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A new approach on the construction of trigonometrically fitted two step hybrid methods

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ABSTRACT

The construction of trigonometrically fitted two step hybrid methods for the numerical solution of second-order initial value problems is considered. These methods are suitable for the numerical integration of problems with periodic or oscillatory behavior of the solution and have variable coefficients depending on the frequency of each problem. The modification of classical two step hybrid methods is done by inserting extra parameters at each stage. We derive the coefficients of the modified methods for the general case of s stages. As examples we present the modifications of three methods of algebraic orders five, six and seven.

1. Introduction

In this work we consider the numerical integration of initial value problems associated to second order ordinary differential equations in which the first derivative does not appear explicitly:

$$y''(x) = f(x, y(x)), \quad x \in [x_0, X], \qquad y(x_0) = y_0, \qquad y'(x_0) = y'_0. \tag{1}$$

This special problem has been solved in the literature by using different approaches, such as one step (Runge–Kutta–Nyström) methods and multistep methods of Numerov type. Hybrid methods of the second category have been proposed by many authors since the pioneering work of Chawla [1], being the construction of these methods based on the evaluation at interpolatory off-step nodes with high accuracy. The maximum algebraic order attained is eight with ten stages, see [2,3]. Coleman [4] has investigated two step hybrid (TSH) methods in the framework of Runge–Kutta methods and derived order conditions; the advantage of using this approach is that we can obtain higher order with fewer stages.

Problems of the form in (1) often exhibit a pronounced oscillatory behavior and arise in many fields of applied sciences as in celestial mechanics and quantum mechanics. Many numerical methods that take into account this property of the solution

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have been developed in recent years by several authors, and can be categorized as methods with constant coefficients (phase lag, amplification error, interval of periodicity) and methods with variable coefficients that depend on the frequency of the problem (phase-fitted, amplification-fitted, trigonometrically-fitted). The explicit Numerov method of Chawla [1] is a three stages method and has algebraic order four. Franco [5] constructed several explicit TSH methods with constant coefficients using four and five stages, obtaining methods with algebraic orders five and six, reduced phase lag and amplification error. Bratsos et al. [6] constructed an explicit TSH method with six stages with variable coefficients, which is phase-fitted and amplification fitted and has algebraic order six. Van de Vyver [7,8] gave the general framework for constructing phase-fitted THS methods that are also dissipative and presented methods with five stages and sixth algebraic order. Trigonometrically fitted (TF) Numerov type methods have a long history, being some of the first works on this subject those of Stiefel–Bettis [9] and Raptis–Allison [10]. Fang and Wu [11,12] considered TF explicit TSH methods, which for each internal stage as well as for the advance stage integrate exactly the trigonometric functions $\{\cos(wx),\ \sin(wx)\}$ and presented TF modifications of two of the methods developed in [5].

In this work we present the general framework for constructing a TF modification of any classical TSH method. As illustration examples we present two modified methods based on a fifth and a sixth order method by Franco [5] with four and five stages. We also develop a seventh algebraic order method with six stages and its TF modification. In Section 2 we revise the theory of TSH methods following the work of Coleman [4]. In Section 3 we give the procedure of deriving modified TF methods from classical TSH methods, introducing in Section 4 some particular methods (which are modifications of the TSH methods in [5], and a new seventh order method). Stability features of the new methods are analyzed in Section 5. Numerical results are presented in Section 6 for the two body problem, a nonlinear oscillator, an oscillatory problem and the computation of the eigenvalues of the Schrödinger equation.

2. Two step hybrid methods

Coleman [4] has written the s stage TSH method in the form

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

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

whose associated Butcher tableau is given by

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{s,s} \\ \hline & b_1 & \cdots & b_s \end{array} \quad \text{or} \quad \begin{array}{c|c} c & A \\ \hline & b^T \end{array}.$$

We define the vector $e = (1, \ldots, 1)^T$ and the diagonal $s \times s$ matrix C with diagonal c (i.e. $C.e = c$).

Assuming the first two simplifying assumptions suggested in [4]

$$Ae = (c^2 + c)/2, \qquad Ac = (c^3 - c)/6,$$

the number of conditions up to algebraic order seven reduces to 14.

We will consider explicit methods (with $c_1 = -1$ and $c_2 = 0$) given by

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \left(b_1 f(x_{n-1}, Y_1) + b_2 f(x_n, Y_2) + \sum_{i=3}^{s} b_i f(x_n + c_i h, Y_i) \right) \tag{3}$$

$$\begin{aligned} Y_1 &= y_{n-1}, \\ Y_2 &= y_n, \\ Y_i &= (1+c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, Y_j), \quad i = 3, 4, \ldots, s. \end{aligned}$$

3. Modified TSH methods

3.1. Trigonometrically fitted conditions

Each internal stage of a RKN method can be seen as a linear multistep method on a non-equidistant grid. Consequently we want our modified methods to integrate exactly at each stage the trigonometric functions $\sin(wx)$ and $\cos(wx)$. The