Applied Mathematics Letters 22 (2009) 1616–1621

Contents lists available at ScienceDirect

Applied Mathematics Letters

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

Closed Newton–Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems

T.E. Simos [*,1]

Laboratory of Computational Sciences, Department of Computer Science and Technology, Faculty of Science and Technology, University of Peloponnese, GR-221 00 Tripolis, Greece

ARTICLE INFO

Article history:
Received 2 February 2009
Received in revised form 16 March 2009
Accepted 27 April 2009

Keywords:
Numerical methods
Orbital problems
Closed Newton–Cotes differential methods
Symplectic integrators
Trigonometric fitting
Energy preservation

ABSTRACT

The connection between closed Newton–Cotes, trigonometrically-fitted differential methods and symplectic integrators is studied in this paper. Several one-step symplectic integrators have been obtained based on symplectic geometry, as is shown in the literature. However, the study of multi-step symplectic integrators is very limited. The well-known open Newton–Cotes differential methods are presented as multilayer symplectic integrators by Zhu et al. [W. Zhu, X. Zhao, Y. Tang, Journal of Chem. Phys. 104 (1996), 2275]. The construction of multi-step symplectic integrators based on the open Newton–Cotes integration methods is investigated by Chiou and Wu [J.C. Chiou, S.D. Wu, Journal of Chemical Physics 107 (1997), 6894]. The closed Newton–Cotes formulae are studied in this paper and presented as symplectic multilayer structures. We also develop trigonometrically-fitted symplectic methods which are based on the closed Newton–Cotes formulae. We apply the symplectic schemes in order to solve Hamilton's equations of motion which are linear in position and momentum. We observe that the Hamiltonian energy of the system remains almost constant as the integration proceeds. Finally we apply the new developed methods to an orbital problem in order to show the efficiency of this new methodology.

1. Introduction

The research area of development of numerical integration methods for ordinary differential equations that preserve qualitative properties of the analytic solution has been of great interest in recent years. Here we consider Hamilton's equations of motion which are linear in position p and momentum q

$$\begin{aligned} \dot{q} &= m\,p \\ \dot{p} &= -m\,q \end{aligned} \tag{1}$$

where m is a constant scalar or matrix. It is well known that Eq. (1) is important in the field of molecular dynamics. In order to preserve the characteristics of the Hamiltonian system in the approximate solution it is necessary to use symplectic integrators. In recent years some work has been done mainly in the construction of one-step symplectic integrators (see [1]). In their work Zhu et al. [2] and Chiou and Wu [3] constructed multi-step symplectic integrators by writing open Newton–Cotes differential schemes as multilayer symplectic structures.

In the past decades, much work has been done on exponential fitting and the numerical solution of periodic initial value problems (see [1,2,4–26,29] and references therein).

* Corresponding address: 10 Konitsis Street, Amfithea - Paleon Faliron, GR-175 64 Athens, Greece.
E-mail addresses: tsimos@mail.ariadne-t.gr, tsimos.conf@gmail.com.

1 Highly Cited Researcher in Mathematics. Active Member of the European Academy of Sciences and Arts. Active Member of the European Academy of Sciences. Corresponding Member of European Academy of Arts, Sciences and Humanities.

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doi:10.1016/j.aml.2009.04.008

In this paper we follow the steps described below:

- The closed Newton–Cotes differential methods are presented as multilayer symplectic integrators.
- The closed Newton–Cotes methods are applied on the Hamiltonian system (1) and as a result, the Hamiltonian energy of the system remains almost constant as the integration proceeds.
- The trigonometrically-fitted methods are constructed.

We note that the aim of this paper is to generate methods that can be used for nonlinear differential equations as well as linear ones.

The construction of the paper is given below. The results about symplectic matrices and schemes are presented in Section 2. In Section 3 we describe closed Newton–Cotes integral rules and differential methods and we develop the new trigonometrically-fitted methods. In Section 4 the conversion of the closed Newton–Cotes differential methods into multilayer symplectic structures is presented. Numerical results are presented in Section 5.

2. Basic theory on symplectic schemes and numerical methods

Based on Zhu et al. [2] we have:

Dividing an interval $[a, b]$ with N points we obtain:

$$x_0 = a, \qquad x_n = x_0 + nh = b, \quad n = 1, 2, \ldots, N. \tag{2}$$

We note that x is the independent variable and a and b in the equation for x_0 (Eq. (2)) are different from the a and b in Eq. (3).

The above division leads to the following discrete scheme:

$$\begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix} = M_{n+1} \begin{pmatrix} p_n \\ q_n \end{pmatrix}, \qquad M_{n+1} = \begin{pmatrix} a_{n+1} & b_{n+1} \\ c_{n+1} & d_{n+1} \end{pmatrix}. \tag{3}$$

Based on the above we can write the n-step approximation to the solution as:

$$\begin{aligned} \begin{pmatrix} p_n \\ q_n \end{pmatrix} &= \begin{pmatrix} a_n & b_n \\ c_n & d_n \end{pmatrix} \begin{pmatrix} a_{n-1} & b_{n-1} \\ c_{n-1} & d_{n-1} \end{pmatrix} \cdots \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} \\ &= M_n M_{n-1} \cdots M_1 \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}. \end{aligned}$$

Defining

$$S = M_n M_{n-1} \cdots M_1 = \begin{pmatrix} A_n & B_n \\ C_n & D_n \end{pmatrix}$$

the discrete transformation can be written as:

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = S \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}.$$

A discrete scheme (3) is a symplectic scheme if the transformation matrix S is symplectic.

A matrix A is symplectic if $A^{\mathrm{T}} J A = J$ where

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The product of symplectic matrices is also symplectic. Hence, if each matrix M_n is symplectic the transformation matrix S is also symplectic. Consequently, the discrete scheme (2) is symplectic if each matrix M_n is symplectic.

Remark 1. The proposed methods can be used for nonlinear differential equations as well as linear ones.

3. Trigonometrically-fitted closed Newton–Cotes differential methods

3.1. General closed Newton–Cotes formulae

The closed Newton–Cotes integral rules are given by:

$$\int_a^b f(x)\mathrm{d}x \approx z\, h \sum_{i=0}^{k} t_i f(x_i)$$

where

$$h = \frac{b-a}{N}, \qquad x_i = a + ih, \quad i = 0, 1, 2, \ldots, N.$$