Computer Physics Communications 185 (2014) 2527–2537

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Optimization of explicit two-step hybrid methods for solving orbital and oscillatory problems

J.M. Franco *, I. Gómez, L. Rández

IUMA, Departamento de Matemática Aplicada, Pza. San Francisco s/n., Universidad de Zaragoza, 50009 Zaragoza, Spain

ARTICLE INFO

Article history:
Received 6 July 2013
Received in revised form
13 May 2014
Accepted 30 May 2014
Available online 7 June 2014

Keywords:
Orbital problems
Oscillatory differential systems
Explicit two-step hybrid methods
Dissipation error
Dispersion error

ABSTRACT

The construction of optimized explicit two-step hybrid methods for solving orbital problems and oscillatory second order IVPs is analyzed. These methods have variable coefficients depending on the parameter $\nu = \omega h$, where h is the integration step-size and ω represents an approximation of the main frequency of the problem. Some optimized explicit two-step hybrid schemes with orders four and six are derived and their stability and phase properties are analyzed. The new methods have the property of being zero dissipative for all the values of the parameter ω whereas their dispersion errors (phase-lag) are optimized in terms of the relative error committed in the approximation of the main frequency of the problem. The numerical experiments carried out with several orbital and oscillatory problems show that the new optimized two-step schemes are more efficient than other methods recently proposed in the scientific literature for solving this class of problems.

1. Introduction

Orbital problems and oscillatory differential systems often arise in different fields of applied sciences and engineering such as celestial mechanics, astronomy and astrophysics, quantum chemistry, electronics, molecular dynamics and so on (see [1]), and they can be modeled by second order initial value problems (IVPs) of the form

$$y''(t) = f(t, y(t)), \qquad y(t_0) = y_0 \in \mathbb{R}^m, \qquad y'(t_0) = y'_0 \in \mathbb{R}^m, \tag{1}$$

where for simplicity $f(t, y)$ is assumed to be sufficiently smooth, so that the IVP (1) has a unique solution. Since the analytical solutions of these IVPs are usually not available, they can be solved by using general purpose numerical methods or using codes specially adapted to the oscillatory behavior of their solutions.

In the last decades, the design and construction of methods with variable coefficients for solving oscillatory IVPs (1) has been considered by several authors (see [2–27] and references therein). The coefficients of these methods usually depend on the parameter $\nu = \omega h$, where h is the integration step-size and ω represents an approximation of the main frequency of the problem. The aim of these methods is to use the available information on the particular structure and/or the behavior of the solutions of the corresponding problems to derive more accurate and efficient algorithms than the general purpose methods for such a type of problems. We mention the pioneering papers of Gautschi [2] and Bettis [3], in which exponentially fitted (EF) linear multistep methods and adapted RK algorithms, respectively, were introduced for solving differential systems with oscillatory solutions. The most representative examples of such algorithms are the phase-fitted methods [7,8] and the exponentially or trigonometrically fitted methods (EF or TF methods) [9–27]. In practical applications, it has been shown that phase-fitted methods and EF or TF 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 [28] have shown that the fitted frequency strongly depends on several factors: the differential equation, the initial conditions and the step-size.

* Corresponding author.
E-mail addresses: jmfranco@unizar.es (J.M. Franco), igomez@unizar.es (I. Gómez), randez@unizar.es (L. Rández).

http://dx.doi.org/10.1016/j.cpc.2014.05.030
0010-4655/

More recently, Kosti et al. [29,30] have optimized explicit Runge–Kutta–Nyström methods (RKN methods) with four stages and algebraic order five for solving oscillatory IVPs. When the main frequency of the problem is known exactly, these methods have the property of being zero dispersive and zero dissipative with zero first derivative of the dissipation error or with zero first derivative of the dispersion error. The numerical experiments given in [29,30] show that these optimized RKN methods are more accurate and efficient than their classical counterparts and a phase-fitted RKN method [8].

The purpose of this paper is the design and construction of explicit two-step hybrid methods which are optimized for solving orbital problems and related oscillatory IVPs. These methods are zero dispersive and zero dissipative when the main frequency of the problem is known exactly. But when the main frequency is known with a certain approximation, the methods have the property of being zero dissipative whereas the dispersion errors are optimized in terms of the relative error committed in this approximation. The paper is organized as follows: Section 2 is devoted to present the basic concepts on explicit two-step hybrid methods as well as the notation to be used in the rest of the paper. In Section 3 we present the optimization process which is based on the expansion of the dispersion and dissipation errors in powers of the relative error committed in the approximation of the main frequency of the problem. In Section 4 we study the construction of explicit two-step hybrid methods based on the optimization process stated in Section 3, and some particular methods with algebraic orders four and six are derived. The stability and phase properties of these new methods are analyzed. In Section 5 we carry out some numerical experiments to show the performance of the new optimized methods when they are compared with other methods proposed in the scientific literature for solving orbital problems and related oscillatory IVPs. Finally, Section 6 is devoted to present some conclusions.

2. Explicit two-step hybrid methods

In this section we present the explicit two-step hybrid methods which are the aim of our study and the notation to be used in the rest of the paper. We consider s-stage explicit two-step methods defined by the scheme [31]

$$\begin{cases} Y_1 = y_{n-1}, \qquad Y_2 = y_n, \\ Y_i = (1+c_i)y_n - c_i\, y_{n-1} + h^2 \sum_{j=1}^{i-1} a_{ij} f(t_n + c_j\, h, Y_j), \quad i = 3, \ldots, s, \\ y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{i=1}^{s} b_i f(t_n + c_i\, h, Y_i), \end{cases} \tag{2}$$

which can be represented by the table of coefficients

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} = \begin{array}{c|ccccc} -1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ c_3 & a_{31} & a_{32} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & 0 \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array} \tag{3}$$

A special feature of this class of explicit two-step methods is that, after the starting procedure, they only require $s-1$ function evaluations in each step, and therefore they can be considered as explicit two-step hybrid methods with $s-1$ stages per step.

We note that the derivation of classical two-step hybrid methods (3) with constant coefficients (up to order six) was analyzed in [31]. In this paper we analyze the derivation of fitted two-step hybrid methods (3) with variable coefficients which are optimized for solving oscillatory problems (see Section 4).

2.1. Classical methods

In the case of classical methods in which the coefficients c_i, b_i and a_{ij} are constants, the order conditions for two-step hybrid methods have been derived by Coleman [32], and these conditions up to order p are given by

$$\mathbf{b}^T \boldsymbol{\Psi}''(t_i) = 1 + (-1)^{\rho(t_i)}, \quad t_i \in T_2,\ \rho(t_i) = 2, \ldots, p+1, \tag{4}$$

where the parameters t_i, $\rho(t_i)$, $\boldsymbol{\Psi}''(t_i)$ and T_2 are defined in [32].

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

$$y''(t) = -\lambda^2 y(t), \quad \lambda > 0. \tag{5}$$

When an explicit two-step hybrid method (2) is applied to solve the linear test model (5), the following recursion is obtained

$$y_{n+1} - S(H)y_n + P(H)y_{n-1} = 0, \quad H = \lambda h, \tag{6}$$

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

$$S(H) = 2 - \mathbf{b}^T(\mathbf{e}+\mathbf{c})H^2 + \mathbf{b}^T\mathbf{A}(\mathbf{e}+\mathbf{c})H^4 - \cdots + (-1)^{s-1}\mathbf{b}^T\mathbf{A}^{s-2}(\mathbf{e}+\mathbf{c})H^{2s-2}, \tag{7}$$

$$P(H) = 1 - (\mathbf{b}^T\mathbf{c})H^2 + (\mathbf{b}^T\mathbf{A}\,\mathbf{c})H^4 - \cdots + (-1)^{s-1}(\mathbf{b}^T\mathbf{A}^{s-2}\,\mathbf{c})H^{2s-2}, \tag{8}$$

and the vector $\mathbf{e} = (1, \ldots, 1)^T \in \mathbb{R}^s$. The stability and phase properties of the methods are determined by the roots of the characteristic polynomial of the recursion (6):

$$\xi^2 - S(H)\xi + P(H). \tag{9}$$