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A class of explicit two-step hybrid methods for second-order IVPs

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Abstract

A class of explicit two-step hybrid methods for the numerical solution of second-order IVPs is presented. These methods require a reduced number of stages per step in comparison with other hybrid methods proposed in the scientific literature. New explicit hybrid methods which reach up to order five and six with only three and four stages per step, respectively, and which have optimized the error constants, are constructed. The numerical experiments carried out show the efficiency of our explicit hybrid methods when they are compared with classical Runge–Kutta–Nyström methods and other explicit hybrid codes proposed in the scientific literature.

MSC: 65L05; 65L06

Keywords: Numerical integration; Two-step methods; Explicit hybrid methods; Second-order IVPs

1. Introduction

In the last two decades there has been a great interest in the research of new methods for the numerical integration of initial value problems associated to second order ODEs

$$y'' = f(t, y), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0, \tag{1}$$

in which the first derivative does not appear explicitly. Such problems often arise in different fields of applied sciences such as celestial mechanics, molecular dynamics, quantum mechanics, spatial

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semi-discretizations of wave equations, electronics, and so on (see Refs. [11,12]), and they can be efficiently solved by using Runge–Kutta–Nyström (RKN) methods or by using special multistep methods for second order ODEs (see [9]).

In the case of special multistep methods for second order ODEs, particular explicit hybrid algorithms have been proposed by several authors [1–3,8,13,14,17,15,16]. A pioneer paper is due to Chawla [1]; in it (by using the explicit two-step Störmer method as an intermediate stage) a modification of the classical Numerov method is presented. In this way he obtains a fourth-order two-stage explicit hybrid method which has better stability properties than the classical Numerov method. In later papers, several authors [2,3,8,13] have obtained explicit hybrid methods with algebraic order four and six in the context of initial-value problems with periodic or oscillating solutions. The maximum algebraic order obtained by the explicit hybrid methods presented in the literature until now is eight (see for example [14,17]). But the main handicap of these methods is that they require a high number of stages per step. So, the sixth-order hybrid methods require at least six stages per step, whereas the eight-order hybrid methods use at least ten stages per step. This fact is due to the technique used in the construction of the methods, which is based on the evaluation of interpolatory off-step nodes with high accuracy, and increases the computational cost. In this paper we investigate the construction of explicit hybrid methods without this drawback.

Recently, Coleman [5] has investigated the order conditions of two-step hybrid methods for differential systems of type (1) by using the theory of B-series. So, this author offers an alternative for the determination of the order of a two-step hybrid method based on checking certain relationships between the coefficients of the method, analogously to the case of RK or RKN methods. He has considered two-step hybrid methods of the form

$$Y_i = (1+c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(t_n + c_j h, Y_j), \quad i = 1, \ldots, s, \tag{2}$$

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{i=1}^{s} b_i f(t_n + c_i h, Y_i), \tag{3}$$

where y_{n-1}, y_n and y_{n+1} represent approximations for $y(t_n - h)$, $y(t_n)$ and $y(t_n + h)$, respectively. These methods are characterized by the coefficients b_i, c_i and a_{ij}, and they can be represented in Butcher notation by the table

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

The order conditions (up to order $\leqslant 8$) for this class of two-step hybrid methods (in terms of their coefficients) are tabulated in [5]. In addition, as is usual in the case of RK or RKN methods, the coefficients of the leading term associated to the local truncation error for a pth-order two-step hybrid method (2)–(3) will be denoted as

$$e_{p+1}(t_i) = \frac{\alpha(t_i)}{(p+2)!}[1 + (-1)^{p+2} - b^{\mathrm{T}} \Psi''(t_i)], \quad t_i \in T_2, \quad \rho(t_i) = p+2, \tag{4}$$

where $\alpha(t_i)$, $\rho(t_i)$, $\Psi''(t_i)$ and T_2 are defined in [5]. The quantity

$$C_{p+1} = \|(e_{p+1}(t_1), \ldots, e_{p+1}(t_k))\|_2,$$

where k is the number of trees of order $p+2$ ($\rho(t_i) = p+2$), will be called the *error constant* for the pth-order method.

An important property for a method to perform efficiently is the accuracy versus the computational cost. In the case of explicit hybrid methods for the numerical integration of (1), this depends on the algebraic order and the number of stages per step used by the method. So, the purpose of this paper is the design and construction of two-step explicit hybrid methods so that the ratio ρ = *algebraic order/number of stages* is as large as possible, which leads to obtain practical and efficient codes. The paper is organized as follows: In Section 2 we present a class of explicit two-step hybrid methods of the form (2)–(3) which requires $s-1$ stages (function evaluations) per step. In Section 3 we derive explicit hybrid methods which reach up to order five and six with only three and four stages per step, respectively. The derivation of these methods is based on the order conditions obtained in [5] and we pay special attention to optimize the error constant C_{p+1} of the methods. In Section 4 we present some numerical experiments that show the efficiency of the new methods when they are compared with other methods proposed in the scientific literature such as RKN methods or explicit hybrid methods. Section 5 is devoted to conclusions.

2. The class of explicit two-step hybrid methods

In this section we present the class of explicit two-step hybrid methods which is the subject of our study. The methods are of the form (2)–(3) and they are defined by

$$Y_1 = y_{n-1}, \quad Y_2 = y_n, \tag{5}$$

$$Y_i = (1+c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{i-1} a_{ij} f(t_n + c_j h, Y_j), \quad i = 3, \ldots, s, \tag{6}$$

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \left[b_1 f_{n-1} + b_2 f_n + \sum_{i=3}^{s} b_i f(t_n + c_i h, Y_i) \right], \tag{7}$$

where f_{n-1} and f_n represent $f(t_{n-1}, y_{n-1})$ and $f(t_n, y_n)$, respectively, and the two first nodes are $c_1 = -1$, $c_2 = 0$.

We note that after the starting procedure, the methods only require the evaluation of $f(t_n, y_n)$, $f(t_n + c_3 h, Y_3), \ldots, f(t_n + c_s h, Y_s)$ in each step ($s-1$ function evaluations). Therefore, they can be considered as two-step hybrid methods with $s-1$ stages per step which can be represented in Butcher notation by the table of coefficients

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|ccccc} -1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ c_3 & a_{31} & a_{32} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & 0 \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array}$$

In order to analyze the phase properties of the two-step hybrid methods above mentioned, we consider the second order homogeneous linear test model (see [6,10])

$$y''(t) = -\lambda^2 y(t), \quad \text{with } \lambda > 0. \tag{8}$$

If an s-stage two-step hybrid method (2)–(3) is applied to the test (8), it may be written in vector form as

$$Y = (e + c)y_n - cy_{n-1} - H^2 AY, \quad H = \lambda h, \tag{9}$$

$$y_{n+1} = 2y_n - y_{n-1} - H^2 b^{\mathrm{T}} Y, \tag{10}$$

where $Y = (Y_1, \ldots, Y_s)^{\mathrm{T}}$ and $e = (1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^s$. Then, solving the stages in (9) we obtain

$$Y = (I + H^2 A)^{-1}(e + c)y_n - (I + H^2 A)^{-1} c y_{n-1},$$

and substituting in (10) we see that the numerical solution satisfies the recursion

$$y_{n+1} - S(H^2)y_n + P(H^2)y_{n-1} = 0, \tag{11}$$

where

$$S(H^2) = 2 - H^2 b^{\mathrm{T}}(I + H^2 A)^{-1}(e + c), \quad P(H^2) = 1 - H^2 b^{\mathrm{T}}(I + H^2 A)^{-1} c.$$

In the case of the explicit two-step hybrid methods (5)–(7), the matrix of coefficients A is nilpotent of degree $s - 1$ ($A^{s-1} = 0$), and therefore we can write

$$(I + H^2 A)^{-1} = I - H^2 A + H^4 A^2 - \cdots + (-1)^{s-2} H^{2s-4} A^{s-2}.$$

So, the coefficients of the difference (11) are polynomials in H^2 which are determined in terms of the coefficients of the method (5)–(7) by the expressions

$$S(H^2) = 2 - H^2 b^{\mathrm{T}}(e + c) + H^4 b^{\mathrm{T}} A(e + c) - \cdots + (-1)^{s-1} H^{2s-2} b^{\mathrm{T}} A^{s-2}(e + c), \tag{12}$$

$$P(H^2) = 1 - H^2 b^{\mathrm{T}} c + H^4 b^{\mathrm{T}} Ac - \cdots + (-1)^{s-1} H^{2s-2} b^{\mathrm{T}} A^{s-2} c. \tag{13}$$

The phase properties of the two-step hybrid methods considered are determined by the characteristic polynomial of the difference (11):

$$\xi^2 - S(H^2)\xi + P(H^2), \tag{14}$$

and following the nomenclature given in [18], the quantities

$$\phi(H) = H - \arccos\left(\frac{S(H^2)}{2\sqrt{P(H^2)}}\right), \quad d(H) = 1 - \sqrt{P(H^2)}, \tag{15}$$

are called the *dispersion error* and the *dissipation error*, respectively. Then, a method is said to be *dispersive of order q* and *dissipative of order r*, if

$$\phi(H) = \mathcal{O}(H^{q+1}), \quad d(H) = \mathcal{O}(H^{r+1}).$$

We remark that the magnitude of the dispersion and dissipation errors is an important feature for solving second-order IVPs (1) with periodic or oscillating solutions. In such problems, it is also desirable that the numerical solution defined by the difference (11) should be periodic, as is the exact solution of the linear test model (8). This last property is equivalent to the fact that the coefficients of polynomial (14) satisfy the conditions

$$P(H^2) \equiv 1, \quad \text{and} \quad |S(H^2)| < 2, \quad \forall H \in (0, H_p), \tag{16}$$

and the interval $(0, H_p)$ is known as the *interval of periodicity* of the method. In [18], the methods which satisfy conditions (16) are called *zero dissipative* ($d(H) = 0$). On the other hand, when the method possesses a finite order of dissipation, the integration process is stable if the coefficients of polynomial (14) satisfy the conditions

$$|P(H^2)| < 1, \quad \text{and} \quad |S(H^2)| < 1 + P(H^2), \quad \forall H \in (0, H_s), \tag{17}$$

and the interval $(0, H_s)$ is known as the *interval of absolute stability* of the method. The first mention to these intervals appears in Refs. [4,10].

As an example we consider the explicit hybrid methods (5)–(7) with $s = 3$ defined by the table of coefficients

$$\begin{array}{c|ccc} -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ c_3 & a_{31} & a_{32} & 0 \\ \hline & b_1 & b_2 & b_3 \end{array}$$

If we impose the order conditions up to algebraic order four (see Coleman [5]) given by

$$Ae = \frac{c^2 + c}{2}, \quad b^{\mathrm{T}}e = 1, \quad b^{\mathrm{T}}c = 0, \quad b^{\mathrm{T}}c^2 = 1/6, \quad b^{\mathrm{T}}c^3 = 0, \quad b^{\mathrm{T}}Ac = 0, \tag{18}$$

for the coefficients of the method we have the unique solution

$$b_1 = b_3 = \frac{1}{12}, \quad b_2 = \frac{5}{6}, \quad c_3 = 1, \quad a_{31} = 0, \quad a_{32} = 1.$$

So, the only fourth-order explicit hybrid method with two stages is given by equations

$$Y_3 = 2y_n - y_{n-1} + h^2 f(t_n, y_n),$$

$$y_{n+1} = 2y_n - y_{n-1} + \frac{h^2}{12}[f_{n-1} + 10f_n + f(t_{n+1}, Y_3)],$$

and it is the explicit version of the Numerov method obtained by Chawla [1]. The coefficients of polynomial (14) for this method are

$$P(H^2) = 1, \quad S(H^2) = 2 - H^2 + \frac{H^4}{12},$$

and therefore it is zero dissipative, dispersive of order four and possesses the interval of periodicity $(0, \sqrt{12})$.

In the next section we analyze the case of explicit hybrid methods (5)–(7) with $s = 4$ and 5 which reach up to order five and six, respectively.

3. Construction of the explicit hybrid methods

Here, we analyze the construction of explicit hybrid methods (5)–(7) which reach up to order five and six, and only require three and four stages per step, respectively. The construction of such methods is carried out paying special attention to optimize the error constant C_{p+1} associated to each method.

3.1. Explicit hybrid methods with three stages ($s = 4$)

We consider the explicit two-step hybrid methods defined by the table of coefficients

$$\begin{array}{c|cccc} -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ c_3 & a_{31} & a_{32} & 0 & 0 \\ c_4 & a_{41} & a_{42} & a_{43} & 0 \\ \hline & b_1 & b_2 & b_3 & b_4 \end{array}$$

The order conditions up to algebraic order five (see Coleman [5]) are given by (18) and the following ones

$$b^{\mathrm{T}}c^4 = 1/15, \quad b^{\mathrm{T}}(c \cdot Ac) = -1/60, \quad b^{\mathrm{T}}Ac^2 = 1/180. \tag{19}$$

If we impose conditions (18) and (19), the coefficients of the methods are determined in terms of the arbitrary parameter c_3 by the expressions

$$b_1 = \frac{c_3 + c_4}{6(1 + c_3 + c_4 + c_3c_4)}, \quad b_2 = \frac{1 - c_3 - c_4 + 6c_3c_4}{6c_3c_4}, \quad b_3 = \frac{1 - c_4}{6c_3(1 + c_3)(c_3 - c_4)},$$

$$b_4 = \frac{-1 + c_3}{6(c_3 - c_4)c_4(1 + c_4)}, \quad a_{31} = \frac{c_3(1 + c_3)}{10(1 - c_4)}, \quad a_{32} = \frac{c_3(1 + c_3)(-4 + 5c_4)}{10(-1 + c_4)},$$

$$a_{41} = -\frac{c_4(1 + c_4)(3 + 2c_3 + c_4)}{30(-1 + c_3^2)}, \quad a_{42} = \frac{c_4(1 + c_4)(-13c_3 + 15c_3^2 + c_4)}{30(-1 + c_3)c_3},$$

$$a_{43} = \frac{(c_3 - c_4)c_4(1 + c_4)}{30c_3(-1 + c_3^2)}, \quad c_4 = \frac{-2 + 5c_3}{-5 + 5c_3},$$

and the coefficients of polynomial (14) are given by

$$S(H^2) = 2 - H^2 + \frac{H^4}{12} - \left(\frac{1}{360} + b^{\mathrm{T}}A^2c\right)H^6, \quad P(H^2) = 1 - (b^{\mathrm{T}}A^2c)H^6.$$

Now, we select the free parameter c_3 so that the error constant C_6 is as small as possible, obtaining the values

$$c_3 = \frac{63}{100}, \quad C_6 = 1.24 \cdot 10^{-3}.$$

This fifth-order explicit two-step hybrid method will be denoted as ETSHM5, it is defined by the table of coefficients

$$
\begin{array}{c|cccc}
-1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\dfrac{63}{100} & \dfrac{126651}{2000000} & \dfrac{900249}{2000000} & 0 & 0 \\
-\dfrac{23}{37} & -\dfrac{43347640}{916464729} & -\dfrac{4864523}{50602347} & \dfrac{213026000}{8248182561} & 0 \\
\hline
 & \dfrac{31}{13692} & \dfrac{1675}{2898} & \dfrac{10000000}{47555739} & \dfrac{1874161}{8947092}
\end{array}
$$

and it possesses the interval of absolute stability $(0, 2.68)$.

Other possibilities are to select the free parameter c_3 so that the order of dispersion or the order of dissipation are increased. If we choose c_3 so that the method is dispersive of order eight, we obtain

$$c_3 = \frac{25}{28}, \quad C_6 = 7.26 \cdot 10^{-2},$$

and the dispersion and dissipation errors are given by

$$\phi(H) = -\frac{13H^9}{7257600} + \mathcal{O}(H^{11}), \quad d(H) = \frac{H^6}{20160} + \mathcal{O}(H^8).$$

This fifth-order method which is dispersive of order eight and dissipative of order five will be denoted as ETSHM5(8, 5), it is defined by the table of coefficients

$$
\begin{array}{c|cccc}
-1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\dfrac{25}{28} & \dfrac{1325}{43904} & \dfrac{35775}{43904} & 0 & 0 \\
-\dfrac{23}{5} & \dfrac{16744}{33125} & \dfrac{383111}{15625} & -\dfrac{13866608}{828125} & 0 \\
\hline
 & \dfrac{173}{1908} & \dfrac{2791}{3450} & \dfrac{307328}{3056775} & -\dfrac{125}{636732}
\end{array}
$$

and it possesses the interval of absolute stability $(0, 2.84)$.

If we select the free parameter c_3 so that the order of dissipation is increased, then the method is zero dissipative

$$b^{\mathrm{T}} A^2 c = 0,$$

obtaining $c_3 = 1$. But unfortunately this value of the parameter c_3 is incompatible with the fifth-order conditions (19), and the algebraic order of the method should be restricted to four. So, we investigate the construction of fourth-order methods which are zero dissipative and dispersive of order six. In order to do this we impose conditions (18) and

$$b^{\mathrm{T}} A^2 c = 0, \quad b^{\mathrm{T}} A^2 e = \frac{1}{360},$$

obtaining the coefficients of the methods in terms of the arbitrary parameters c_3 and c_4

$$b_1=\frac{c_3+c_4}{6(1+c_3+c_4+c_3c_4)},\quad b_2=\frac{1-c_3-c_4+6c_3c_4}{6c_3c_4},\quad b_3=\frac{1-c_4}{6c_3(1+c_3)(c_3-c_4)},$$

$$b_4=\frac{-1+c_3}{6(c_3-c_4)c_4(1+c_4)},\quad a_{42}=\frac{c_4(1+c_4)(-16c_3+15c_3^2+c_4)}{30(-1+c_3)c_3},\quad a_{32}=\frac{c_3(1+c_3)}{2},$$

$$a_{41}=-\frac{(c_3-c_4)c_4(1+c_4)}{30(-1+c_3^2)},\quad a_{31}=0,\quad a_{43}=\frac{(c_3-c_4)c_4(1+c_4)}{30c_3(-1+c_3^2)}.$$

We note that the last two conditions imposed (zero dissipation and dispersion of order six) are the conditions $C_3=0$ and $U_3=1/360$ in the notation of Section 9 of [5].

First, we select the free parameters c_3 and c_4 so that the error constant C_5 is as small as possible, obtaining the values

$$c_4=\frac{-2+5c_3}{-5+5c_3},\quad C_5=1.66\cdot 10^{-2}.$$

Now, the free parameter c_3 is chosen so that the resulting method is optimized for linear systems of ODEs $(f(t,y)=Ky+g(t))$ and possesses order five for this class of differential systems, obtaining

$$c_3=\frac{33}{50},\quad C_6^*=3.26\cdot 10^{-4},$$

where C_6^* is the error constant for the class of linear differential systems.

The resulting fourth-order explicit hybrid method which is zero dissipative (dissipative of order infinity) and dispersive of order six will be denoted as ETSHM4(6,∞), and it is defined by the table of coefficients

$$\begin{array}{c|cccc}
-1 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0\\
\frac{33}{50} & 0 & \frac{2739}{5000} & 0 & 0\\
-\frac{13}{17} & \frac{314860}{20796729} & -\frac{1058746}{8268579} & \frac{15743000}{686292057} & 0\\
\hline
 & -\frac{89}{1992} & \frac{545}{858} & \frac{625000}{3316929} & \frac{83521}{377832}
\end{array}$$

The dispersion and dissipation errors for this method are

$$\phi(H)=-\frac{H^7}{40320}+\mathcal{O}(H^9),\quad d(H)=0,$$

and it possesses the interval of periodicity (0, 2.75).

We remark that for the nodes $c_3=1$ and $c_4=0$, Chawla and Rao [2] have derived an explicit hybrid method of this class with algebraic order four which is also zero dissipative and dispersive of order six. But this method only has algebraic order four for the class of linear differential systems and its error constant is $C_5=3.28\cdot 10^{-2}$ (it is greater than the error constant of our method).

3.2. Explicit hybrid methods with four stages ($s = 5$)

Now we analyze the case of explicit two-step hybrid methods defined by the table of coefficients

$$\begin{array}{c|ccccc}
-1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
c_3 & a_{31} & a_{32} & 0 & 0 & 0 \\
c_4 & a_{41} & a_{42} & a_{43} & 0 & 0 \\
c_5 & a_{51} & a_{52} & a_{53} & a_{54} & 0 \\
\hline
 & b_1 & b_2 & b_3 & b_4 & b_5
\end{array}$$

The order conditions up to algebraic order six (see [5]) are given by the following expressions

$$b^{\mathrm{T}} e = 1, \quad b^{\mathrm{T}} c = 0, \quad b^{\mathrm{T}} c^2 = 1/6, \quad b^{\mathrm{T}} c^3 = 0, \quad b^{\mathrm{T}} c^4 = 1/15, \tag{20}$$

$$b^{\mathrm{T}} A c^2 = 1/180, \quad b^{\mathrm{T}} c^5 = 0, \quad b^{\mathrm{T}} (c \cdot A c^2) = 1/72, \quad b^{\mathrm{T}} A c^3 = 0, \tag{21}$$

together with the simplifying conditions

$$Ae = \frac{c^2 + c}{2}, \quad Ac = \frac{c^3 - c}{6}. \tag{22}$$

If we impose conditions (20)–(22), the coefficients of the methods are determined in terms of the arbitrary parameters c_3 and c_4, which define a two-parameter family of sixth-order explicit hybrid methods, where the coefficients of polynomial (14) are given by

$$S(H^2) = 2 - H^2 + \frac{H^4}{12} - \frac{H^6}{360} + b^{\mathrm{T}} A^3 (e + c) H^8, \quad P(H^2) = 1 + (b^{\mathrm{T}} A^3 c) H^8.$$

First we select the free parameters so that the error constant C_7 is as small as possible, obtaining the values

$$c_3 = -\frac{1}{5}, \quad c_4 = -\frac{2}{5}, \quad C_7 = 2.51 \cdot 10^{-3}.$$

This sixth-order explicit hybrid method will be denoted as ETSHM6, it is defined by the table of coefficients

$$\begin{array}{c|ccccc}
-1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{1}{5} & -\frac{4}{125} & -\frac{6}{125} & 0 & 0 & 0 \\
-\frac{2}{5} & -\frac{133}{3000} & -\frac{13}{750} & -\frac{7}{120} & 0 & 0 \\
\frac{2}{3} & -\frac{1115}{52488} & \frac{4175}{4374} & -\frac{2275}{1944} & \frac{5200}{6561} & 0 \\
\hline
 & \frac{1}{60} & \frac{23}{24} & -\frac{125}{156} & \frac{125}{192} & \frac{729}{4160}
\end{array}$$

and it possesses the interval of absolute stability (0, 3).

We remark that for the nodes $c_3 = 1/2$ and $c_4 = -1/2$, Tsitouras [16] has derived an explicit hybrid method of this class with algebraic order six and error constant $C_7 = 3.45 \cdot 10^{-3}$ which is greater than the error constant of our method.

Other possibilities consist of selecting the nodes c_3 and c_4 so that the order of dispersion or the order of dissipation or both orders are increased. If we choose c_3 and c_4 so that the method is dispersive of order eight with the error constant being as small as possible, we obtain

$$c_3 = \frac{3}{4}, \quad c_4 = -\frac{25}{42}, \quad C_7 = 4.91 \cdot 10^{-3},$$

and the dispersion and dissipation errors are given by

$$\phi(H) = -\frac{11H^9}{14515200} + \mathcal{O}(H^{11}), \quad d(H) = \frac{H^8}{483840} + \mathcal{O}(H^{10}).$$

This sixth-order method which is dispersive of order eight and dissipative of order seven will be denoted as ETSHM6(8, 7), it is defined by the table of coefficients

$$\begin{array}{c|ccccc}
-1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
\frac{3}{4} & \frac{7}{128} & \frac{77}{128} & 0 & 0 & 0 \\
-\frac{25}{42} & -\frac{1107125}{21781872} & -\frac{30175}{345744} & \frac{48025}{2722734} & 0 & 0 \\
\frac{7}{13} & \frac{13215760}{246167259} & \frac{71321558}{217206405} & \frac{33220000}{4908864753} & \frac{1177085448}{46361500445} & 0 \\
\hline
 & \frac{403}{71400} & \frac{2861}{5250} & \frac{7936}{130515} & \frac{32672808}{148637375} & \frac{4826809}{28597800}
\end{array}$$

and it possesses the interval of absolute stability (0, 2.98).

If we select the nodes c_3 and c_4 so that the order of dissipation is increased, then the method is zero dissipative ($b^{\mathrm{T}}A^3c = 0$), obtaining

$$c_3 = \frac{-2 + 3c_4}{-3 + 5c_4}.$$

But unfortunately, for this value of the parameter c_3 the term of order eight associated to the dispersion error is not zero for all $c_4 \in \mathbb{R}$, and the dispersion order of the method is restricted to six. So, we use the free parameter c_4 so that the error constant is as small as possible, obtaining the values

$$c_4 = \frac{7}{10}, \quad C_7 = 5.73 \cdot 10^{-3}.$$

This sixth-order method which is zero dissipative and dispersive of order six will be denoted as ETSHM6(6, ∞), and it is defined by the table of coefficients

$$\begin{array}{c|ccccc}
-1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{5} & \frac{4}{125} & \frac{11}{125} & 0 & 0 & 0 \\
\frac{7}{10} & \frac{119}{2000} & \frac{1071}{2000} & 0 & 0 & 0 \\
-\frac{1}{2} & -\frac{11}{204} & -\frac{7}{144} & -\frac{7}{144} & \frac{4}{153} & 0 \\
\hline
 & \frac{1}{68} & \frac{11}{42} & \frac{25}{84} & \frac{50}{357} & \frac{2}{7}
\end{array}$$

The dispersion and dissipation errors for this method are

$$\phi(H) = -\frac{H^7}{40320} + \mathcal{O}(H^9), \quad d(H) = 0.$$

and it possesses the interval of periodicity (0, 2.75).

4. Numerical experiments

In order to evaluate the effectiveness of the new explicit hybrid methods derived above, we consider several model problems. The new methods have been compared with other explicit hybrid codes proposed in Refs. [2,16], and with classic RKN integrators. The criterion used in the numerical comparisons is the usual test based on computing the maximum global error over the whole integration interval. In Figs. 1–8 we have depicted the efficiency curves for the tested codes. These figures show the decimal logarithm of the maximum global error ($\log_{10}(GE)$) versus the computational effort measured by the number of

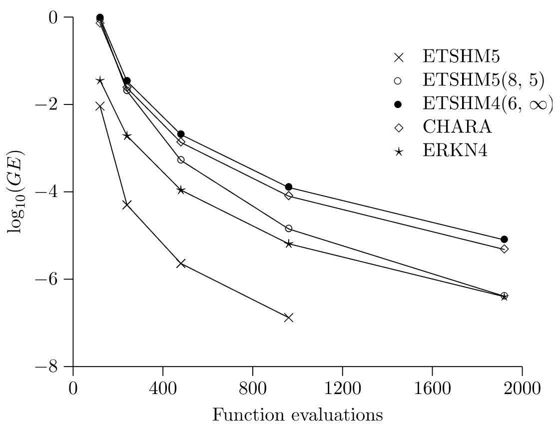

Fig. 1. Methods with three stages per step in Problem 1.

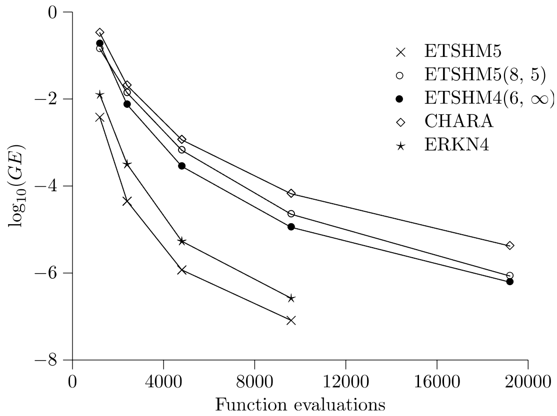

Fig. 2. Methods with three stages per step in Problem 2.

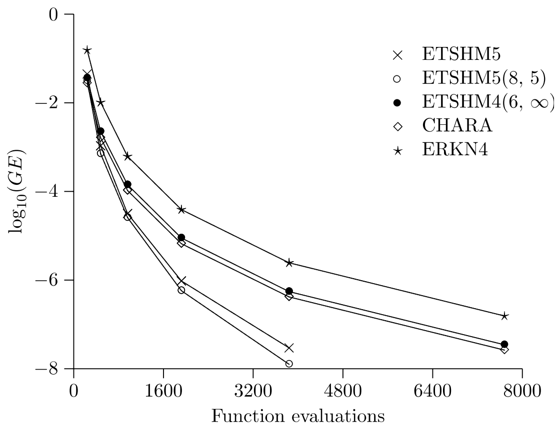

Fig. 3. Methods with three stages per step in Problem 3.

function evaluations required by each code. The codes used in the comparisons have been denoted by:

(i) *Methods with three stages per step*

(a) ETSHM5: The first explicit hybrid method derived in Section 3.1 ($\rho = 5/3$).
(b) ETSHM5(8,5): The second explicit hybrid method derived in Section 3.1 ($\rho = 5/3$).
(c) ETSHM4(6, ∞): The third explicit hybrid method derived in Section 3.1 ($\rho = 4/3$).
(d) CHARA: The explicit hybrid method derived by Chawla and Rao [2] ($\rho = 4/3$).
(e) ERKN4: The explicit fourth-order RKN method obtained in [7] ($\rho = 4/3$).

(ii) *Methods with four stages per step*

(a) ETSHM6: The first explicit hybrid method derived in Section 3.2 ($\rho = 3/2$).
(b) ETSHM6(8, 7): The second explicit hybrid method derived in Section 3.2 ($\rho = 3/2$).
(c) ETSHM6(6, ∞): The third explicit hybrid method derived in Section 3.2 ($\rho = 3/2$).
(d) TSITOURAS: The explicit hybrid method derived by Tsitouras [16] ($\rho = 3/2$).
(e) ERKN5: The explicit fifth-order RKN method given in [9] ($\rho = 5/4$).

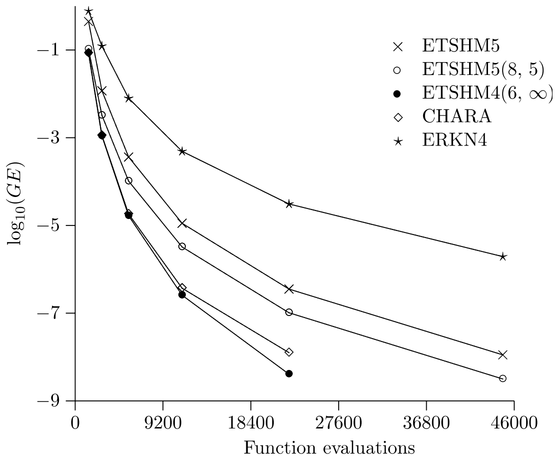

Fig. 4. Methods with three stages per step in Problem 4.

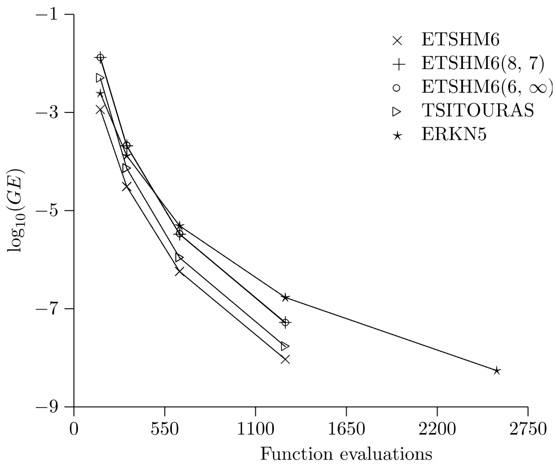

Fig. 5. Methods with four stages per step in Problem 1.

We have used the following four model problems:

Problem 1. We consider the nonlinear system

$$y_1'' = y_1(\log^2(y_2) - \log(y_1)), \quad y_1(0) = \mathrm{e}, \quad y_1'(0) = 0, \quad t \in [0, t_{\mathrm{end}}],$$
$$y_2'' = y_2(\log^2(y_1) - \log(y_2)), \quad y_2(0) = 1, \quad y_2'(0) = 1,$$

whose analytic solution is given by

$$y_1(t) = \mathrm{e}^{\cos(t)}, \quad y_2(t) = \mathrm{e}^{\sin(t)}.$$

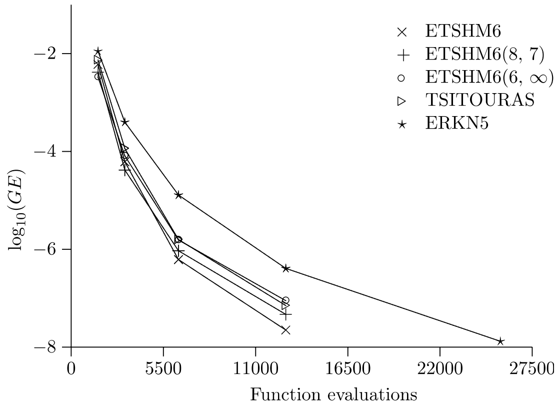

Fig. 6. Methods with four stages per step in Problem 2.

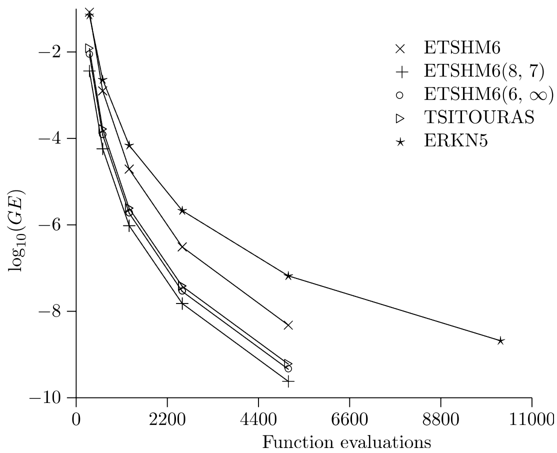

Fig. 7. Methods with four stages per step in Problem 3.

In our test we choose the parameter value $t_{\mathrm{end}} = 10$, and the numerical results stated in Figs. 1 and 5 have been computed with integration steps $h = 1/2^i$, $i \geqslant 2$.

Problem 2. We consider the two body gravitational problem

$$y_1'' = -\frac{y_1}{(y_1^2 + y_2^2)^{3/2}}, \quad y_1(0) = 1 - e, \quad y_1'(0) = 0,$$

$$y_2'' = -\frac{y_2}{(y_1^2 + y_2^2)^{3/2}}, \quad y_2(0) = 0, \quad y_2'(0) = \sqrt{\frac{1+e}{1-e}},$$

where e represents the eccentricity of the orbit. This problem has been solved in the interval [0, 20] with the parameter value $e = 0.7$, and the numerical results stated in Figs. 2 and 6 have been computed with integration steps $h = 0.1/2^i$, $i \geqslant 1$.

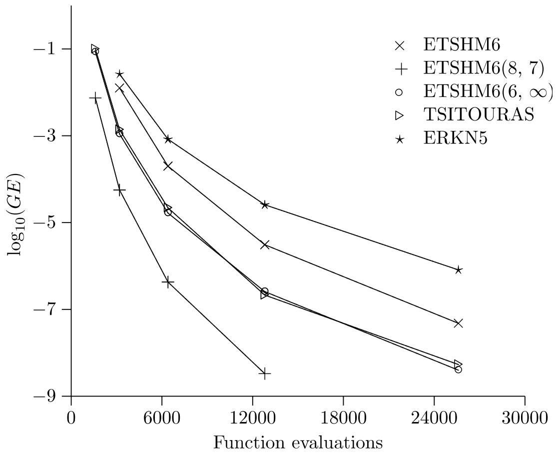

Fig. 8. Methods with four stages per step in Problem 4.

Problem 3. We consider the oscillatory nonlinear system

$$y_1'' = -4t^2 y_1 - \frac{2y_2}{\sqrt{y_1^2 + y_2^2}}, \quad y_1(0) = 1, \quad y_1'(0) = 0, \quad t \in [0, t_{\mathrm{end}}],$$

$$y_2'' = -4t^2 y_2 + \frac{2y_1}{\sqrt{y_1^2 + y_2^2}}, \quad y_2(0) = 0, \quad y_2'(0) = 0,$$

whose analytic solution is given by

$$y_1(t) = \cos(t^2), \quad y_2(t) = \sin(t^2).$$

This solution represents a periodic motion with variable frequency. In our test we choose the parameter value $t_{\mathrm{end}} = 8$, and the numerical results stated in Figs. 3 and 7 have been computed with integration steps $h = 0.1/2^i$, $i \geqslant 0$.

Problem 4. We consider the oscillatory linear system

$$y''(t) + \begin{pmatrix} 13 & -12 \\ -12 & 13 \end{pmatrix} y(t) = \begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix}, \quad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} -4 \\ 8 \end{pmatrix}, \tag{23}$$

with $f_1(t) = 9\cos(2t) - 12\sin(2t)$, $f_2(t) = -12\cos(2t) + 9\sin(2t)$, and whose analytic solution is given by

$$y(t) = \begin{pmatrix} \sin(t) - \sin(5t) + \cos(2t) \\ \sin(t) + \sin(5t) + \sin(2t) \end{pmatrix}. \tag{24}$$

This problem has been solved in the interval $[0, t_{\mathrm{end}}]$ and in our test we choose the parameter value $t_{\mathrm{end}} = 100$. The numerical results stated in Figs. 4 and 8 have been computed with integration steps $h = 1/2^i$, $i \geqslant 2$.

4.1. Efficiency curves for the methods with three stages per step

Now we will show the efficiency for the methods with three stages per step. Figs. 1 and 2 show that for general nonlinear differential systems (Problems 1 and 2) the code ETSHM5, which has optimized the error constant, is the most efficient of the tested methods, whereas the code ERKN4 performs better than the remaining codes. On the other hand, in the case of oscillatory problems (Problems 3 and 4) the code ERKN4 is the least efficient of the methods being compared. We note that the method ERKN4 was derived in the context of embedded pairs providing a mechanism for error estimation, and therefore it presents a poor behaviour in the integration of oscillatory problems. When the oscillatory problem is nonlinear (Problem 3) the code ETSHM5(8,5), which is dispersive of high order, results to be the most efficient, whereas in the oscillatory linear system (Problem 4) the codes ETSHM4(6, ∞) and CHARA, which are optimized for this class of problems, perform very well. Finally, we note that in general the methods whose ratio ρ is greater show a more efficient behaviour.

4.2. Efficiency curves for the methods with four stages per step

Now we will show the efficiency for the methods with four stages per step. In this case, Figs. 5 and 6 show again that for general nonlinear differential systems (Problems 1 and 2) the codes which have optimized the error constant perform more efficiently. So, the code ETSHM6 results to be the most efficient for these problems, and the code TSITOURAS performs well, whereas the code ERKN5 is the least efficient of the methods being compared. On the other hand, in the case of oscillatory problems (Problemss 3 and 4) the results are different. For these problems, the sixth-order codes which have optimized the dispersion error or the dissipation error or both errors perform more efficiently. So, in this case the code ETSHM6(8, 7) results to be the most efficient and the codes ETSHM6(6, ∞) and TSITOURAS perform well. Again, for the methods with four stages per step, those whose ratio ρ is greater show a more efficient behaviour. Finally, we note that the code TSITOURAS performs well in most cases, even though it is not the most efficient in any of the problems solved.

5. Conclusions

A class of explicit two-step hybrid methods for solving second-order IVPs which require a reduced number of stages per step is analyzed. New explicit hybrid methods which reach up to order five and six with the smallest possible computational cost are derived. The derivation of these methods is based on the order conditions obtained in [5] (similar to order conditions for RK methods), paying special attention to optimize the error constant of the methods as well as the dispersion and the dissipation.

The numerical experiments carried out show that the new explicit hybrid methods perform more efficiently than classical RKN methods and other explicit hybrid methods proposed in the scientific literature which require the same computational cost per step. In general, for methods with the same computational cost per step, those whose ratio ρ is greater result to be the most efficient. In the case of second-order general differential systems the methods which have optimized the error constant show a more efficient behaviour, whereas for oscillatory problems the methods which have also optimized the dispersion and the dissipation are preferable.

Finally, we conclude that the class of explicit hybrid methods analyzed represents an alternative to explicit RKN methods in order to solve second-order IVPs. So, in a future research we intend to derive explicit hybrid methods of this class with higher algebraic order.

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