with $0 < r < 1 < s < 2$ for approximating the solution of (1.1) on $[x_n, x_{n+2}]$ at the points x_n, x_{n+1}, x_{n+2} . To do that, consider the approximation in (2.1) and its first derivative (2.2a) applied to the point x_n , its second derivative in (2.2b) applied to the points $x_n, x_{n+r}, x_{n+1}, x_{n+s}, x_{n+2}$, and its third derivative (2.2c) applied to the points x_n, x_{n+2} . In this way, we have a system of nine equations with nine real unknowns $a_n, n = 0, 1, \dots, 8$, given by

$$\begin{aligned} p(x_n) &= y_n, & p'(x_n) &= y'_n, \\ p''(x_n) &= f_n, & p''(x_r) &= f_{n+r}, & p''(x_{n+1}) &= f_{n+1}, & p''(x_s) &= f_{n+s}, & p''(x_{n+2}) &= f_{n+2}, \\ p'''(x_n) &= f'_n, & p'''(x_{n+2}) &= f'_{n+2}, \end{aligned}$$

where the notations y_{n+j}, f_{n+j} and f'_{n+j} stand for approximations of $y(x_{n+j}), y''(x_{n+j})$ and $y'''(x_{n+j})$ respectively. This system of nine equations may be written in a matrix form as

$$\begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 & x_n^6 & x_n^7 & x_n^8 \\ 0 & 1 & 2x_n & 3x_n^2 & 4x_n^3 & 5x_n^4 & 6x_n^5 & 7x_n^6 & 8x_n^7 \\ 0 & 0 & 2 & 6x_n & 12x_n^2 & 20x_n^3 & 30x_n^4 & 42x_n^5 & 56x_n^6 \\ 0 & 0 & 2 & 6x_{n+r} & 12x_{n+r}^2 & 20x_{n+r}^3 & 30x_{n+r}^4 & 42x_{n+r}^5 & 56x_{n+r}^6 \\ 0 & 0 & 2 & 6x_{n+1} & 12x_{n+1}^2 & 20x_{n+1}^3 & 30x_{n+1}^4 & 42x_{n+1}^5 & 56x_{n+1}^6 \\ 0 & 0 & 2 & 6x_{n+s} & 12x_{n+s}^2 & 20x_{n+s}^3 & 30x_{n+s}^4 & 42x_{n+s}^5 & 56x_{n+s}^6 \\ 0 & 0 & 2 & 6x_{n+2} & 12x_{n+2}^2 & 20x_{n+2}^3 & 30x_{n+2}^4 & 42x_{n+2}^5 & 56x_{n+2}^6 \\ 0 & 0 & 0 & 6 & 24x_n & 60x_n^2 & 120x_n^3 & 210x_n^4 & 336x_n^5 \\ 0 & 0 & 0 & 6 & 24x_{n+2} & 60x_{n+2}^2 & 120x_{n+2}^3 & 210x_{n+2}^4 & 336x_{n+2}^5 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \\ a_7 \\ a_8 \end{pmatrix} = \begin{pmatrix} y_n \\ y'_n \\ f_n \\ f_{n+r} \\ f_{n+1} \\ f_{n+s} \\ f_{n+2} \\ f'_n \\ f'_{n+2} \end{pmatrix}.$$

Solving the above system of equations, we obtain the values of the unknowns $a_n, n = 0, 1, \dots, 8$, which we do not include here because they are very cumbersome expressions. After obtaining the values of these unknowns and doing the change of variables $x = x_n + th$, the polynomial in (2.1) may be written as

$$\begin{aligned} p(x_n + th) &= \alpha_0 y_n + h\alpha_1 y'_n + h^2(\beta_0 f_n + \beta_r f_{n+r} + \beta_1 f_{n+1} \\ &\quad + \beta_s f_{n+s} + \beta_2 f_{n+2}) + h^3(\gamma_0 f'_n + \gamma_2 f'_{n+2}), \end{aligned} \tag{2.3}$$

where

$$\begin{aligned} \alpha_0 &= 1, & \alpha_1 &= t, \\ \beta_0 &= -\frac{t^2}{3360r^2s^2} \left(st^2(-4s(-70 + 84t - 35t^2 + 5t^3)) + t(-168 + 224t - 100t^2 + 15t^3) \right. \\ &\quad + 2r^2(2t^2(70 - 84t + 35t^2 - 5t^3) - 4st^2(-70 + 84t - 35t^2 + 5t^3) \\ &\quad + 7s^2(-120 + 55t^2 - 27t^3 + 4t^4)) + rt^2(-8s^2(-70 + 84t - 35t^2 + 5t^3) \\ &\quad \left. + t(-168 + 224t - 100t^2 + 15t^3) + s(280 - 672t + 588t^2 - 220t^3 + 30t^4) \right), \end{aligned}$$

Then, taking $t = 2$ in the derivative of the above formula we evaluate $p'(x)$ at the point x_{n+2} , thus obtaining an approximation for the first derivative of the solution $y(x)$ at the point x_{n+2} :

$$\begin{aligned}
 hy'_{n+2} = & \left\{ h \left[-16f_{n+s}h(-2+r)^2(-1+r)r^2 + f_nh(-2+r)^2(-1+r)(-2+s)^2(-1+s)\dots \right. \right. \\
 & \cdot (4s^2+8rs^2+49r^3s^2-r^2(4+8s+49s^3)) + s \left[f'_n h^2(-2+r)^2(-1+r)r(-2+s)^2\dots \right. \\
 & \cdot (-1+s)(4s+7r^2s-r(4+7s^2)) + s \left(16f_{n+r}h(-2+s)^2(-1+s)+r^2(r-s)\dots \right. \\
 & \cdot (16f_{n+1}h(-2+r)^2)(8+7r(-1+s)-7s)(-2+s)^2 + (-1+r)(-1+s)\dots \\
 & \cdot (f_{n+2}h(736+49r^2(-2+s)^2-764s+196s^2-4r(191-194s+49s^2))) \\
 & \left. \left. \left. \left. \left. -(-2+r)(-2+s)(f'_{n+2}h^2(24+7r(-2+s)-14s)-105(-2+r)\dots \right. \right. \right. \right. \right. \\
 & \left. \left. \left. \left. \left. \cdot (-2+s)y'_n \right) \right) \right) \right) \right) \right] \left. \right\} / (105(-2+r)^2(-1+r)r^2(r-s)(-2+s)^2(-1+s)s^2). \quad (2.5)
 \end{aligned}$$

The above approximations depend on the parameters r, s , which are related to the intermediate points x_r, x_s . In order to obtain appropriate values of r and s , we consider to optimize the local truncation errors in the formulas (2.4) and (2.5). The reason to consider the local truncation errors in y_{n+2} and y'_{n+2} to obtain the optimized values of r and s is that at the end of the block $[x_n, x_{n+2}]$, the values of y_{n+2} and y'_{n+2} are the only ones needed for advancing the integration on the next block. It is clear that optimizing in this way, we will gain at least an order in each of the above formulas, as it is shown below.

To get the local truncation errors we expand in Taylor series about x_n the above formulas. The local truncation error in the formula in (2.4) is given by

$$\mathcal{L}(y(x_{n+2}), h) = \frac{(2-3rs)y^{(9)}(x_n)h^9}{99225} + \mathcal{O}(h^{10}). \quad (2.6)$$

Similarly, for the formula in (2.5) the local truncation error is given by

$$\mathcal{L}(hy'(x_{n+2}), h) = \frac{(2-r-s)y^{(9)}(x_n)h^9}{33075} + \mathcal{O}(h^{10}). \quad (2.7)$$

Equating to zero the principal terms of the local truncation errors given in (2.6) and (2.7) respectively, that is, the coefficients of h^9 , we obtain the following system of equations

$$2 - 3rs = 0, \quad 2 - r - s = 0.$$

It is easy to verify that the above implicit system of equations corresponds to rs -plane curves which are symmetric with respect to the diagonal $r = s$, thus there is a unique solution with the constraints $0 < r < 1 < s < 2$. After solving the above system of equations, we obtain the optimized values of r and s as follow

$$r = 1 - \frac{\sqrt{3}}{3} \simeq 0.42265, \quad s = 1 + \frac{\sqrt{3}}{3} \simeq 1.57735.$$

We note that these values are the zeros of the second order Legendre polynomial shifted to the interval $[0, 2]$. Substituting these values of r and s in the local truncation errors of the formulas (2.4) and (2.5), we obtain

$$\begin{aligned} \mathcal{L}(y(x_{n+2}), h) &= \frac{y^{(11)}(x_n)h^{11}}{58939650} + \mathcal{O}(h^{12}), \\ \mathcal{L}(hy'(x_{n+2}), h) &= \frac{-y^{(12)}(x_n)h^{12}}{589396500} + \mathcal{O}(h^{13}). \end{aligned}$$

Until now, we have two formulas, one for approximating the solution and one for approximating the first derivative at the final point of the block $[x_n, x_{n+2}]$. Note that we have eight unknowns, that is, $\{y_{n+j}, y'_{n+j}\}$, $j = r, 1, s, 2$. Therefore, to obtain a two-step hybrid block method we need to consider other six formulas. For this, we consider the evaluation of $p'(x)$ at the points $x_{n+r}, x_{n+1}, x_{n+s}$, and the evaluation of $p(x)$ at the points x_{n+r}, x_{n+1} and x_{n+s} . In this way, we obtain the complete block method consisting of the following eight equations

$$\begin{aligned} y_{n+r} = y_n + \frac{(3 + \sqrt{3})hy'_n}{3(2 + \sqrt{3})} + \frac{h^2}{11340(2 + \sqrt{3})} & \left((1801 + 559\sqrt{3})f_n + (630 + 315)f_{n+r} \right. \\ & + (400 - 376\sqrt{3})f_{n+1} + (990 - 477\sqrt{3})f_{n+s} - (41 + 21\sqrt{3})f_{n+2} \\ & \left. + h((107 + 36\sqrt{3})f'_n + (7 + 4\sqrt{3})f'_{n+2}) \right), \end{aligned} \tag{2.8a}$$

$$\begin{aligned} y_{n+1} = y_n + hy'_n + \frac{h^2}{6720} & \left(1171f_n + (945 + 576\sqrt{3})f_{n+r} + 280f_{n+1} + (945 - 576\sqrt{3})f_{n+s} \right. \\ & \left. + 19f_{n+2} + h(67f'_n - 3f'_{n+2}) \right), \end{aligned} \tag{2.8b}$$

$$\begin{aligned} y_{n+s} = y_n + \frac{(-3 + \sqrt{3})hy'_n}{3(-2 + \sqrt{3})} + \frac{h^2}{11340(-2 + \sqrt{3})} & \left((-1801 + 559\sqrt{3})f_n - (990 + 477\sqrt{3})f_{n+r} \right. \\ & - (400 + 376\sqrt{3})f_{n+1} + (-630 + 315\sqrt{3})f_{n+s} + (41 - 21\sqrt{3})f_{n+2} \\ & \left. + h((-107 + 36\sqrt{3})f'_n + (-7 + 4\sqrt{3})f'_{n+2}) \right), \end{aligned} \tag{2.8c}$$

$$\begin{aligned} y_{n+2} = y_n + 2hy'_n + \frac{h^2}{105} & \left(37f_n + (54 + 18\sqrt{3})f_{n+r} + 64f_{n+1} + (54 - 18\sqrt{3})f_{n+s} \right. \\ & \left. + f_{n+2} + 2hf'_n \right), \end{aligned} \tag{2.8d}$$

$$\begin{aligned} hy'_{n+r} = hy'_n + \frac{h^2}{3780(2 + \sqrt{3})} & \left((1726 + 885\sqrt{3})f_n + (1656 + 780\sqrt{3})f_{n+r} \right. \\ & + (96 - 320\sqrt{3})f_{n+1} + (396 - 60\sqrt{3})f_{n+s} - (94 + 25\sqrt{3})f_{n+2} \\ & \left. + h((124 + 65\sqrt{3})f'_n + (16 + 5\sqrt{3})f'_{n+2}) \right), \end{aligned} \tag{2.8e}$$

$$\begin{aligned} hy'_{n+1} = hy'_n + \frac{h^2}{1680} & \left(257f_n + (432 + 315)f_{n+r} + 512f_{n+1} + (432 - 315)f_{n+s} \right. \\ & \left. + 47f_{n+2} + 8h(f'_n - f'_{n+2}) \right), \end{aligned} \tag{2.8f}$$

$$\begin{aligned}
 hy'_{n+s} = & hy'_n + \frac{h^2}{3780(-2 + \sqrt{3})} \left((-1726 + 885\sqrt{3})f_n - (396 + 60\sqrt{3})f_{n+r} \right. \\
 & - (96 + 320\sqrt{3})f_{n+1} + (-1656 + 780\sqrt{3})f_{n+s} + (94 - 25\sqrt{3})f_{n+2} \\
 & \left. + h((-124 + 65\sqrt{3})f'_n + (-16 + 5\sqrt{3})f'_{n+2}) \right), \tag{2.8g}
 \end{aligned}$$

$$hy'_{n+2} = hy'_n + \frac{h^2}{105} \left(19f_n + 54f_{n+r} + 64f_{n+1} + 54f_{n+s} + 19f_{n+2} + h(f'_n - f'_{n+2}) \right). \tag{2.8h}$$

Note that if we are not particularly interested in approximations of derivatives (except the last one y'_{n+2}), as in the case of solving special second order equations $y'' = f(x, y)$, then the number of equations may be reduced. In this case, the system is reduced in five equations in five unknowns, that is, we will only consider the five equations related with unknowns $y_{n+r}, y_{n+1}, y_{n+s}, y_{n+2}, y'_{n+2}$. As mentioned above, to find the approximation of the solution at the next block, only the values of the solution and its first derivative are required at the final point of the previous block, which are provided after solving the new reduced system. For solving the differential equations where the right hand side of Eq. (1.1) does not contain the first derivative this strategy is less costly from a computational point of view.

3. Main characteristics of the method

This section is concerned with main characteristics, for instance, accuracy, consistency, zero-stability and linear stability analysis of the block method. The proposed block method (2.8) may be written in the following convenient matrix form

$$\mathbf{A} \mathbf{Y}_n = \mathbf{h} \mathbf{B} \mathbf{Y}'_n + \mathbf{h}^2 \mathbf{C} \mathbf{F}_n + \mathbf{h}^3 \mathbf{D} \mathbf{G}_n, \tag{3.1}$$

where $\mathbf{A}, \mathbf{B}, \mathbf{C}$ and \mathbf{D} are the corresponding matrices of coefficients of dimensions 8×5 , and

$$\begin{aligned}
 \mathbf{Y}_n &= (y_n, y_{n+r}, y_{n+1}, y_{n+s}, y_{n+2})^T, \\
 \mathbf{Y}'_n &= (y'_n, y'_{n+r}, y'_{n+1}, y'_{n+s}, y'_{n+2})^T, \\
 \mathbf{F}_n &= (f_n, f_{n+r}, f_{n+1}, f_{n+s}, f_{n+2})^T, \\
 \mathbf{G}_n &= (f'_n, f'_{n+r}, f'_{n+1}, f'_{n+s}, f'_{n+2})^T.
 \end{aligned}$$

3.1. Accuracy

Let $z(x)$ be a sufficiently differentiable function. Consider the following difference operator associated with the block hybrid method given in (3.1)

$$\begin{aligned}
 \mathcal{L}[z(x); h] = & \sum_j \bar{\alpha}_j z(x_n + jh) - h \bar{\beta}_j z'(x_n + jh) - h^2 \bar{\gamma}_j z''(x_n + jh) \\
 & - h^3 \bar{\delta}_j z'''(x_n + jh), \quad j = 0, r, 1, s, 2,
 \end{aligned}$$

where $\bar{\alpha}_j, \bar{\beta}_j, \bar{\gamma}_j, \bar{\delta}_j$ are respectively the vector columns of matrices $\mathbf{A}, \mathbf{B}, \mathbf{C}$ and \mathbf{D} . The block method (2.8) for solving (1.1) and the associated difference operator are said to have order

p if after expanding $z(x_n + jh), z'(x_n + jh), z''(x_n + jh)$ and $z'''(x_n + jh)$ in Taylor series about x_n , we obtain

$$\mathcal{L}[z(x); h] = \bar{C}_0 z(x_n) + \bar{C}_1 h z'(x_n) + \bar{C}_2 h^2 z''(x_n) + \dots + \bar{C}_q h^q z^{(q)}(x_n) + \dots$$

with $\bar{C}_0 = \bar{C}_1 = \dots = \bar{C}_{p+1} = 0$ and $\bar{C}_{p+2} \neq 0$. The \bar{C}_i are vectors and \bar{C}_{p+2} is called the error constant. For the block method (2.8), we have $\bar{C}_0 = \bar{C}_1 = \dots = \bar{C}_8 = 0$ and

$$\bar{C}_9 = \left(\frac{-1}{1837080\sqrt{3}}, 0, \frac{1}{1837080\sqrt{3}}, 0, \frac{-1}{612360}, \frac{1}{362880}, \frac{-1}{612360}, 0 \right)^T.$$

Hence, the proposed block method has seventh algebraic order of convergence. As the order of the method is no less than 1, therefore the method is also consistent with Eq. (1.1).

3.2. Zero-stability

Zero-stability is concerned with the stability of the difference schemes (3.1) as the step-size approaches to zero, that is, $h \rightarrow 0$. Consider $h \rightarrow 0$ in (3.1), then the difference scheme may be written in a more convenient form as

$$A^{(0)}\bar{Y}_\mu - A^{(1)}\bar{Y}_{\mu-1} = 0,$$

where $A^{(0)}$ and $A^{(1)}$ are constant matrices given by

$$A^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad A^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

$$\bar{Y}_\mu = (y_{n+2}, y_{n+s}, y_{n+1}, y_{n+r})^T, \quad \bar{Y}_{\mu-1} = (y_n, y_{n+s-2}, y_{n-1}, y_{n+r-2})^T.$$

The block method is zero stable if roots R_j of the first characteristic polynomial $\rho(R)$ given by $\rho R = \det[A^{(0)}R - A^{(1)}]$ satisfy $|R_j| \leq 1$ and for those roots with $|R_j| = 1$, the multiplicity does not exceed 2 (see [4]). For the proposed block method (3.1), the first characteristic polynomial is $\rho(R) = R^3(R - 1)$. Hence, the proposed block method (3.1) is zero-stable. As we have seen that the block method (3.1) is consistent and zero-stable then it implies the convergence of the method.

3.3. Linear stability analysis

As pointed out above, zero-stability of a numerical method is concerned with the behavior of the numerical method when $h \rightarrow 0$. In practice, we deal with some $h > 0$. In order to determine whether a numerical scheme will produce acceptable results for a given value of $h > 0$, we need a notion of stability that is different from zero-stability. The stability properties of a numerical scheme for a special second order equation are usually analyzed by considering the linear test equation introduced by Lambert and Watson [10]

$$y''(x) = -\mu^2 y(x) \quad \text{with} \quad \mu > 0. \tag{3.2}$$

As our method is concerned with general second order differential equations and Lambert and Watson's equation does not contain the first order derivative, for linear stability analysis, we will consider the following linear test equation (see [12])

$$y''(x) = -2\mu y'(x) - \mu^2 y(x). \quad (3.3)$$

This test equation has bounded solutions for $\mu \geq 0$ that tend to zero as $x \rightarrow \infty$. We will determine the region in which the numerical method reproduces the behavior of the true solutions.

Let us describe the procedure to obtain such region. Our method has eight equations in which there are five different terms of derivatives: $y'_n, y'_{n+r}, y'_{n+1}, y'_{n+s}, y'_{n+2}$, and two intermediate values y_{n+r}, y_{n+s} . Using the Mathematica system we have eliminated these terms from the system of equations, and get a recurrence equation in the terms y_n, y_{n+1}, y_{n+2} . This recurrence equation reads

$$P(H)y_{n+2} - Q(H)y_{n+1} + P(-H)y_n = 0, \quad (3.4)$$

where $H = \mu h$, and

$$\begin{aligned} P(H) &= H^{11} + 21H^{10} + 155H^9 + 225H^8 - 2415H^7 - 4515H^6 + 61740H^5 + 220500H^4 \\ &\quad - 793800H^3 - 7144200H^2 - 19051200H - 19051200, \\ Q(H) &= 48(H^{10} - 30H^8 + 455H^6 - 7350H^4 + 99225H^2 - 793800). \end{aligned}$$

We study the magnitude boundedness of their solutions through its characteristic equation to determine the stability region. The roots of the characteristic equation must be less than 1, for the method to be stable. The roots of the characteristic equation

$$P(H)r^2 - Q(H)r + P(-H) = 0 \quad (3.5)$$

are

$$r_{1,2} = \frac{1}{D}(24H^{10} - 720H^8 + 10920H^6 - 176400H^4 + 2381400H^2 - 19051200 \pm R)$$

with

$$\begin{aligned} R &= H^5(H^{12} + 445H^{10} - 24815H^8 + 556395H^6 - 8037225H^4 + 85631175H^2 - 450084600)^{\frac{1}{2}}, \\ D &= H^{11} + 21H^{10} + 155H^9 + 225H^8 - 2415H^7 - 4515H^6 + 61740H^5 \\ &\quad + 220500H^4 - 793800H^3 - 7144200H^2 - 19051200H - 19051200. \end{aligned}$$

Fig. 1 shows a plot of the absolute values of the roots $r_{1,2}$ versus H . We see that one of them limits the interval and thus the region of absolute stability, shown in Fig. 2.

If $\mu \in \mathbb{C}$ then the stability region is a region in the complex μh -plane, but if $\mu \in \mathbb{R}$ then the region of stability consists in a subset of the real line where the interval of the form

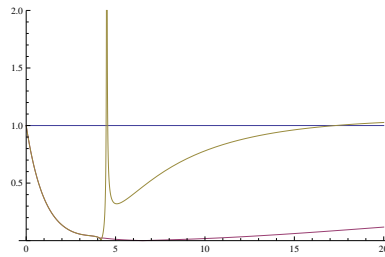


Figure 1: Absolute values of the roots of the characteristic equation in (3.5) versus H .

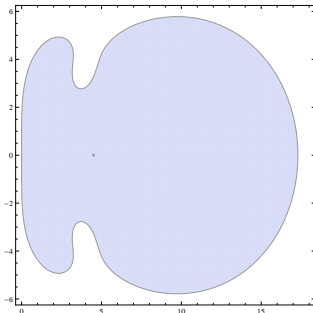


Figure 2: Stability region in the complex μh -plane for the method in (2.8) using the equation test in (3.3).

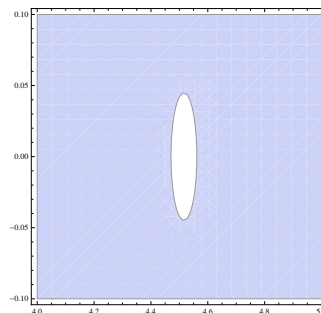


Figure 3: Detailed of the gap of the stability region in the complex μh -plane.

$(0, b)$ is known as the primary interval of stability. In Fig. 2 it is shown the stability region for the method considered in this article, being the real stability region given by

$$(0, 4.470686490605611) \cup (4.561384194246628, 17.296288514195407).$$

This region is that in the complex H -plane where the roots of the characteristic equation associated to the recurrence equation in (3.4) are bounded in modulus by unity. Or in other words, it is the set of H -values in the complex plane such that the solution of (3.1) is decaying for the test equation in (3.3) [5]. We note that there is a gap in the stability region, whose detailed plot is shown in Fig. 3.

4. Formulation in variable step-size mode

The proposed block method (3.1) may be formulated in variable step-size mode by considering a lower order method to estimate the local error at the final point in each block of the form $[x_n, x_{n+2}]$. The procedure will be less costly if the second method uses function evaluations that have been already calculated. To get a reliable estimate of the local error we follow a similar approach to that adopted by L. F. Shampine et al. [23].

Let us consider another method of order q to get another approximation at the final point of the current block, y_{n+2}^* , and let the local error le_{n+2} in using it given by

$$le_{n+2} = y(x_n + 2h) - y_{n+2}^*, \tag{4.1}$$

where $y(x)$ is the true solution.

Now, if we apply our proposed method of order $p > q$ to compute the approximation y_{n+2} on the current step then we have that $y(x_n + 2h) - y_{n+2} = \mathcal{O}(h^{p+2})$, and thus,

$$\begin{aligned} est &= y_{n+2} - y_{n+2}^* \\ &= [y(x_n + 2h) - y_{n+2}^*] - [y(x_n + 2h) - y_{n+2}] \\ &= le_{n+2} + \mathcal{O}(h^{p+2}). \end{aligned} \tag{4.2}$$

This is a computable estimate of the local error of the lower order method because le_{n+2} is $\mathcal{O}(h^{q+2})$ and so it dominates in (4.2) for small enough values of h . We can estimate the error in y_{n+2}^* by comparing it to the more accurate solution y_{n+2} . The approach adopted here is similar to that used in embedded pairs, where to make the local error estimation practical one has to look for a pair of methods that share as many function evaluations as possible. In implementation of embedded pairs, the lower order method is used to estimate the local error and the higher order method is used to advance the integration. Advancing the integration with the more accurate result y_{n+2} is called *local extrapolation*. In this way of proceeding, we do not know precisely how small the local error is at each step of integration, but we may assume that it is rather smaller than the estimated local error [23].

For the proposed block method in (3.1), the multi-step method given by

$$\begin{aligned} y_{n+2} &= (2 + 3\sqrt{3})y_n - 3(3 + \sqrt{3})y_{n+r} + 8y_{n+1} + \frac{h^2}{30} \left((-1 - \sqrt{3})f_n \right. \\ &\quad \left. + (-12 - 13\sqrt{3})f_{n+r} + 4(7 - 3\sqrt{3})f_{n+1} + (15 - 4\sqrt{3})f_{n+s} \right) \end{aligned}$$

with local truncation error $LTE = (1 + \sqrt{3})y^{(7)}(x_n)h^7/56700 + \mathcal{O}(h^8)$ has been used to estimate the local error at the final point in each block. This error estimate, est , provides the basis for determining the step-size for the next step. In the implementation, for a given tolerance, tol , the algorithm will change the step-size, from old to new as

$$h_{new} = \nu h \left(\frac{tol}{\|est\|} \right)^{1/(q+2)}, \tag{4.3}$$

where q is order of the lower order method and $0 < \nu < 1$ is a safety factor whose purpose is to avoid failed steps.

Normally some restrictions must be considered in order to avoid large fluctuations in step-size: step-size is not allowed to decrease by more than h_{mini} (minimum step-size allowed) or increase by more than h_{maxi} (maximum step-size allowed). This may be included in the implementation using an *If* statement:

$$\text{If } h_{mini} \leq h_{new} \leq h_{maxi}, \text{ then } h_{old} = h_{new}.$$

This strategy is applied successively to predict the step-size for the next step after a successful step, i.e. when $\|est\| < tol$. There are different strategies for selecting the size of the initial step h_{ini} (see Shampine *et. al.* [23] and Watts [27]), but one can simply take a very small starting step-size as in Sedgwick [22], and then the algorithm will correct this value if necessary, according to the strategy for changing the step-size.

4.1. Implementation details

In order to implement the proposed block method (3.1), we consider the method and calculate at the beginning of the process with the help of a computer algebra system like *Mathematica* the function f' using that $y''(x) = f(x, y(x), y'(x))$. In this way, we do not have to evaluate the higher derivatives appearing in the method on each step. This results in seven function evaluations per step, those of $f_n, f_{n+r}, f_{n+1}, f_{n+s}, f_{n+2}, f'_n, f'_{n+2}$.

The presence of $f'_{n+j}, j = 0, 2$, in the formulas of the block method, which approximates the third derivative at x_{n+j} , that is, $f'_{n+j} \simeq y'''(x_{n+j})$, requires the calculation of

$$f'(x) = \frac{df(x, y, y')}{dx} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}y' + \frac{\partial f}{\partial y'}f,$$

which can be easily obtained by hand, or in more difficult cases, with the use of a computer algebra system like *Mathematica*.

We note that the above method may also be used for solving systems of second-order differential equations, by considering a component-wise implementation. For a system of m equations, given in vector form as

$$y'' = \mathbf{f}(x, \mathbf{y}^T, \mathbf{y}'^T), \quad \mathbf{y}(a) = \mathbf{y}_0, \quad \mathbf{y}'(a) = \dot{\mathbf{y}}_0, \quad a = x_0 \leq x \leq b = x_N,$$

where $\mathbf{y} = (y_1, \dots, y_m)^T, \mathbf{y}' = (y'_1, \dots, y'_m)^T$,

$$\mathbf{f}(x, \mathbf{y}^T, \mathbf{y}'^T) = (f_1(x, \mathbf{y}^T, \mathbf{y}'^T), \dots, f_m(x, \mathbf{y}^T, \mathbf{y}'^T))^T,$$

and $\mathbf{y}_0 = (y_{1,0}, \dots, y_{m,0})^T, \dot{\mathbf{y}}_0 = (\dot{y}_{1,0}, \dots, \dot{y}_{m,0})^T$, we apply the method to each of the scalar equations in the differential system. In the general case this would result in an algebraic system of $8m$ equations, that may be solved using the Newton's method. To get the approximate values of the third derivative of each component at x_{n+j} , denoted by $f'_{i,n+j} = f'_i(x_{n+j}) \simeq y_i'''(x_{n+j}), i = 1, \dots, m$, we use the formula

$$f'_i(x) = \frac{df_i}{dx}(x, y_1, \dots, y_m, y'_1, \dots, y'_m) = \frac{\partial f_i}{\partial x} + \sum_{j=1}^m \frac{\partial f_i}{\partial y_j}y'_j + \sum_{j=1}^m \frac{\partial f_i}{\partial y'_j}f'_j.$$

5. Numerical experiments

To test performance of the proposed optimized hybrid block method, some numerical experiments have been presented. The following notations have been used in the tables:

- FEval: Number of function evaluations (including derivatives);
- EMAX: Maximum norm of the absolute errors on the grid points along the integration interval;
- N: Total number of steps taken when solving a particular problem;

Table 1: Data for problem 5.1.

Method	FEval	EMAX
SCOWE(6)	9038	4.29×10^{-9}
I3P1B	16755	4.10×10^{-9}
OPTBM	2100	1.13×10^{-12}

- h_{ini} : Initial step-size taken.

We note that in the examples presented we have considered both the fixed step-size method, denoted by OPTBM, and the variable step-size formulation presented above, which is denoted by VOPTBM.

5.1. Orbital problem of Stiefel and Bettis

As a first problem, we consider the well-known orbital problem which was firstly studied by Stiefel and Bettis [26] and later discussed by many other researchers [16–18]

$$y''(x) + y(x) = 0.001 \exp(ix); \quad y(0) = 1, \quad y'(0) = \frac{9995i}{10000}, \quad x \in [0, 40\pi].$$

The true solution of this problem is

$$y(x) = \frac{x \sin(x)}{2000} + \cos(x) + i \left(\sin(x) - \frac{x \cos(x)}{2000} \right).$$

The true solution represents the motion of a perturbation of a circular orbit in the complex plane. For comparison purposes, we have considered the new optimized block method named as OPTBM, the seventh order six variable-step Störmer-Cowell method named as SCOWE(6) in [18], and the implicit 3-point block method in [7], named as I3P1B. The data given in Table 1 demonstrate that the proposed method has very good performance compared to the methods used for comparison.

5.2. Bessel type IVP

Consider the following Bessel type problem appeared many times in the literature [1, 9, 19]

$$x^2 y''(x) + x y'(x) + (x^2 - 0.25)y(x) = 0, \quad x \in [1, 8],$$

$$y(1) = \sqrt{\frac{2}{\pi}} \sin(1), \quad y'(1) = \frac{2 \cos(1) - \sin(1)}{\sqrt{2\pi}}.$$

The true solution of this problem is $y(x) = J_{1/2} = \sqrt{\frac{2}{\pi x}} \sin(x)$. For comparison purpose, we have considered the seventh order hybrid block method in [9] and the variable-step

Table 2: Maximum absolute error ($EMAX = \max_j |y(x_j) - y_j|$) for problem 5.2.

N	OPTBM	Vigo-Ramos [1]	Jator [9]
67	5.5178×10^{-14}	7.1122×10^{-7}	6.5286×10^{-11}
82	7.5495×10^{-15}	9.2632×10^{-8}	1.3679×10^{-11}
112	4.4408×10^{-16}	1.2108×10^{-10}	1.1897×10^{-12}

Falkner method of eighth order implemented in predictor-corrector mode in [1]. In Table 2, maximum absolute errors along the integration interval for different number of steps have been considered. The data given in Table 2 show that the proposed method has better performance.

5.3. Damped wave equation

Consider the damped wave equation with periodic boundary conditions [11]

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} + \delta \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f(u), & -1 < x < 1, \quad t > 0, \\ u(-1, t) = u(1, t). \end{cases}$$

According to [11] the semi-discretization in the spatial variable by second order symmetric differences leads to the following system of second order ODEs in time

$$\ddot{U} + KU = F(U, \dot{U}), \quad 0 < t \leq t_{end},$$

where $U(t) = (u_1(t), u_2(t), \dots, u_N(t))^T$ with $u_i(t) \approx u(x_i, t)$, $i = 1, \dots, N$.

$$K = \frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & & -1 & 2 & -1 \\ -1 & & & & -1 & 2 \end{pmatrix},$$

where $\Delta x = \frac{2}{N}$, $x_i = -1 + i\Delta x$ and $F(U, \dot{U}) = (f(u_1) - \delta \dot{u}_1, \dots, f(u_N) - \delta \dot{u}_N)^T$. In this experiment, we take $f(u) = \sin u$, $\delta = 0.08$ and the initial conditions as

$$U(0) = (\pi)_{i=1}^N, \quad U_t(0) = \sqrt{N} \left(0.01 + \sin \left(\frac{2\pi i}{N} \right) \right)_{i=1}^N.$$

We have solved this problem in order to compare the proposed method with those in the article [11]. We have taken $N = 40$ and solved on the interval $[0, 100]$ the problem with the proposed method for $h = 1/10, 1/20, 1/30$. For this problem, we have presented the efficiency curves indicating the good performance of the proposed method compared

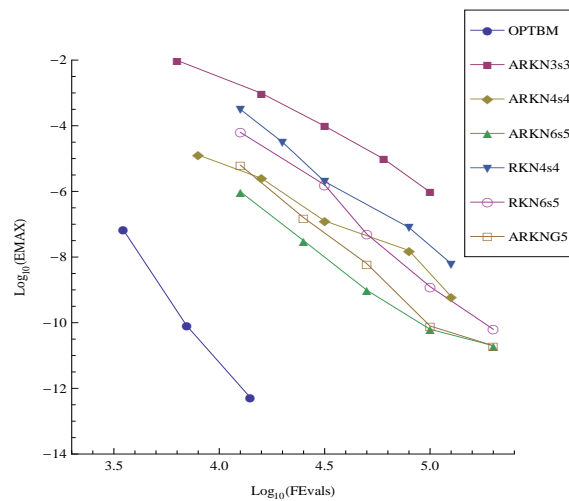


Figure 4: For Problem 5.3.

with the methods considered for comparison in terms of accuracy and number of function evaluations.

Note. In the following examples, we have considered the variable step-size implementation of the proposed block method, named as VOPTBM using the strategy given in Section 4. A similar strategy has also been considered for the variable step-size implementation of the seventh order method in [9], named as VJATOR. The following problems have also been solved by variable step-size ODE solvers ode45 and ode113 in MATLAB. The solver ode45 is the well-known Dormand-Prince 5(4) pair [24], or Dopri 5(4), which is formed by Runge-Kutta methods with orders 5 and 4. It can also be found as the algorithm ode45 in MATLAB. The code ode113 is a variable step variable order method which uses Adams-Bashforth-Moulton predictor-correctors of order 1 to 13. For more details about these solvers, see [24]. In the Tables, the maximum absolute error of the computed solution, $EMAX = \max_j |y(x_j) - y_j|$, the number of steps taken, N , and the total number of function evaluations (including derivatives) have been included.

5.4. A linear problem

Consider the following linear problem which was discussed many times in the scientific literature [1, 9, 19]

$$y''(x) = -100y(x) + 99 \sin(x), \quad y(0) = 1, \quad y'(0) = 11, \quad x \in [0, 2].$$

The true solution of the problem is $y(x) = \cos(10x) + \sin(10x) + \sin(x)$. The numerical results have been obtained by considering $h_{ini} = 10^{-j}$, $j = 2, 3$. The data given in Table 3 is a numerical evidence for the good performance of the optimized block method.

Table 3: Data for problem 5.4.

h_{ini}	Method	EMAX	N	FEval
10^{-2}	VOPTBM	9.7699×10^{-15}	136	476
	VJATOR	4.3126×10^{-13}	249	581
	ode45	7.4607×10^{-14}	3731	22387
	ode113	1.5610×10^{-13}	349	695
10^{-3}	VOPTBM	5.4400×10^{-15}	138	483
	VJATOR	4.3498×10^{-13}	252	588
	ode45	7.2164×10^{-14}	3730	22381
	ode113	5.9286×10^{-14}	398	793

Table 4: Data for problem 5.5.

h_{ini}	Method	EMAX	N	FEval
10^{-2}	VOPTBM	4.8319×10^{-13}	78	273
	VJATOR	6.8742×10^{-12}	204	476
	ode45	2.2993×10^{-12}	807	4849
	ode113	3.3940×10^{-11}	260	525
10^{-4}	VOPTBM	8.7833×10^{-13}	116	406
	VJATOR	8.6447×10^{-12}	216	504
	ode45	3.6483×10^{-12}	809	4855
	ode113	9.1131×10^{-12}	255	515

5.5. A nonlinear problem

Consider the following nonlinear problem taken from [21]

$$y''(x) = 6y(x)^2, \quad y(0) = 1, \quad y'(0) = -2, \quad x \in [0, 10].$$

The true solution of the problem is $y(x) = (1 + x)^{-2}$. The numerical results have been obtained by considering $h_{ini} = 10^{-j}, j = 2, 4$. The data given in Table 4 is a numerical evidence for the good performance of the optimized block method.

5.6. A second order nonlinear system

Consider the following second order system [15] given by

$$\begin{cases} y_1''(x) = \frac{-y_1(x)}{r}, & y_1(0) = 1, \quad y_1'(0) = 0, \\ y_2''(x) = \frac{-y_2(x)}{r}, & y_2(0) = 0, \quad y_2'(0) = 1, \\ r = \sqrt{y_1(x)^2 + y_2(x)^2}, & x \in [0, 15\pi]. \end{cases}$$

The true solution of this system is $y_1(x) = \cos(x), y_2(x) = \sin(x)$. The numerical results have been obtained by considering different initial step-sizes, $h_{ini} = 10^{-j}, j = 2, 3$ for all

Table 5: Data for problem 5.6.

h_{ini}	Method	EMAX($y_1(x)$)	EMAX($y_2(x)$)	N	FEval
10^{-2}	VOPTBM	4.9445×10^{-12}	5.4417×10^{-12}	168	588
	VJATOR	1.3323×10^{-10}	1.3328×10^{-10}	309	721
	ode45	4.9056×10^{-8}	5.2537×10^{-8}	877	5263
	ode113	1.7028×10^{-8}	1.9331×10^{-8}	433	871
10^{-3}	VOPTBM	4.9453×10^{-12}	5.4391×10^{-12}	170	595
	VJATOR	1.3139×10^{-10}	1.3182×10^{-10}	309	721
	ode45	4.9040×10^{-8}	5.2533×10^{-8}	878	5269
	ode113	1.7028×10^{-8}	1.9331×10^{-8}	433	871

Table 6: Data for problem 5.7.

h_{ini}	Method	EMAX($y_1(x)$)	EMAX($y_2(x)$)	N	FEval
10^{-2}	VOPTBM	2.6557×10^{-10}	2.6193×10^{-10}	114	399
	VJATOR	4.1251×10^{-8}	4.1240×10^{-8}	207	483
	ode45	4.4402×10^{-8}	4.4460×10^{-8}	646	3877
	ode113	1.9523×10^{-6}	1.9507×10^{-6}	207	419
10^{-3}	VOPTBM	1.3096×10^{-10}	1.3096×10^{-10}	116	406
	VJATOR	2.3328×10^{-8}	2.3304×10^{-8}	213	497
	ode45	4.4638×10^{-8}	4.4696×10^{-8}	647	3883
	ode113	2.0514×10^{-6}	2.0505×10^{-6}	212	429

the methods. Results in Table 5 clearly show that the proposed method performs better than the other methods in terms of accuracy, number of steps taken for solving the problem and number of function evaluations.

5.7. A second order system

Consider the following second order system [14] given by

$$\begin{cases} y_1''(x) = -y_2(x) + \sin(\pi x), & y_1(0) = 0, \quad y_1'(0) = -1, \\ y_2''(x) = -y_1(x) + 1 - \pi^2 \sin(\pi x), & y_2(0) = 1, \quad y_2'(0) = 1 + \pi, \end{cases}$$

where $x \in [0, 10]$. The true solution of this system is

$$y_1(x) = 1 - e^x, \quad y_2(x) = e^x + \sin(\pi x).$$

The numerical results have been obtained by considering different initial step-sizes, $h_{ini} = 10^{-j}$, $j = 2, 3$ for all the methods. Results in Table 6 clearly show that the proposed method performs better than the other methods in terms of accuracy, number of steps taken for solving the problem and number of function evaluations.

Table 7: Data for problem 5.8.

h_{ini}	Method	EMAX($y_1(x)$)	EMAX($y_2(x)$)	N	FEval
10^{-2}	VOPTBM	9.0785×10^{-13}	8.8062×10^{-13}	3220	11270
	VJATOR	1.2903×10^{-11}	1.2897×10^{-11}	5904	13776
	ode45	7.4385×10^{-12}	7.1543×10^{-12}	91654	549925
	ode113	4.5137×10^{-11}	4.6031×10^{-11}	8290	16577
10^{-3}	VOPTBM	9.4679×10^{-13}	9.0910×10^{-13}	3224	11284
	VJATOR	1.2968×10^{-11}	1.3037×10^{-11}	5907	13783
	ode45	3.9891×10^{-12}	3.5701×10^{-12}	91653	549919
	ode113	4.5754×10^{-11}	4.5812×10^{-11}	8844	17685

5.8. An Oscillatory problem

As our last example, consider the following oscillatory problem studied in [18]

$$\begin{cases} y_1''(x) = -13y_1(x) + 12y_2(x) + 9\cos(2x) - 12\sin(2x), \\ y_2''(x) = 12y_1(x) - 13y_2(x) - 12\cos(2x) + 9\sin(2x) \end{cases}$$

with initial conditions $y_1(0) = 1$, $y_2(0) = 0$ and $y_1'(0) = -4$, $y_2'(0) = 8$. The true solution of this system is

$$y_1(x) = \sin(x) - \sin(5x) + \cos(2x), \quad y_2(x) = \sin(x) + \sin(5x) + \sin(2x).$$

The system has been integrated in the interval $x \in [0, 100]$. The numerical results have been obtained by considering $h_{ini} = 10^{-j}$, $j = 2, 3$. The data given in Table 7 is a numerical evidence to show the good performance of the new proposed method in terms of accuracy, number of steps taken for solving the problem and used function evaluations.

5.9. Efficiency curves

In this section, we present efficiency curves comparing the new proposed variable step-size optimized block method (VOPTBM) and the variable step-size Jator's block method (VJATOR) showing maximum absolute errors (EMAX) versus total number of function evaluations (including derivatives), (FEvals). The corresponding plots are given for problems 5.4 up to 5.8 in Fig. 5. These efficiency curves clearly show that the new proposed method is the most efficient one for solving the type of problems considered for comparisons.

6. Conclusions

In this article, we have developed an optimized two-step hybrid block method for integrating general second order initial value problems numerically. The obtained method is self-starting and has good characteristics that make it suitable for solving second order differential systems. The method is derived by considering a polynomial approximation of

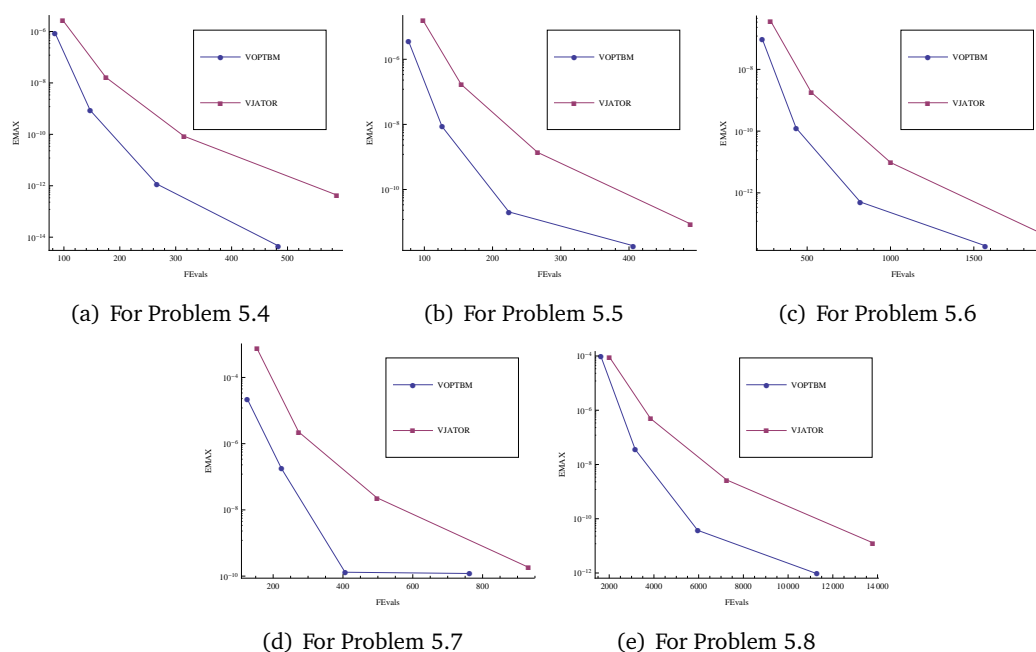


Figure 5: Efficiency curves for Problems 5.4–5.8.

the true solution and two intra-step points x_{n+r} and x_{n+s} . We have further obtained the appropriate values of these intra-step points after optimizing the local truncation errors concerning the two main formulas for approximating y_{n+2} and y'_{n+2} . We have also developed a variable step-size formulation, which is more effective from a computational point of view. Some numerical experiments have been presented to illustrate the good performance of the proposed method in comparison with some methods existing in the scientific literature.

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