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Multistep numerical methods for the integration of oscillatory problems in several frequencies

F. García-Alonso [a,*], J.A. Reyes [a], J.M. Ferrándiz [a], J. Vigo-Aguiar [b]

[a] Departamento de Matemática Aplicada, Universidad de Alicante, Apartado 99, E-03080 Alicante, Spain
[b] Dept. of Applied Mathematics, University of Salamanca, Plaza de los Caídos s/n (37008) Salamanca, Spain

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ABSTRACT

The perturbed harmonic oscillator appear frequently in the mathematical modelling of many problems in physics and engineering. The harmonic oscillator has a special purpose in Astrodynamics, because the Kunstaanheimo–Stiefel (KS) and Burdet–Ferrándiz (BF) transformations reduce the Kepler problem to harmonic oscillators.

A new multi-step methods of numerical integration are introduced that generalize SMF ones. They are defined for arbitrary order and have similar properties to the former methods.

Modified methods allowing step variations, whose coefficients are computed from relations of recurrence, are derived, what considerably improve the implementation of the algorithms.

These methods are based in a sequence of analytical φ-functions dependent on two parameters α and β that generalizes the Scheifele's G-functions and that, under wide hypothesis, allow us obtain the solution of harmonic oscillator.

In this paper a new methodology is generated to solve the problem which the φ-functions series create regarding the calculus of recurrence relations transforming the method into a multistep scheme. The methodology is implemented in a computational algorithm, which lets us solve in a general way the problems of physics and engineering which are modalized by means of the study of the harmonic oscillators.

Numerical examples already used by other authors are presented. They show how the new developed methods in this paper may compete in accuracy or efficiency with other well-reputed algorithms.

1. Introduction

In 1970, Scheifele [1,2] designed an algorithm able to integrate without truncation error the harmonic oscillator. The solution was expressed as series of the so-called G-functions. Scheifele's G-functions were used by Martín and Ferrándiz [3,4] to introduce a multistep fixed step method (SMF) to integrate perturbed harmonic oscillators. In last years, Vigo-Aguiar and Ferrándiz, introduced new VSVO multistep methods [5,6] using scalar G-functions, and with additional good properties.

On the other hand, around 1970, Stiefel and Bettis [7–9] introduced several fixed step multistep method. Stiefel and Bettis method changes a pair of coefficients of a classic Adams–Bashforth, Adams–Moulton [10] or Störmer–Cowell [11] algorithms for each oscillation that is exactly integrated. A general theory including those and other special integrators was developed by Vigo-Aguiar and Ferrándiz [5].

In the present paper our attention is focused on the issue of the numerical integration of equations of the form:

$$x'' + \alpha^2 x = \varepsilon \cdot f(x(t), x'(t), t), \qquad (1)$$
$$x(0) = x_0 \quad \text{and} \quad x'(0) = x'_0,$$

where α is a constant coefficient, ε being a small parameter of perturbation.

In [12], a numerical method is presented aiming at solving (1), which is consistent with the proper limiting behaviour of the perturbed solution because it integrates exactly the unperturbed problem. The most important asset is that it substantially reduces the accumulated error in many circumstances and values of the integration parameters. This method of φ-functions series not only integrates exactly the homogeneous problem, but also enables to eliminate somehow the perturbation term. In spite of the good behaviour of φ-functions series method, it is only practical for use in cases in which the function of perturbation is simple, given the complexity of the preliminary calculations needed to obtain the recurrence formulas.

This problem is resolved in this article by converting the φ-functions series method into a multistep scheme. The derivatives

* Corresponding author. Tel.: +34 965 903400x2050; fax: +34 965 909707.
E-mail address: Fernando.Garcia@ua.es (F. García-Alonso).

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will be substituted by expressions in term of divided differences and next to some coefficients d_{ij}, elements of a matrix A_p^{-t}, whose recurrence relation does not know. Similarly for the implicit case, it will be denoted by B_p^{-t}, the matrix whose coefficients d_{ij} are extracted.

Once the matrices A_p^{-t} and B_p^{-t} are know in, we will set up a recurrent calculus, through matrices $S_{p,n}$ and $S_{p,n+1}$.

The general good behaviour and the long term accuracy of the new method is shown through several examples, including the Duffing problem [3] and the highly oscillatory Denk's problem [13] and Petzold's problem [14,15]. The comparisons show that the new methods provide significantly higher accuracy and efficiency than a selection of classic well-reputed general-purpose integrators as GEAR, MGEAR or LSODE.

2. Construction of φ-functions and numerical methods

If we consider the IVP (1) corresponding to one forced oscillation of frequency α^2 and function of perturbation $f = f(x(t), x'(t), t)$.

Let us assume for the sake of simplicity that f and therefore the solution $x(t; x_0, x'_0, t_0)$ obtained with the initial conditions is analytical in $I = [-T, T]$. If we suppose that the partial derivatives of the function of perturbation are continuous in the independent variables x, x', t in I; with these conditions, the function of perturbation reduces along the solution to a function:

$$g(t) = f(x(t; x_0, x'_0, t_0), x'(t; x_0, x'_0, t_0), t) \tag{2}$$

that can be expressed $g(t)$ as an convergent power series.

By applying the differential operator $D^2 + \beta^2$ at the IVP (1), in order to cancel the perturbation, we obtain

$$D^4x + (\alpha^2 + \beta^2)D^2x + \alpha^2\beta^2x = (D^2 + \beta^2)\varepsilon g(t) \tag{3}$$

at the solution $x(t; x_0, x'_0, t_0)$.

The two first initial values are

$$x(0) = x_0, x'(0) = x'_0 \tag{4}$$

and from IVP(1) is deduced:

$$x''(0) = -\alpha^2x_0 + \varepsilon f(x_0, x'_0, 0) = x''_0 \tag{5}$$

and as

$$x'''(0) = -\alpha^2x'_0 + \varepsilon\,\vec{\nabla} f(x_0, x'_0, 0)\cdot(x'_0, x''_0, 1) = x'''_0. \tag{6}$$

A new IVP is considered:

$$(D^2 + \beta^2)(D^2 + \alpha^2)x = (D^2 + \beta^2)\varepsilon g(t), \tag{7}$$

$$x(0) = x_0,\quad x'(0) = x'_0,\quad x''(0) = x''_0,\quad x'''(0) = x'''_0.$$

The notation used is

$$L_4(x) = (D^2 + \beta^2)(D^2 + \alpha^2)x. \tag{8}$$

Based on the Taylor expansion we can write

$$g(t) = \sum_{n=0}^{\infty} c_n \frac{t^n}{n!} \tag{9}$$

and (9) at (7) replacing, the IVP (7) is expressed as

$$L_4(x) = \varepsilon\sum_{n=0}^{\infty}(c_{n+2} + \beta^2c_n)\frac{t^n}{n!}. \tag{10}$$

The solution $x(t)$ for the IVP (7) might be split in two parts: that corresponding to associated homogeneous IVP (7), $x_H(t)$, and that non-linear inhomogeneous equation with vanishing initial values, respectively.

In order to obtain a solution to the inhomogeneous equation, we recall that it can be cast as a superposition of solutions to the sequence of initial value problems:

$$L_4(x_n) = \frac{t^n}{n!}$$
$$x_n(0) = x'_n(0) = x''_n(0) = x'''_n(0) = 0. \tag{11}$$

If we define: $\Psi_n(t) = x_n$, for $n \geqslant 0$, yields

$$L_4(\Psi_n(t)) = \frac{t^n}{n!}$$
$$\Psi_n(0) = \Psi'_n(0) = \Psi''_n(0) = \Psi'''_n(0) = 0. \tag{12}$$

It is easy to prove that

$$\Psi'_n(t) = \Psi_{n-1}(t) \quad \text{for } n \geqslant 1 \tag{13}$$

and

$$\Psi_n(t) + (\alpha^2 + \beta^2)\Psi_{n+2}(t) + \alpha^2\beta^2\Psi_{n+4}(t) = \frac{t^{n+4}}{(n+4)!} \quad \text{for } n \geqslant 0. \tag{14}$$

The explicit and analytical expression for the Ψ_n-functions depend on the frequencies α and β.According to them five cases must be discussed:

2.1. Case I. ($\alpha \neq 0$, $\beta \neq 0$, $\alpha \neq \beta$)

The $\Psi_n(t)$-functions can be expressed as a series

$$\Psi_n(t) = \sum_{m=0}^{\infty}\frac{(-1)^m}{(2m+4+n)!}\frac{\beta^{2m+2} - \alpha^{2m+2}}{\beta^2 - \alpha^2}t^{2m+4+n}. \tag{15}$$

The derivation is simple. It is enough to suppose that

$$\Psi_n(t) = \sum_{k=0}^{\infty} b_k^{[n]}t^k. \tag{16}$$

By substituting it into (12) and identifying coefficients we obtain the equation

$$(k+4)(k+3)(k+2)(k+1)b_{k+4}^{[n]} + (\alpha^2 + \beta^2)(k+1)(k+2)b_{k+2}^{[n]} + \alpha^2\beta^2b_k^{[n]} = \frac{\delta_{k,n}}{k!} \tag{17}$$

with the initial conditions

$$b_0^{[n]} = b_1^{[n]} = b_2^{[n]} = b_3^{[n]} = 0. \tag{18}$$

Let us remark that the leading term of Ψ_n has the order t^{n+4}. A more compact form, can be get through suitable changes of the dummy indices. It results

$$\Psi_n(t) = \sum_{m=0}^{\infty} b_m^{[n]}t^{2m+4+n}, \tag{19}$$

where

$$b_m^{[n]} = \frac{(-1)^m}{(2m+4+n)!}\frac{\beta^{2m+2} - \alpha^{2m+2}}{\beta^2 - \alpha^2}. \tag{20}$$

In order to obtain the solution to the homogeneous equation, the "canonical" IVP's is introduced:

$$L_4(\varphi_i(t)) = 0, \tag{21}$$
$$\varphi_i^{j)}(0) = \delta_{ij} \quad i,j = 0,1,2,3,$$

$\delta_{i,j}$ being Kronecker deltas.

The functions $\varphi_n(t)$ for $n = 0,1,2,3$, can be expressed for the trigonometric functions