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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.

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 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

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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

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

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

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. The Eqs. (2) will be referred to as the internal stages, and Eq. (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

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