A class of explicit high-order exponentially-fitted two-step methods for solving oscillatory IVPs

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Abstract: The derivation of new exponentially fitted (EF) modified two-step hybrid (MTSH) methods for the numerical integration of oscillatory second-order IVPs is analyzed. These methods are modifications of classical two-step hybrid methods so that they integrate exactly differential systems whose solutions can be expressed as linear combinations of the set of functions $\{\exp(\lambda t),\ \exp(-\lambda t)\}$, $\lambda \in \mathbb{C}$, or equivalently $\{\sin(\omega t),\ \cos(\omega t)\}$ when $\lambda = i\omega$, $\omega \in \mathbb{R}$, where λ represents an approximation of the main frequency of the problem. The EF conditions and the conditions for this class of EF schemes to have algebraic order p (with $p \leq 8$) are derived. With the help of these conditions we construct explicit EFMTSH methods with algebraic orders seven and eight which require five and six function evaluation per step, respectively. These new EFMTSH schemes are optimal among the two-step hybrid methods in the sense that they reach a certain order of accuracy with minimal computational cost per step. In order to show the efficiency of the new high order explicit EFMTSH methods in comparison to other EF and standard two-step hybrid codes from the literature some numerical experiments with several orbital and oscillatory problems are presented.

Keywords: Exponential fitting; modified two-step hybrid methods; oscillatory second-order IVPs.

Mathematics Subject Classification: 65L05, 65L06

1 Introduction

In this paper we deal with the construction of exponentially fitted (EF) modified two-step hybrid (MTSH) methods for the numerical integration of orbital and oscillatory initial value problems (IVPs) associated to second order ODEs

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

where the right-hand side of (1) does not depend on the first derivative. Such problems often arise in different fields of applied sciences such as celestial mechanics, astrophysics, chemistry, molecular dynamics, quantum mechanics, electronics, and so on (see [1, 2]). The numerical solution of this class of problems can be carried out by using general purpose methods (they have constant coefficients) or codes specially adapted to the oscillatory behavior

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of their solutions (they have variable coefficients depending on the frequency of each problem). Examples of such specially adapted algorithms are the exponentially or trigonometrically fitted methods (EF or TF methods) [3–22]. After the pioneering papers of Gautschi [6] and others [3, 5, 7, 13], the theory on EF linear multistep methods and EF Runge-Kutta (RK) type methods for first and second order differential systems is well known and a detailed survey on this subject can be found in Ixaru and Vanden Berghe [22].

The derivation of EF methods is usually based on the selection of the coefficients of the methods so that they are exact (within round-off error) for a set of linearly independent functions which are chosen according to the a-priori known information on the nature of the solutions of the differential system to be solved. Some authors [3, 4, 7, 9, 10, 13] have derived EFRK methods with frequency-dependent coefficients that are able to integrate exactly first or second order differential systems whose solutions belong to the linear space (fitting space) generated by the set of functions $\{1, t, \ldots, t^k, \exp(\pm\lambda t), t\ \exp(\pm\lambda t), \ldots, t^p\ \exp(\pm\lambda t)\}$, where λ is a prescribed frequency. The construction of explicit EFRK-Nyström methods has been analyzed in [5, 11, 16], and methods up to order five have been derived. Recently, the construction of explicit EF two-step hybrid methods of high order as an alternative to EFRKN methods has been investigated for some authors [20, 21], and they have derived methods up to order seven. In practical applications, it has been shown that EF methods are more accurate and efficient than non-fitted ones provided that the main frequency of the problem or a good approximation of it is known in advance. Therefore, the problem of how to choose a good approximation of the fitted frequency is crucial for an efficient implementation of these methods. Some procedures for the frequency determination in EF methods have been analyzed in [14, 15], but this problem is very difficult and it is still pending to be solved. Recently, Ramos and Vigo-Aguiar [18] have shown that the fitted frequency strongly depends on several factors: the differential equation, the initial conditions and the step-size.

In this paper, we investigate the derivation of explicit EFMTSH methods with algebraic orders seven and eight and reduced number of stages. The MTSH methods were recently introduced by Kalogiratou et al. [21] and these authors have derived TF schemes up to order seven. The EFMTSH methods integrate exactly second–order differential systems whose solutions can be expressed as linear combinations of the set of functions $\{\exp(\lambda t),\ \exp(-\lambda t)\}$, $\lambda \in \mathbb{C}$, or equivalently $\{\sin(\omega t),\ \cos(\omega t)\}$ when $\lambda = i\omega$, $\omega \in \mathbb{R}$. One important property for a method to perform efficiently is the accuracy versus the computational cost. In general, this fact depends on the algebraic order and the number of stages per step used by each method. So, the purpose of this paper is the design and construction of explicit EFMTSH methods so that the ratio *number of stages/algebraic order* is as small as possible, which leads to obtain practical and efficient codes.

The paper is organized as follows: In section 2 we present the MTSH methods and we derive the EF conditions and the conditions for this class of EFMTSH methods to have algebraic order p (with $p \leq 8$). These order conditions, up to order four, were already justified in [21]. With the help of these order conditions and the EF conditions, in section 3 we derive explicit EFMTSH methods with algebraic orders seven and eight. In section 4 we present some numerical experiments with several orbital and oscillatory IVPs that show the efficiency of the new EFMTSH methods when they are compared with other EF and standard two-step hybrid codes proposed in the scientific literature. Section 5 is devoted to present some conclusions.

2 Exponentially fitted modified two-step hybrid methods

In this section we present the EFMTSH methods which are the goal of our study as well as the notation to be used in the rest of the paper. First we recall the basic concepts on classical two-step hybrid (TSH) methods. Next we introduce the modified TSH methods (MTSH methods) and we derive the EF conditions and the conditions for this class of EFMTSH methods to have algebraic order p (with $p \leq 8$).

2.1 Two-step hybrid methods

We consider s-stage two–step hybrid methods for solving the IVP (1) defined by the equations

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

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

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. The equations (2) will be referred to as the internal stages, and equation (3) as the advance formula of the two–step hybrid method. These methods are characterized by the real parameters b_i, c_i and a_{ij}, and they can be represented in Butcher notation by the tableau

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} \quad = \quad \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \tag{4}$$

or equivalently by the triplet $(\mathbf{c}, \mathbf{A}, \mathbf{b})$. The conditions for a two–step hybrid method to have algebraic order of accuracy p have been investigated in Coleman [23] by using the theory of B-series. So, as it is usual in the case of RK or RKN methods, this author obtains an expansion of the local truncation error in the form

$$y(t_{n+1}) - y_{n+1} = \sum_{j \geq 1} h^{j+1} \left(\sum_{\rho(\tau_i)=j+1} e_j(\tau_i)\, F(\tau_i)(y_n) \right), \tag{5}$$

where $F(\tau_i)$ denotes the elementary differential associated to tree τ_i, and

$$e_j(\tau_i) = \frac{\alpha(\tau_i)}{(j+1)!} \left[1 + (-1)^{j+1} - \mathbf{b}^T \mathbf{\Psi}''(\tau_i) \right], \qquad \tau_i \in T_2, \qquad \rho(\tau_i) = j+1, \tag{6}$$

with $\alpha(\tau_i)$, $\rho(\tau_i)$, $\mathbf{\Psi}''(\tau_i)$ and T_2 defined in [23]. Therefore, a two–step hybrid method possesses algebraic order p iff

$$e_{\rho(\tau_i)-1}(\tau_i) = 0, \qquad \forall\, \tau_i \in T_2, \quad \text{with} \quad 2 \leq \rho(\tau_i) \leq p+1, \tag{7}$$

or equivalently

$$\mathbf{b}^T \mathbf{\Psi}''(\tau_i) = 1 + (-1)^{\rho(\tau_i)}, \qquad \forall\, \tau_i \in T_2, \quad \text{with} \quad 2 \leq \rho(\tau_i) \leq p+1. \tag{8}$$

Assuming the following two simplifying conditions are satisfied (stage order ≥ 3)

$$\mathbf{A}\,\mathbf{e} = \frac{1}{2}\left(\mathbf{c}^2 + \mathbf{c}\right), \qquad \mathbf{A}\,\mathbf{c} = \frac{1}{6}\left(\mathbf{c}^3 - \mathbf{c}\right), \tag{9}$$

the order conditions (8) (up to order ≤ 8) are listed in Table 1 (see [23]). Here $\mathbf{e}$ represents the vector $\mathbf{e} = (1, \ldots, 1)^T \in \mathbb{R}^s$ and the operation " $\cdot$ " represents the componentwise product: $\mathbf{v} \cdot \mathbf{w} = (v_1 w_1, \ldots, v_s w_s)^T \in \mathbb{R}^s$, $\mathbf{v}^k = \mathbf{v} \cdot \mathbf{v} \cdots \mathbf{v} \in \mathbb{R}^s$ (k-times).

Table 1: Order conditions for TSH methods up to order ≤ 8

Order p	Conditions
1–4	$\mathbf{b}^T\mathbf{e} = 1, \quad \mathbf{b}^T\mathbf{c} = 0, \quad \mathbf{b}^T\mathbf{c}^2 = 1/6, \quad \mathbf{b}^T\mathbf{c}^3 = 0,$
5	$\mathbf{b}^T\mathbf{c}^4 = 1/15, \quad \mathbf{b}^T\mathbf{A}\,\mathbf{c}^2 = 1/180,$
6	$\mathbf{b}^T\mathbf{c}^5 = 0, \quad \mathbf{b}^T\left(\mathbf{c}\cdot\mathbf{A}\,\mathbf{c}^2\right) = 1/72, \quad \mathbf{b}^T\mathbf{A}\,\mathbf{c}^3 = 0,$
7	$\mathbf{b}^T\mathbf{c}^6 = 1/28, \quad \mathbf{b}^T\left(\mathbf{c}^2\cdot\mathbf{A}\,\mathbf{c}^2\right) = 1/336, \quad \mathbf{b}^T\left(\mathbf{c}\cdot\mathbf{A}\,\mathbf{c}^3\right) = -11/1680,$ $\mathbf{b}^T\mathbf{A}\,\mathbf{c}^4 = 1/840, \quad \mathbf{b}^T\mathbf{A}^2\,\mathbf{c}^2 = 1/10080,$
8	$\mathbf{b}^T\mathbf{c}^7 = 0, \quad \mathbf{b}^T\left(\mathbf{c}^3\cdot\mathbf{A}\,\mathbf{c}^2\right) = 1/180, \quad \mathbf{b}^T\left(\mathbf{c}^2\cdot\mathbf{A}\,\mathbf{c}^3\right) = 0,$ $\mathbf{b}^T\left(\mathbf{c}\cdot\mathbf{A}\,\mathbf{c}^4\right) = 1/180, \quad \mathbf{b}^T\left(\mathbf{c}\cdot\mathbf{A}^2\,\mathbf{c}^2\right) = -1/1080, \quad \mathbf{b}^T\mathbf{A}\,\mathbf{c}^5 = 0,$ $\mathbf{b}^T\mathbf{A}\left(\mathbf{c}\cdot\mathbf{A}\,\mathbf{c}^2\right) = 1/2160, \quad \mathbf{b}^T\mathbf{A}^2\,\mathbf{c}^3 = 0$

The analysis of the phase properties for classical two-step methods is carried out by using the linear test model

$$y''(t) = -\theta^2\,y(t), \quad \theta > 0. \tag{10}$$

When a two-step hybrid method (4) is applied to solve the linear test model (10), the following recursion is obtained

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

where the coefficients $S(H)$ and $P(H)$ are given by

$$S(H,\nu) = 2 - H^2\,\mathbf{b}^T\,(\mathbf{I} + H^2\,\mathbf{A})^{-1}\,(\mathbf{e} + \mathbf{c}), \tag{12}$$

$$P(H,\nu) = 1 - H^2\,\mathbf{b}^T\,(\mathbf{I} + H^2\,\mathbf{A})^{-1}\,\mathbf{c}. \tag{13}$$

Therefore, the phase properties of these methods are determined by the roots of the characteristic polynomial

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

So, in the scientific literature the following concepts are used:

- $I_s = \{H > 0 \,|\, P(H) < 1 \text{ and } |S(H)| < 1 + P(H)\}$ is called the *stability interval.*
- $I_p = \{H > 0 \,|\, P(H) = 1 \text{ and } |S(H)| < 2\}$ is called the *periodicity interval.*
- The interval $I = (0, H_0)$, where H_0 is the maximum value such that $I \subset I_s$ or $I \subset I_p$ is called the *primary stability interval* or the *primary periodicity interval*, respectively.
- If $I_s = (0, \infty)$, the method is called *A-stable.*
- If $I_p = (0, \infty)$, the method is called *P-stable.*

In addition, the quantities

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

are called the *dispersion error* and the *dissipation error*, respectively. If these quantities satisfy

$$\phi(H) = \mathcal{O}(H^{q+1}), \qquad d(H) = \mathcal{O}(H^{r+1}), \tag{16}$$

then the method is said to be *dispersive of order* q and *dissipative of order* r, respectively.

2.2 Modified two–step hybrid methods

In order to derive TF schemes which integrate exactly the trigonometric functions $\sin(\lambda t)$ and $\cos(\lambda t)$, Kalogiratou et al. [21] have introduced some modifications of the classical TSH methods in the following form

$$Y_i = \beta_i(h)(1 + c_i)y_n - \gamma_i(h)c_i y_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(t_n + c_j h, Y_j), \quad i = 1, \ldots, s \tag{17}$$

$$y_{n+1} = 2\beta_{s+1}(h)y_n - \gamma_{s+1}(h)y_{n-1} + h^2 \sum_{i=1}^{s} b_i f(t_n + c_i h, Y_i), \tag{18}$$

where the real parameters b_i, c_i and a_{ij} are constant as in the case of classical TSH methods. Now these modified TSH methods can be represented in Butcher notation by the table

$$\begin{array}{c|cc|c} \mathbf{c} & \beta(h) & \gamma(h) & \mathbf{A} \\ \hline & \beta_{s+1}(h) & \gamma_{s+1}(h) & \mathbf{b}^T \end{array} \quad = \quad \begin{array}{c|cc|ccc} c_1 & \beta_1(h) & \gamma_1(h) & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & \beta_s(h) & \gamma_s(h) & a_{s1} & \cdots & a_{ss} \\ \hline & \beta_{s+1}(h) & \gamma_{s+1}(h) & b_1 & \cdots & b_s \end{array} \tag{19}$$

and when $\beta_i(h) = \gamma_i(h) = 1$, $i = 1, \ldots, s + 1$, the algorithm (17)–(18) reduces to a classical TSH method (2)–(3).

The idea of constructing methods which integrate exactly a set of linearly independent functions different from the polynomials has been proposed by several authors (see for example [3, 5, 6, 7, 9, 10, 12]). This idea consists of selecting the available parameters of the modified TSH method (17)–(18) in order to make the method exact for a linear space of functions with basis

$$\mathcal{F} = \langle u_1(t),\, u_2(t),\, \ldots\, ,\, u_r(t)\rangle.$$

In such case, the following conditions should be satisfied:

$$u_k(t_n+h) = 2\beta_{s+1}(h)u_k(t_n) - \gamma_{s+1}(h)u_k(t_n-h) + h^2\sum_{i=1}^{s} b_i\, u_k''(t_n+c_i\,h), \tag{20}$$

$$u_k(t_n+c_i\,h) = \beta_i(h)(1+c_i)\,u_k(t_n) - \gamma_i(h)c_i\,u_k(t_n-h) + h^2\sum_{j=1}^{s} a_{ij}\,u_k''(t_n+c_j\,h), \tag{21}$$

$$i=1,\dots,s, \quad k=1,\dots,r.$$

The most usual case is to consider exponential or trigonometric functions as reference set of functions:

$$\mathcal{F}_1 = \{\exp(\lambda t),\ \exp(-\lambda t)\} \quad \text{or} \quad \mathcal{F}_2 = \{\sin(\omega t),\ \cos(\omega t)\}.$$

The trigonometric case $\mathcal{F}_2$ is obtained from $\mathcal{F}_1$ with $\lambda = i\omega$. For the reference set of functions $\mathcal{F}_1$ the linear relations (20)–(21) reduce to

$$\gamma_{s+1}(z) = 1 - \frac{z^2}{\sinh(z)}\,\mathbf{b}^T\,\sinh(\mathbf{c}\,z), \tag{22}$$

$$\beta_{s+1}(z) = \frac{1}{2}\left((1+\gamma_{s+1}(z))\,\cosh(z) - z^2\,\mathbf{b}^T\,\cosh(\mathbf{c}\,z)\right), \tag{23}$$

$$\mathbf{c}\cdot\gamma(z) = \frac{1}{\sinh(z)}\left(\sinh(\mathbf{c}\,z) - z^2\,\mathbf{A}\,\sinh(\mathbf{c}\,z)\right), \tag{24}$$

$$(\mathbf{e}+\mathbf{c})\cdot\beta(z) = \mathbf{c}\cdot\gamma(z)\,\cosh(z) + \cosh(\mathbf{c}\,z) - z^2\,\mathbf{A}\,\cosh(\mathbf{c}\,z), \tag{25}$$

where $z = \lambda\,h$ and

$$\sinh(\mathbf{c}\,z) = (\sinh(c_1\,z),\dots,\sinh(c_s\,z))^T, \quad \cosh(\mathbf{c}\,z) = (\cosh(c_1\,z),\dots,\cosh(c_s\,z))^T.$$

The conditions defined by equations (22)–(25) characterize when a modified TSH method (17)–(18) is exponentially–fitted, and therefore they will be called exponential fitting conditions (EF conditions). A modified TSH method (17)–(18) which satisfies the EF conditions (22)–(25) will be called an EF modified TSH method (EFMTSH method).

Now we present an analysis on the variable coefficients $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ and $\beta(z)$ which will be of great utility in order to study the algebraic order reached by an EFMTSH method. From the EF conditions (22)–(25) we have that these coefficients are smooth even functions of the parameter $z = \lambda\,h$ and they have expansions of the form

$$\gamma_{s+1}(z) = 1 + \gamma_{s+1}^{(2)}\,z^2 + \gamma_{s+1}^{(4)}\,z^4 + \gamma_{s+1}^{(6)}\,z^6 + \cdots, \quad \gamma(z) = \mathbf{e} + \gamma^{(2)}\,z^2 + \gamma^{(4)}\,z^4 + \gamma^{(6)}\,z^6 + \cdots,$$

$$\beta_{s+1}(z) = 1 + \beta_{s+1}^{(2)}\,z^2 + \beta_{s+1}^{(4)}\,z^4 + \beta_{s+1}^{(6)}\,z^6 + \cdots, \quad \beta(z) = \mathbf{e} + \beta^{(2)}\,z^2 + \beta^{(4)}\,z^4 + \beta^{(6)}\,z^6 + \cdots.$$

From the EF condition (22) and the expansions of the hyperbolic functions we have

$$\gamma_{s+1}(z) = 1 - \frac{z}{\sinh(z)}\sum_{k\geq 1}\left(\mathbf{b}^T\,\mathbf{c}^{2k-1}\right)\frac{z^{2k}}{(2k-1)!}.$$

So, if we assume that the triplet $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ defines a classical TSH method with algebraic order p we have the following conclusion:

• If p is even, $p = 2\,r$, then $\mathbf{b}^T\,\mathbf{c}^{2k-1} = 0$, $k = 1, \ldots, r$ (see Table 1) and having in mind that

$$\frac{z}{\sinh(z)} = 1 + \mathcal{O}\left(z^2\right),$$

we have $\gamma_{s+1}(z) = 1 + \mathcal{O}\left(z^{2r+2}\right) = 1 + \mathcal{O}\left(z^{p+2}\right)$.

• If p is odd, $p = 2\,r - 1$, then $\mathbf{b}^T\,\mathbf{c}^{2k-1} = 0$, $k = 1, \ldots, r-1$, and we have

$$\gamma_{s+1}(z) = 1 + \gamma_{s+1}^{(2r)}\, z^{2r} + \mathcal{O}\left(z^{2r+2}\right), \qquad \gamma_{s+1}^{(2r)} = -\frac{1}{(2r-1)!}\left(\mathbf{b}^T\,\mathbf{c}^{2r-1}\right),$$

i.e., $\gamma_{s+1}(z) = 1 + \mathcal{O}\left(z^{p+1}\right)$.

Similarly, from (23) and the expansions of $\gamma_{s+1}(z)$ and the hyperbolic functions we have

$$\beta_{s+1}(z) = 1 + \frac{1}{2}\sum_{k\geq 0}\left(\frac{2}{(2k+2)(2k+1)} - \mathbf{b}^T\,\mathbf{c}^{2k}\right)\frac{z^{2k+2}}{2k!} + \frac{1}{2}\gamma_{s+1}^{(2r)}\, z^{2r} + \mathcal{O}\left(z^{2r+2}\right),$$

where

$$\gamma_{s+1}^{(2r)} = \begin{cases} 0, & \text{if } p = 2r \text{ (even)} \\ -\frac{1}{(2r-1)!}\left(\mathbf{b}^T\,\mathbf{c}^{2r-1}\right), & \text{if } p = 2r-1 \text{ (odd).} \end{cases}$$

• If p is even, $p = 2\,r$, then

$$\mathbf{b}^T\,\mathbf{c}^{2k} = \frac{2}{(2k+2)(2k+1)}, \quad k = 0, \ldots, r-1,$$

(see Table 1) and we have $\beta_{s+1}(z) = 1 + \mathcal{O}\left(z^{2r+2}\right) = 1 + \mathcal{O}\left(z^{p+2}\right)$.

• If p is odd, $p = 2\,r - 1$, then we also have

$$\mathbf{b}^T\,\mathbf{c}^{2k} = \frac{2}{(2k+2)(2k+1)}, \quad k = 0, \ldots, r-1,$$

and $\beta_{s+1}(z) = 1 + \frac{1}{2}\gamma_{s+1}^{(2r)}\, z^{2r} + \mathcal{O}\left(z^{2r+2}\right) = 1 + \mathcal{O}\left(z^{p+1}\right)$.

So, we have the following property on the coefficients $\gamma_{s+1}(z)$ and $\beta_{s+1}(z)$ of an EFMTSH method:

Property 2.1 *For an EFMTSH method (17)–(18) such that the triplet* $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ *defines a classical TSH method with algebraic order p, their coefficients* $\gamma_{s+1}(z)$ *and* $\beta_{s+1}(z)$ *satisfy*

$$\gamma_{s+1}(z) = \begin{cases} 1 + \mathcal{O}\left(z^{p+2}\right), & \text{if } p \text{ is even} \\ 1 + \mathcal{O}\left(z^{p+1}\right), & \text{if } p \text{ is odd.} \end{cases} \tag{26}$$

$$\beta_{s+1}(z) = \begin{cases} 1 + \mathcal{O}\left(z^{p+2}\right), & \text{if } p \text{ is even} \\ 1 + \frac{1}{2}\gamma_{s+1}^{(p+1)}\, z^{p+1} + \mathcal{O}\left(z^{p+3}\right), & \text{if } p \text{ is odd.} \end{cases} \tag{27}$$

From the expansion of $\gamma(z)$, the EF condition (24) and the expansions of the hyperbolic functions we have the following relationships:

$$\mathbf{c}\cdot\gamma^{(2)} = \frac{1}{6}\left(\mathbf{c}^3-\mathbf{c}\right) - \mathbf{A}\,\mathbf{c}, \tag{28}$$

$$\mathbf{c}\cdot\gamma^{(4)} = \frac{1}{3!}\left(\frac{1}{20}\left(\mathbf{c}^5-\mathbf{c}\right) - \mathbf{A}\,\mathbf{c}^3 - \mathbf{c}\cdot\gamma^{(2)}\right), \tag{29}$$

$$\mathbf{c}\cdot\gamma^{(6)} = \frac{1}{5!}\left(\frac{1}{42}\left(\mathbf{c}^7-\mathbf{c}\right) - \mathbf{A}\,\mathbf{c}^5 - 20\,\mathbf{c}\cdot\gamma^{(4)} - \mathbf{c}\cdot\gamma^{(2)}\right). \tag{30}$$

Similarly, from (25) and the expansions of $\beta(z)$ and the hyperbolic functions we obtain

$$\beta^{(2)} + \mathbf{c}\cdot\beta^{(2)} - \mathbf{c}\cdot\gamma^{(2)} = \frac{1}{2}\left(\mathbf{c}^2+\mathbf{c}\right) - \mathbf{A}\,\mathbf{e}, \tag{31}$$

$$\beta^{(4)} + \mathbf{c}\cdot\beta^{(4)} - \mathbf{c}\cdot\gamma^{(4)} = \frac{1}{2!}\left(\frac{1}{12}\left(\mathbf{c}^4+\mathbf{c}\right) - \mathbf{A}\,\mathbf{c}^2 + \mathbf{c}\cdot\gamma^{(2)}\right), \tag{32}$$

$$\beta^{(6)} + \mathbf{c}\cdot\beta^{(6)} - \mathbf{c}\cdot\gamma^{(6)} = \frac{1}{4!}\left(\frac{1}{30}\left(\mathbf{c}^6+\mathbf{c}\right) - \mathbf{A}\,\mathbf{c}^4 + 12\,\mathbf{c}\cdot\gamma^{(4)} + \mathbf{c}\cdot\gamma^{(2)}\right). \tag{33}$$

So, we have the following property on the coefficients $\gamma(z)$ and $\beta(z)$ of an EFMTSH method:

Property 2.2 *For an EFMTSH method (17)–(18) such that the triplet* $(\mathbf{c},\mathbf{A},\mathbf{b})$ *defines a classical TSH method satisfying the two simplifying conditions (9), their coefficients* $\gamma(z)$ *and* $\beta(z)$ *satisfy*

$$\gamma^{(2)} = 0, \qquad \mathbf{c}\cdot\gamma^{(4)} = \frac{1}{3!}\left(\frac{1}{20}\left(\mathbf{c}^5-\mathbf{c}\right) - \mathbf{A}\,\mathbf{c}^3\right), \tag{34}$$

$$\mathbf{c}\cdot\gamma^{(6)} = \frac{1}{5!}\left(\frac{1}{42}\left(\mathbf{c}^7-\mathbf{c}\right) - \mathbf{A}\,\mathbf{c}^5 - 20\,\mathbf{c}\cdot\gamma^{(4)}\right), \tag{35}$$

$$\beta^{(2)} = 0, \qquad \beta^{(4)} + \mathbf{c}\cdot\beta^{(4)} - \mathbf{c}\cdot\gamma^{(4)} = \frac{1}{2!}\left(\frac{1}{12}\left(\mathbf{c}^4+\mathbf{c}\right) - \mathbf{A}\,\mathbf{c}^2\right), \tag{36}$$

$$\beta^{(6)} + \mathbf{c}\cdot\beta^{(6)} - \mathbf{c}\cdot\gamma^{(6)} = \frac{1}{4!}\left(\frac{1}{30}\left(\mathbf{c}^6+\mathbf{c}\right) - \mathbf{A}\,\mathbf{c}^4 + 12\,\mathbf{c}\cdot\gamma^{(4)}\right). \tag{37}$$

Finally, we study the algebraic order of accuracy for EFMTSH methods. These methods integrate exactly IVPs whose solutions belong to linear spaces generated by the basis $\{\exp(\lambda t), \exp(-\lambda t)\}$ or $\{\cos(\omega t), \sin(\omega t)\}$, but for IVPs with more general solutions they present local truncation errors. Therefore, an EFMTSH method possesses algebraic order p iff the local truncation error satisfies

$$y(t_{n+1}) - y_{n+1} = \mathcal{O}\left(h^{p+2}\right). \tag{38}$$

The local truncation error for classical TSH methods (2)–(3) has been analyzed by Coleman [23] by using the theory of B-series (see subsection 2.1) and the order conditions (up to order eight) are listed in Table 1. In the case of EFMTSH methods, the local truncation error has an expansion in the form

$$y(t_{n+1}) - y_{n+1} = \sum_{j\geq 1} h^{j+1} \left(\sum_{\rho(\tau_i)=j+1} e_j(\tau_i)\, F(\tau_i)(y_n) + \sum_{\rho(\tau_i^*)=j+1} e_j^*(\tau_i^*)\, F^*(\tau_i^*)(y_n) \right), \quad (39)$$

where the tree τ_i^*, the elementary differential $F^*(\tau_i^*)$ and the coefficients $e_j^*(\tau_i^*)$ appear because of the variable coefficients $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ and $\beta(z)$, and these additional terms lead to some additional order conditions.

Assuming that the triplet $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ defines a pth-order classical TSH method satisfying the two simplifying conditions (9) and taking into account Properties 2.1 and 2.2, i.e.,

$$\gamma^{(2)} = 0, \quad \beta^{(2)} = 0, \quad \beta_{s+1}^{(p+1)} = \frac{1}{2}\,\gamma_{s+1}^{(p+1)} \quad \text{if } p \text{ is odd},$$

we have computed the additional order conditions for EFMTSH methods (up to order ≤ 8), which are listed in Table 2.

Table 2: Additional order conditions for EFMTSH methods up to order ≤ 8

Order p	Conditions
5	$\mathbf{b}^T \left(\beta^{(4)} + \mathbf{c}\cdot\beta^{(4)} - \mathbf{c}\cdot\gamma^{(4)}\right) = 0,$
6	$\mathbf{b}^T \left(\mathbf{c}\cdot\beta^{(4)} + \mathbf{c}^2\cdot\beta^{(4)} - \mathbf{c}^2\cdot\gamma^{(4)}\right) = 0, \quad \mathbf{b}^T \left(\mathbf{c}\cdot\gamma^{(4)}\right) = 0,$
7	$\mathbf{b}^T \left(\mathbf{c}^2\cdot\beta^{(4)} + \mathbf{c}^3\cdot\beta^{(4)} - \mathbf{c}^3\cdot\gamma^{(4)}\right) = 0, \quad \mathbf{b}^T \left(\mathbf{c}^2\cdot\gamma^{(4)}\right) = 0,$ $\mathbf{b}^T \left(\beta^{(6)} + \mathbf{c}\cdot\beta^{(6)} - \mathbf{c}\cdot\gamma^{(6)}\right) = 0,$
8	$\mathbf{b}^T \left(\mathbf{c}^3\cdot\beta^{(4)} + \mathbf{c}^4\cdot\beta^{(4)} - \mathbf{c}^4\cdot\gamma^{(4)}\right) = 0, \quad \mathbf{b}^T \left(\mathbf{c}^3\cdot\gamma^{(4)}\right) = 0,$ $\mathbf{b}^T \left(\mathbf{c}\cdot\beta^{(6)} + \mathbf{c}^2\cdot\beta^{(6)} - \mathbf{c}^2\cdot\gamma^{(6)}\right) = 0, \quad \mathbf{b}^T \left(\mathbf{c}\cdot\gamma^{(6)}\right) = 0,$

So, we have the following theorem on the algebraic order:

Theorem 2.3 *An EFMTSH method (17)–(18) such that the triplet* $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ *defines a classical TSH method satisfying the two simplifying conditions (9) and their coefficients satisfy the conditions given in Tables 1 and 2 has algebraic order* p *(with* p *up to eight).*

We note that the case of algebraic order up to $p = 4$ for TF modified TSH methods (TFMTSH methods) has been analyzed in Kalogiratou et al. [21]. These authors have found that if a classical TSH method defined by the triplet $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ has algebraic order four then the corresponding TFMTSH method has the same algebraic order (see Remark 3 of [21]). However, they have derived TFMTSH methods based on classical TSH methods $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ of orders 5, 6 and 7 but they have not justified the algebraic order of these new TF schemes. In the following theorem we give a justification of the algebraic order reached by an EFMTSH method (up to order eight) with regard to its classic counterpart.

Theorem 2.4 *If a classical TSH method defined by the triplet* $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ *and satisfying the two simplifying conditions (9) has algebraic order p (with p up to eight) then the corresponding EFMTSH method with coefficients* $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ *and* $\beta(z)$ *computed from the EF conditions (22)–(25) has the same algebraic order.*

Proof: We will see that if the order conditions given in Table 1 are satisfied then the additional order conditions given in Table 2 are also satisfied.

From Property 2.2 and Table 1 the fifth-order additional condition given in Table 2 is satisfied:

$$\mathbf{b}^T \left(\beta^{(4)} + \mathbf{c} \cdot \beta^{(4)} - \mathbf{c} \cdot \gamma^{(4)}\right) = \frac{1}{2!} \left(\frac{1}{12} \left(\mathbf{b}^T \mathbf{c}^4 + \mathbf{b}^T \mathbf{c}\right) - \mathbf{b}^T \mathbf{A} \mathbf{c}^2 \right) = \frac{1}{2!} \left(\frac{1}{12} \frac{1}{15} - \frac{1}{180} \right) = 0.$$

Similarly, for the sixth-order additional condition:

$$\mathbf{b}^T \left(\mathbf{c} \cdot \gamma^{(4)}\right) = \frac{1}{3!} \left(\frac{1}{20} \left(\mathbf{b}^T \mathbf{c}^5 - \mathbf{b}^T \mathbf{c}\right) - \mathbf{b}^T \mathbf{A} \mathbf{c}^3 \right) = \frac{1}{3!} (0 - 0) = 0.$$

For the following seventh-order additional condition we have

$$\begin{aligned} \mathbf{b}^T \left(\beta^{(6)} + \mathbf{c} \cdot \beta^{(6)} - \mathbf{c} \cdot \gamma^{(6)}\right) &= \frac{1}{4!} \left(\frac{1}{30} \left(\mathbf{b}^T \mathbf{c}^6 + \mathbf{b}^T \mathbf{c}\right) - \mathbf{b}^T \mathbf{A} \mathbf{c}^4 + 12 \, \mathbf{b}^T \left(\mathbf{c} \cdot \gamma^{(4)}\right) \right) \\ &= \frac{1}{4!} \left(\frac{1}{30} \frac{1}{28} - \frac{1}{840} + 0 \right) = 0. \end{aligned}$$

Finally we see that the following eighth-order additional condition is satisfied

$$\begin{aligned} \mathbf{b}^T \left(\mathbf{c}^3 \cdot \beta^{(4)} + \mathbf{c}^4 \cdot \beta^{(4)} - \mathbf{c}^4 \cdot \gamma^{(4)}\right) &= \frac{1}{2!} \left(\frac{1}{12} \left(\mathbf{b}^T \mathbf{c}^7 + \mathbf{b}^T \mathbf{c}^4\right) - \mathbf{b}^T \left(\mathbf{c}^3 \cdot \mathbf{A} \mathbf{c}^2\right) \right) \\ &= \frac{1}{2!} \left(\frac{1}{12} \frac{1}{15} - \frac{1}{180} \right) = 0. \end{aligned}$$

The remaining additional conditions given in Table 2 can be checked in a similar way. □

In next section we apply the above mentioned ideas to the construction of explicit EFMTSH methods with algebraic orders seven and eight.

3 Explicit EFMTSH methods of high order

In this section we analyze the construction of explicit EFMTSH methods of high order (orders seven and eight) with the help of Theorem 2.4 and the order conditions listed in the previous section. Therefore, we only need to construct the classic TSH methods defined by the triplet $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ and then to compute the coefficients $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ and $\beta(z)$ from the EF conditions (22)–(25). The construction of such TSH methods is carried out by paying special attention to optimize the number of function evaluations required in each step and the error terms associated to each method. So, we consider the class of explicit TSH methods presented in [24]

$$\begin{aligned} Y_1 &= y_{n-1}, \quad Y_2 = y_n, && (40)\\ Y_i &= (1+c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{i-1} a_{ij} f(t_n + c_j h, Y_j), \quad i = 3,\dots,s && (41)\\ y_{n+1} &= 2y_n - y_{n-1} + h^2 \left[b_1 f_{n-1} + b_2 f_n + \sum_{i=3}^{s} b_i f(t_n + c_i h, Y_i) \right], && (42) \end{aligned}$$

where f_{n-1} and f_n represent $f(t_{n-1}, y_{n-1})$ and $f(t_n, y_n)$, respectively, the two first nodes are $c_1 = -1$, $c_2 = 0$, and which can be represented by the table of coefficients

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

These methods (after the starting procedure) only require $s-1$ function evaluations in each step, and therefore they can be considered as two–step hybrid methods with $s-1$ stages per step.

3.1 Explicit EFMTSH methods with $s = 6$

First we analyze the case of explicit EFMTSH methods such that their classical counterparts $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ are defined by the table of coefficients

$$\begin{array}{c|cccccc} -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c_3 & a_{31} & a_{32} & 0 & 0 & 0 & 0 \\ c_4 & a_{41} & a_{42} & a_{43} & 0 & 0 & 0 \\ c_5 & a_{51} & a_{52} & a_{53} & a_{54} & 0 & 0 \\ c_6 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & 0 \\ \hline & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 \end{array}$$

In addition to the two simplifying conditions (9) we impose the following condition (stage order four):

$$\mathbf{A}\,\mathbf{c}^2 = \frac{1}{12}\left(\mathbf{c}^4 + \mathbf{c}\right). \quad (43)$$

This condition implies that the second condition of fifth order, the second condition of sixth order and the second and fifth conditions of seventh order in Table 1 are superfluous and the order conditions up to seven are reduced to

$$\mathbf{b}^T\mathbf{e} = 1, \quad \mathbf{b}^T\mathbf{c} = 0, \quad \mathbf{b}^T\mathbf{c}^2 = \frac{1}{6}, \quad \mathbf{b}^T\mathbf{c}^3 = 0, \quad \mathbf{b}^T\mathbf{c}^4 = \frac{1}{15}, \quad \mathbf{b}^T\mathbf{c}^5 = 0, \quad \mathbf{b}^T\mathbf{c}^6 = \frac{1}{28}, \quad (44)$$

$$\mathbf{b}^T\mathbf{A}\,\mathbf{c}^3 = 0, \quad \mathbf{b}^T\left(\mathbf{c}\cdot\mathbf{A}\,\mathbf{c}^3\right) = -\frac{11}{1680}, \quad \mathbf{b}^T\mathbf{A}\,\mathbf{c}^4 = \frac{1}{840}. \quad (45)$$

From (44) we can determine the coefficients b_i, $i = 1, \ldots, 6$ and c_6 in terms of the nodes c_3, c_4, and c_5.

From the simplifying conditions (9) and (43) we obtain $c_3 = (-1 \pm \sqrt{5})/2$ and the first three columns of the matrix A in terms of the nodes c_4, and c_5.

From (45) we obtain the coefficients a_{54}, a_{64} and a_{65} in terms of the nodes c_4, and c_5.

These coefficients define a two-parameter family of seventh-order classical TSH methods depending on the parameters c_4 and c_5. Now, by using the node $c_3 \in [-1, 1]$ (i.e., $c_3 = (-1 + \sqrt{5})/2$), we select the free parameters c_4 and c_5 so that the method is dissipative of order 9 and the dispersion error constant and the error terms associated to eighth-order conditions given in Table 1 are small, obtaining the values

$$c_4 = -0.98000000000000000000000000000000, \quad c_5 = -0.88127876738280697491311139563585,$$

$$\phi(H) = -2.28121 \times 10^{-7}\, H^9 + \mathcal{O}(H^{11}), \qquad d(H) = 6.41313 \times 10^{-8}\, H^{10} + \mathcal{O}(H^{12}),$$

and the remaining coefficients are given by

$$c_3 = 0.61803398874989484820458683436564, \quad c_6 = 0.82165281775952009354402306742730,$$

$$b_1 = 3.08581683313492242704871615018 71, \quad b_2 = 0.60562295108227648794883358065301,$$

$$b_3 = 0.19112149606479325234807733152312, \quad b_4 = -4.09264071271053622939797859642 32,$$

$$b_5 = 1.19638148649856132474262122841 71, \quad b_6 = 0.01369794592998273730973030564 2824,$$

$$a_{31} = 0.06366100187501752529923552760 5727, \quad a_{41} = -0.00543875915694865844752531866 40120,$$

$$a_{51} = 0.08408946964780400637280435905 8738, \quad a_{61} = -17.5000525437663280012799377972 64,$$

$$a_{32} = 0.43633899812498247470076447239427, \quad a_{42} = -0.00602658750971800821914134800 26547,$$

$$a_{52} = -0.02916385902685101495143843820 6684, \quad a_{62} = -0.14749883816470291408921337124 048,$$

$$a_{43} = 0.00166534666666666666666666666666667, \quad a_{53} = 0.00738448298096264444306049601 02130,$$

$$a_{63} = 0.35014332832278721606850445584170, \quad a_{54} = -0.11462334437343931989728478177952,$$

$$a_{64} = 18.81632828597707401107142930081 9, \quad a_{65} = -0.77053714702299069578178560132982.$$

The coefficients $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ and $\beta(z)$ of the EFMTSH method can be computed from the EF conditions (22)–(25) and the triplet of coefficients $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ determined above (see Appendix). The new EF scheme will be denoted as EFMTSH7a and for values of $|z| < 0.1$ series expansions for the coefficients $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ and $\beta(z)$ must be used.

Another possibility consists of selecting the free parameters c_4 and c_5 so that the coefficients of the method be small (for example, smaller than 5 in magnitude) and the error terms associated to eighth-order conditions given in Table 1 are small, obtaining the values

$$c_4 = -\frac{3}{10}, \quad c_5 = -\frac{1}{10},$$

and the remaining coefficients are given by

$c_3 = 0.61803398874989484820458683436564$, $\quad c_6 = 0.28099647054043483555828608347380$,

$b_1 = 0.02005375319819834763108355383907\text{2}$, $\quad b_2 = 3.78109038570970752079878592254\text{24}$,

$b_3 = 0.26764469079851380122569867462216$, $\quad b_4 = 1.35046625444693559799552348741\text{41}$,

$b_5 = -3.94117875329752040831851145462\text{47}$, $\quad b_6 = -0.47807633085583485933258018379310$,

$a_{31} = 0.06366100187501752529923552760572\text{7}$, $\quad a_{41} = -0.03241313028822097658926787378230\text{8}$,

$a_{51} = -0.01642296377907634041869671557716\text{9}$, $\quad a_{61} = 0.07950086842275285584614835530019\text{3}$,

$a_{32} = 0.43633899812498247470076447239427$, $\quad a_{42} = -0.09376186971177902341073212621769\text{2}$,

$a_{52} = -0.07212083148903433254133247299970\text{2}$, $\quad a_{62} = 0.26117422791895349662194453594602$,

$a_{43} = 0.02117500000000000000000000000000$, $\quad a_{53} = 0.01431338595562251348893068562077\text{9}$,

$a_{63} = -0.06954019178961195944065329096967\text{3}$, $\quad a_{54} = 0.02923040931248815947109850295609\text{1}$,

$a_{64} = -0.35114238413861755314330469352195$, $\quad a_{65} = 0.25998522308483130909795190943103$.

The coefficients $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ and $\beta(z)$ of the EFMTSH method can be computed from the EF conditions (22)–(25) and the triplet of coefficients $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ determined above (see Appendix). The new EF scheme will be denoted as EFMTSH7b and for values of $|z| < 0.1$ series expansions for the coefficients $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ and $\beta(z)$ must be used.

3.2 Explicit EFMTSH methods with $s = 7$

Now we analyze the case of explicit EFMTSH methods with $s = 7$ stages and algebraic order $p = 8$. As the number of stages is odd, we may consider that their classical counterparts $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ have symmetric nodes and weights. The use of symmetric nodes and weights produce a significant simplification on the order conditions given in Table 1, which make easier the determination of the methods. For example, these conditions of symmetry imply that the order conditions $\mathbf{b}^T\,\mathbf{c}^{2j-1} = 0$, $j \geq 1$ are satisfied. So, the TSH methods considered are defined by the table of coefficients

$$
\begin{array}{c|ccccccc}
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
c_3 & a_{31} & a_{32} & 0 & 0 & 0 & 0 & 0 \\
c_4 & a_{41} & a_{42} & a_{43} & 0 & 0 & 0 & 0 \\
-c_4 & a_{51} & a_{52} & a_{53} & a_{54} & 0 & 0 & 0 \\
-c_3 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & 0 & 0 \\
1 & a_{71} & a_{72} & a_{73} & a_{74} & a_{75} & a_{76} & 0 \\
\hline
 & b_1 & b_2 & b_3 & b_4 & b_4 & b_3 & b_1
\end{array}
$$

As in the previous case we impose stage order four, i.e., the simplifying conditions (9) and (43) are satisfied. This fact implies that the order conditions up to eight are reduced to

$$\mathbf{b}^T\mathbf{e} = 1, \qquad \mathbf{b}^T\mathbf{c}^2 = \frac{1}{6}, \qquad \mathbf{b}^T\mathbf{c}^4 = \frac{1}{15}, \qquad \mathbf{b}^T\mathbf{c}^6 = \frac{1}{28}, \tag{46}$$

$$\mathbf{b}^T \mathbf{A}\, \mathbf{c}^3 = 0, \qquad \mathbf{b}^T \left(\mathbf{c} \cdot \mathbf{A}\, \mathbf{c}^3 \right) = -\frac{11}{1680}, \qquad \mathbf{b}^T \mathbf{A}\, \mathbf{c}^4 = \frac{1}{840}, \tag{47}$$

$$\mathbf{b}^T \left(\mathbf{c}^2 \cdot \mathbf{A}\, \mathbf{c}^3 \right) = 0, \qquad \mathbf{b}^T \left(\mathbf{c} \cdot \mathbf{A}\, \mathbf{c}^4 \right) = \frac{1}{180}, \qquad \mathbf{b}^T \mathbf{A}\, \mathbf{c}^5 = 0, \qquad \mathbf{b}^T \mathbf{A}^2\, \mathbf{c}^3 = 0. \tag{48}$$

From (46) we can determine the weights b_i, $i = 1, \ldots, 4$ in terms of the nodes c_3, and c_4.

From the simplifying conditions (9) and (43) we obtain $c_3 = (-1 \pm \sqrt{5})/2$ and the first three columns of the matrix A in terms of the node c_4.

From (47) we obtain the coefficients a_{54}, a_{64} and a_{65} in terms of the node c_4.

From (48) we obtain the coefficients a_{74}, a_{75} and a_{76} in terms of the node c_4 and this node is given by the solution of a polynomial equation. By using the node $c_3 \in [-1, 1]$ (i.e., $c_3 = (-1 + \sqrt{5})/2$), the solutions of this polynomial equation are

$$c_4 = \frac{1}{102} \left(-51 + 31\sqrt{5} \mp \sqrt{18014 - 5202\sqrt{5}} \right).$$

The first solution of c_4 (sign $-$) produces a classical TSH method of order eight which has a stability interval I = (0, 2.98), whereas the second solution (sign $+$) produces an eighth-order method which has an empty stability interval. Therefore, we take the first solution of c_4 (sign -) and the coefficients of the eighth-order classical TSH method are given by

$c_3 = 0.6180339887498948482045868343656$4, $\quad c_4 = -0.60361914843378467005821789391586$,

$b_1 = 0.011651728688930353027299666937631$, $\quad b_2 = 0.51947751687932440043114591744000$,

$b_3 = -0.65949479954651251899793764693423$, $\quad b_4 = 0.88810431241791996575506502127660$,

$a_{31} = 0.063661001875017525299235527605727$, $\quad a_{41} = -0.048676708161310607769243506817295$,

$a_{51} = 0.049173998832250328388575859388615$, $\quad a_{61} = -0.062293944614421084490136695298785$,

$a_{71} = 0.039472354440919364453059750618307$, $\quad a_{32} = 0.43633899812498247470076447239427$,

$a_{42} = -0.095663985355783978667718213793155$, $\quad a_{52} = 0.40156534362389296645399661944370$,

$a_{62} = -0.11486701806504414582013691616516$, $\quad a_{72} = 0.20871568187537993404275699541582$,

$a_{43} = 0.024709157478165936457939939165124$, $\quad a_{53} = 0.0043346869436031400359458063709320$,

$a_{63} = 0.079841832378202140731191303674826$, $\quad a_{73} = -3.0135229557356315769798758973816$,

$a_{54} = 0.028913582995109585200677827267291$, $\quad a_{64} = 0.029384441951982111748783178458801$,

$a_{74} = 5.6896089441316356692133881504757$, $\quad a_{65} = -0.050099300400613870374287705035320$,

$a_{75} = 3.3945986758246996404491087296343$, $\quad a_{76} = -5.3188727005370030311784377287625$.

The coefficients $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ and $\beta(z)$ of the EFMTSH method can be computed from the EF conditions (22)–(25) and the triplet of coefficients $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ determined above (see Appendix). The new EF scheme will be denoted as EFMTSH8 and for values of $|z| < 0.1$ series expansions for the coefficients $\gamma_{s+1}(z)$, $\beta_{s+1}(z)$, $\gamma(z)$ and $\beta(z)$ must be used.

4 Numerical experiments

In this section we are going to present some numerical results to show the behaviour of the new explicit EFMTSH methods studied in section 3 when they are applied to some orbital problems and related oscillatory IVPs. The new EF integrators EFMTSH7a, EFMTSH7b and EFMTSH8 have been compared with the following standard and EF schemes denoted by:

- ETSHM7TF: The seventh-order TF two-step hybrid method derived by of Kalogiratou et al. [21].
- TSHM8_1: The eighth-order standard two-step hybrid method derived by Tsitouras [25].
- TSHM8_2: The eighth-order standard two-step hybrid method derived by Famelis [26].
- EFTSH8: The eighth-order EF two-step hybrid method recently derived in [27].

As usual, we employ efficiency plots, the so-called work-precision diagrams, computing the maximum global error ($\text{MGE} = \log_{10}(\max \|y(t_n)-y_n\|)$) over the whole integration interval and plotted against the number of required function evaluations. The algorithms were implemented in `python` by using the `mpmath` library with a precision of thirty two significant digits. All the figures have been represented in a log-log scale.

Problem 1. We consider the two-body gravitational problem (Kepler's plane problem) defined by the IVP

$$q_1'' = -\frac{q_1}{(q_1^2+q_2^2)^{3/2}}, \quad q_1(0) = 1-e, \quad q_1'(0) = 0,$$

$$q_2'' = -\frac{q_2}{(q_1^2+q_2^2)^{3/2}}, \quad q_2(0) = 0, \quad q_2'(0) = \sqrt{\frac{1+e}{1-e}},$$

where e $(0 \leq e < 1)$ represents the eccentricity of the orbit and whose exact solution is a 2π-periodic elliptic orbit with semimajor axis 1 given by

$$q_1(t) = \cos(u(t)) - e, \qquad q_2(t) = \sqrt{1-e^2}\,\sin(u(t)),$$

where $u(t)$ is the solution of Kepler's equation: $t = u(t) - e\,\sin(u(t))$. The integration is carried out on the interval $[0, 200\,\pi]$ with fitting parameter $\omega = 1$ $(\lambda = i\omega)$, and we select the eccentricity values $e = 0.05$ and $e = 0.25$. The numerical results obtained for this problem are presented in Figures 1a and 1b.

Problem 2. We consider a perturbed Kepler's problem defined by the IVP

$$q_1'' = -\frac{q_1}{(q_1^2+q_2^2)^{3/2}} - \delta\,\frac{(2+\delta)\,q_1}{(q_1^2+q_2^2)^{5/2}}, \quad q_1(0) = 1, \quad q_1'(0) = 0,$$

$$q_2'' = -\frac{q_2}{(q_1^2+q_2^2)^{3/2}} - \delta\,\frac{(2+\delta)\,q_2}{(q_1^2+q_2^2)^{5/2}}, \quad q_2(0) = 0, \quad q_2'(0) = 1+\delta,$$

where δ is a small positive parameter and whose analytic solution is

$$q_1(t) = \cos(t+\delta\,t), \qquad q_2(t) = \sin(t+\delta\,t).$$

The numerical results presented in Figure 2 have been computed with fitting parameter $\omega = 1$ ($\lambda = i\omega$), parameter of the perturbation $\delta = 10^{-2}$, and the problem is integrated up to $t_{end} = 400$.

Problem 3. We consider the Duffing's equation

$$q''(t) = -(\omega^2 + k^2)\, q(t) + 2\, k^2 q^3(t), \quad q(0) = 0, \quad q'(0) = \omega,$$

where the parameters satisfy $\omega > 0$, $0 \leq k < \omega$.

The solution of this oscillatory IVP represents a periodic motion in terms of a Jacobi's elliptic function given by

$$q(t) = \mathrm{sn}(\omega\, t, k/\omega).$$

In our test we choose the parameter values $\omega = 5$, $k = 0.03$, $t_{end} = 500$, and the numerical results are presented in Figure 3.

Problem 4. We consider the popular Bessel equation [26]

$$q''(t) + \left(100 + \frac{1}{4\, t^2}\right) q(t) = 0, \quad q(1) = J_0(10), \quad q'(1) = J_0(10)/2 - 10\, J_1(10),$$

where J_0 is the Bessel function of the first kind of order zero and whose analytic solution is

$$q(t) = \sqrt{t}\, J_0(10\, t).$$

This oscillatory IVP is solved until $t_{end} = 100$ and the numerical results are presented in Figure 4.

From the numerical results obtained in Figures 1–4 it follows that for the orbital problems and oscillatory IVPs under consideration the new explicit EF two-step hybrid integrators of high order (EFMTSH7a, EFMTSH7b and EFMTSH8) show an efficient behavior. In general, it can be observed that the new integrator EFMTSH8 and the recently published integrator EFTSH8 turn out to be the most efficient (when low accuracy or high accuracy is required) of all tested codes. This is due to the fact that the schemes EFMTSH8 and EFTSH8 have a larger accuracy order than the fitted schemes ETSHM7TF, EFMTSH7a and EFMTSH7b and the same accuracy order as the standard schemes $\mathrm{TSHM8}_1$ and $\mathrm{TSHM8}_2$. We note that the scheme EFMTSH8 requires six f-evaluations per step while EFTSH8 requires seven f-evaluations, and this fact is reflected in the computational cost shown in Figures 1–4. Among the seventh-order EF integrators, the codes EFMTSH7a and EFMTSH7b turn out to be more efficient than ETSHM7TF in some cases and in others the opposite happens, but in conclusion they show a very similar behaviour. Finally, we can observe that for oscillatory IVPs in which the linear terms are dominant (Problems 3 and 4) the eighth-order standard methods $\mathrm{TSHM8}_1$ and $\mathrm{TSHM8}_2$ specially designed for solving this type of problems may be more efficient than seventh-order fitted methods EFMTSH7a, EFMTSH7b and ETSHM7TF when a very high accuracy is required.

5 Conclusions

A detailed analysis on the construction of explicit EF modified two-step hybrid methods for solving orbital problems and second order oscillatory IVPs has been carried out. This analysis is based on combining the EF conditions with the triplet of coefficients $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ of optimal classical two-step hybrid methods in order to obtain efficient high order methods. New seventh-order and eighth-order explicit EF modified two-step schemes which are EF versions of new classical two-step hybrid methods are constructed. These new explicit EF modified two-step integrators show to be reliable alternatives to high-order standard [25, 26] and fitted [21, 27] two-step hybrid methods specially designed for solving oscillatory problems. The numerical experiments carried out with several orbital problems and related oscillatory IVPs show that the new high order explicit EF modified two-step integrators improve the computational efficiency obtained with standard and fitted two-step hybrid methods of high order from the scientific literature.

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Appendix

Here we present an algorithm to compute the coefficients $\gamma_i(z)$ and $\beta_i(z)$ of the EFMTSH methods (17)–(18) assuming that the triplet of coefficients $(\mathbf{c}, \mathbf{A}, \mathbf{b})$ is known:

For $i = 1, \ldots, s$

- If $c_i = -1$ or $c_i = 0$ *then*

$$\gamma_i(z) = 1, \quad \beta_i(z) = 1 \quad \text{and} \quad a_{ij} = 0, \quad j = 1, \ldots, s$$

- *else*

$$\gamma_i(z) = \frac{1}{c_i \sinh(z)} \left(\sinh(c_i\, z) - z^2 \sum_{j=1}^{s} a_{ij} \sinh(c_j\, z) \right),$$

$$\beta_i(z) = \left(c_i\, \gamma_i(z) \cosh(z) + \cosh(c_i\, z) - z^2 \sum_{j=1}^{s} a_{ij} \cosh(c_j\, z) \right) / (1 + c_i),$$

For $i = s + 1$

$$\gamma_{s+1}(z) = 1 - \frac{z^2}{\sinh(z)} \sum_{j=1}^{s} b_i \sinh(c_i\, z),$$

$$\beta_{s+1}(z) = \frac{1}{2} \left((1 + \gamma_{s+1}(z)) \cosh(z) - z^2 \sum_{j=1}^{s} b_i \cosh(c_i\, z) \right).$$

In the particular case of the explicit EFMTSH methods derived in section 3 we have: $c_1 = -1$, $c_2 = 0$, $a_{21} = 0$, $a_{ij} = 0$, $j \geq i = 1, \ldots, s$ and $c_3, \ldots, c_s$ different of -1 and 0. So, the algorithm reduces to

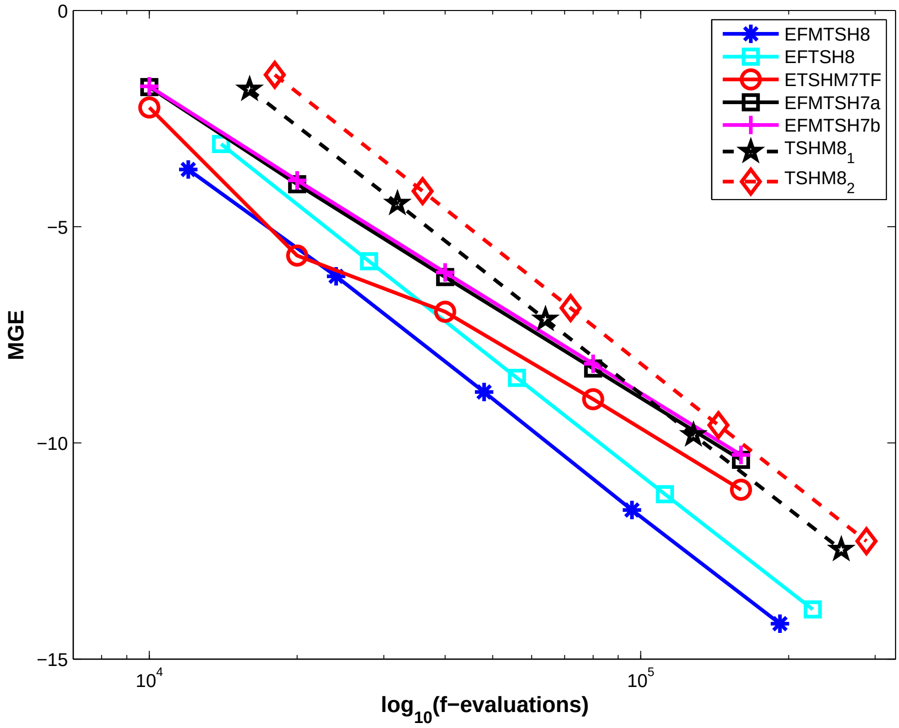

Figure 1a. Efficiency curves for Problem 1 with $e = 0.05$.

For $i = 1, 2$

$$\gamma_i(z) = 1, \quad \beta_i(z) = 1$$

For $i = 3, \ldots, s$

$$\gamma_i(z) = \frac{1}{c_i \, \sinh(z)} \left(\sinh(c_i \, z) - z^2 \sum_{j=1}^{i-1} a_{ij} \, \sinh(c_j \, z) \right),$$

$$\beta_i(z) = \left(c_i \, \gamma_i(z) \, \cosh(z) + \cosh(c_i \, z) - z^2 \sum_{j=1}^{i-1} a_{ij} \, \cosh(c_j \, z) \right) / (1 + c_i),$$

For $i = s + 1$

$$\gamma_{s+1}(z) = 1 - \frac{z^2}{\sinh(z)} \sum_{j=1}^{s} b_i \, \sinh(c_i \, z),$$

$$\beta_{s+1}(z) = \frac{1}{2} \left((1 + \gamma_{s+1}(z)) \, \cosh(z) - z^2 \sum_{j=1}^{s} b_i \, \cosh(c_i \, z) \right).$$

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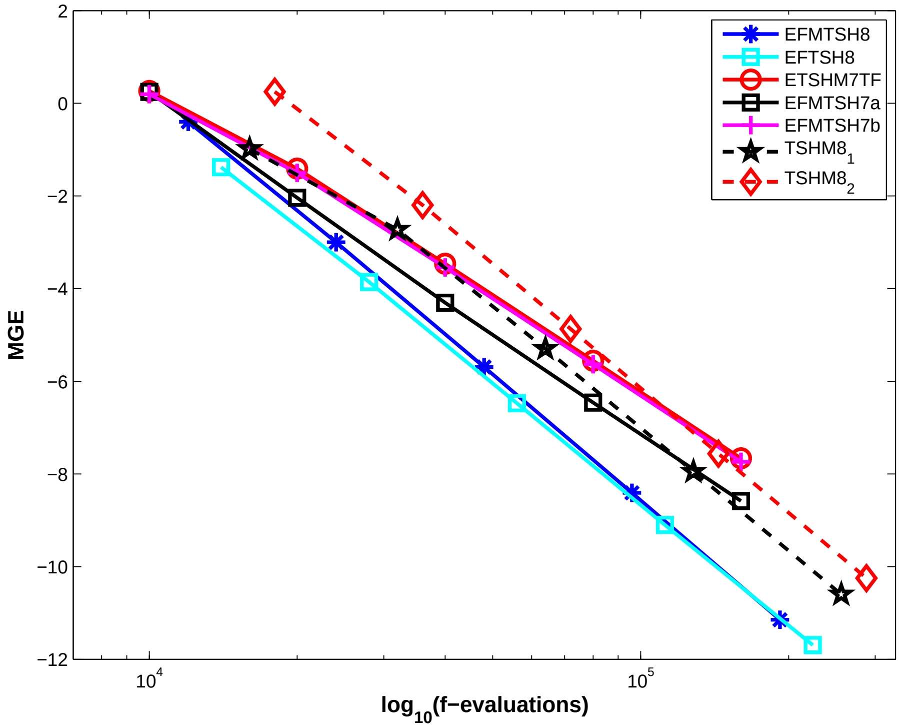

Figure 1b. Efficiency curves for Problem 1 with $e = 0.25$.

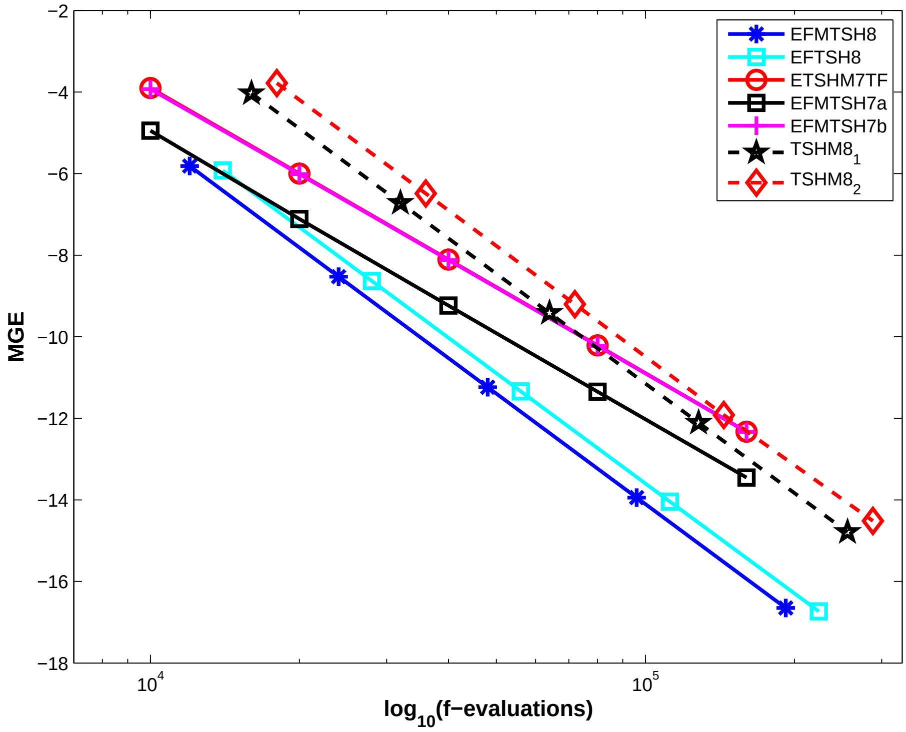

Figure 2. Efficiency curves for Problem 2.

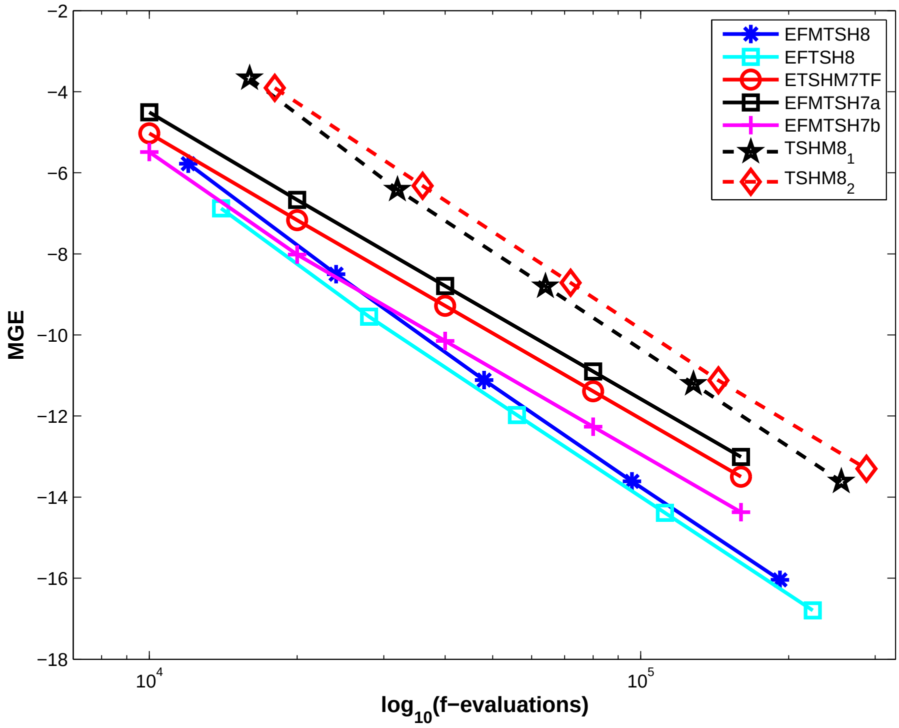

Figure 3. Efficiency curves for Problem 3.

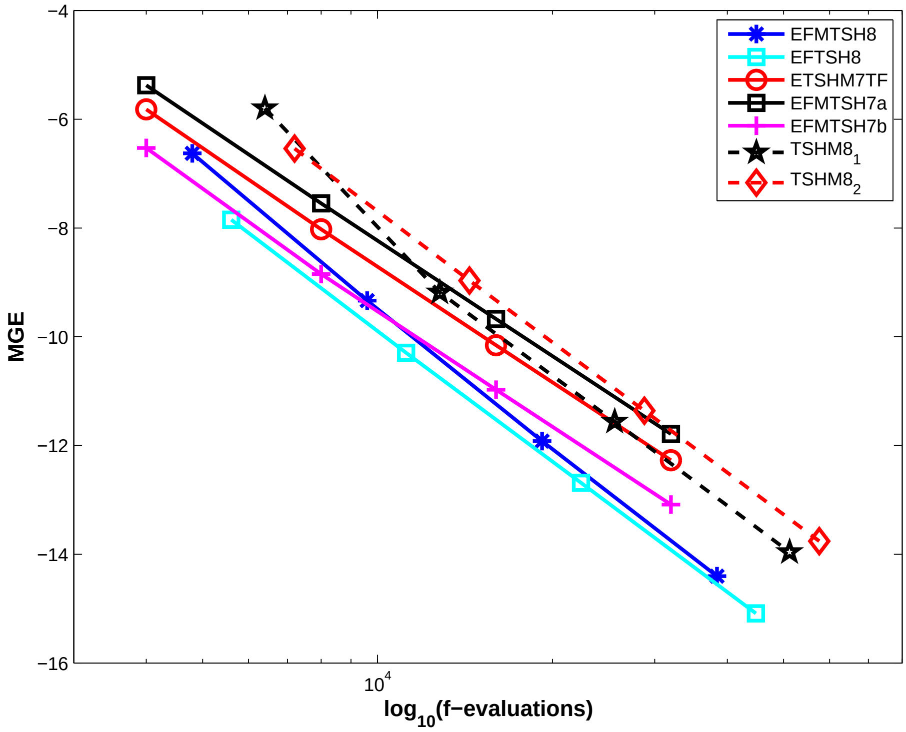

Figure 4. Efficiency curves for Problem 4.

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