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Research Article

New Stable Closed Newton-Cotes Trigonometrically Fitted Formulae for Long-Time Integration

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The closed Newton-Cotes differential methods of high algebraic order for small number of function evaluations are unstable. In this work, we propose a new closed Newton-Cotes trigonometrically fitted differential method of high algebraic order which gives much more efficient results than the well-know ones.

1. Introduction

In the recent years, there is a great interest in the construction of numerical methods for ordinary differential equations that preserve qualitative properties of the analytic solution.

Symplectic integrators are necessary in the case that we wish to preserve the characteristics of the Hamiltonian system in the approximate solution. Much research has been done recently mainly on the development of one-step symplectic integrators (see [1, 2]). In their work, Zhu et. al [3] and Chiou and Wu [4] constructed multistep symplectic integrators by writing open Newton-Cotes differential schemes as multilayer symplectic structures.

Last decades much work has been done on trigonometrically fitting and the numerical solution of periodic initial value problems (see [5–20] and references therein).

In this paper, we follow the steps described below.

(i) The new condition is described.

(ii) The trigonometrically fitted method is developed.

(iii) The closed Newton-Cotes differential methods are presented as multilayer symplectic integrators.

(iv) The closed Newton-Cotes methods are applied to nonlinear problems and the efficiency of the new methods is presented.

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.

(i) The theory for the symplectic schemes is presented in Section 2.

(ii) In Section 3, we present the closed Newton-Cotes differential methods and the new condition for the development of the methods. We also develop the new trigonometrically-fitted methods.

(iii) In Section 4, the conversion of the closed Newton-Cotes differential methods into multilayer symplectic structures is presented.

(iv) Numerical results are presented in Section 5.

2. Basic Theory on Symplectic Schemes and Numerical Methods

Based on Zhu et al. [3] and on the division of the interval $[a, b]$ with N points, we have the following discrete scheme for the n-step approximation to the solution:

$$\begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix} = M_{n+1} \begin{pmatrix} p_n \\ q_n \end{pmatrix}, \quad M_{n+1} = \begin{pmatrix} w_{n+1} & y_{n+1} \\ z_{n+1} & g_{n+1} \end{pmatrix}. \tag{2.1}$$

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

$$\begin{aligned} \begin{pmatrix} p_n \\ q_n \end{pmatrix} &= \begin{pmatrix} w_n & y_n \\ z_n & g_n \end{pmatrix} \begin{pmatrix} w_{n-1} & y_{n-1} \\ z_{n-1} & g_{n-1} \end{pmatrix} \cdots \begin{pmatrix} w_1 & y_1 \\ z_1 & g_1 \end{pmatrix} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} \\ &= M_n M_{n-1} \cdots M_1 \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}. \end{aligned} \tag{2.2}$$

Defining

$$S = M_n M_{n-1} \cdots M_1 = \begin{pmatrix} W_n & Y_n \\ Z_n & G_n \end{pmatrix}, \tag{2.3}$$

the discrete transformation can be written as

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = S \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}. \tag{2.4}$$

Table 1: Closed Newton-Cotes integral rules.

k	z	t_0	t_1	t_2	t_3	t_4	t_5	t_6	t_7	t_8
0	1	1								
1	1/2	1	1							
2	1/3	1	4	1						
3	3/8	1	3	3	1					
4	2/45	7	32	12	32	7				
5	5/288	19	75	50	50	75	19			
6	1/140	41	216	27	272	27	216	41		
7	7/17280	751	3577	1323	2989	2989	1323	3577	751	
8	4/14175	989	5888	−928	10496	−4540	10496	−928	5888	989

A discrete scheme (2.1) is a symplectic scheme if the transformation matrix S is symplectic. A matrix A is symplectic if $A^T JA = J$, where

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{2.5}$$

The product of symplectic matrices is also symplectic. Hence, if each matrix M_n is symplectic the transformation matrix S is symplectic. Consequently, the discrete scheme (3.5) is symplectic if each matrix M_n is symplectic.

Remark 2.1. 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 can be presented with the formula:

$$\int_a^b f(x)dx \approx zh\sum_{i=0}^{k} t_i f(x_i), \tag{3.1}$$

where

$$h = \frac{b-a}{N}, \qquad x_i = a + ih, \quad i = 0, 1, 2, \ldots, N. \tag{3.2}$$

The coefficient z as well as the weights t_i are given in Table 1.

Remark 3.1. It is easy for one to see that the coefficients t_i in the Table 1 are symmetric, that is, one has the following relation:

$$t_i = t_{k-i}, \quad i = 0, 1, \ldots, \frac{k}{2}. \tag{3.3}$$

The closed Newton-Cotes differential methods are produced from the integral rules. From Table 1 we have the following differential methods:

$$
\begin{aligned}
k=1 \qquad & y_{n+1}-y_n=\frac{h}{2}\left(f_{n+1}+f_n\right),\\
k=2 \qquad & y_{n+1}-y_{n-1}=\frac{h}{3}\left(f_{n-1}+4f_n+f_{n+1}\right),\\
k=3 \qquad & y_{n+1}-y_{n-2}=\frac{3h}{8}\left(f_{n-2}+3f_{n-1}+3f_n+f_{n+1}\right),\\
k=4 \qquad & y_{n+2}-y_{n-2}=\frac{2h}{45}\left(7f_{n-2}+32f_{n-1}+12f_n+32f_{n+1}+7f_{n+1}\right),\\
k=5 \qquad & y_{n+2}-y_{n-3}=\frac{5h}{288}\left(19f_{n-3}+75f_{n-2}+50f_{n-1}+50f_n\right.\\
& \qquad\left.+75f_{n+1}+19f_{n+2}\right),\\
k=6 \qquad & y_{n+3}-y_{n-3}=\frac{h}{140}\left(41f_{n-3}+216f_{n-2}+27f_{n-1}+272f_n\right.\\
& \qquad\left.+27f_{n+1}+216f_{n+2}+41f_{n+3}\right),\\
k=7 \qquad & y_{n+3}-y_{n-4}=\frac{7h}{17280}\left(751f_{n-4}+3577f_{n-3}+1323f_{n-2}+2989f_{n-1}\right.\\
& \qquad\left.+2989f_n+1323f_{n+1}+3577f_{n+2}+751f_{n+3}\right),\\
k=8 \qquad & y_{n+4}-y_{n-4}=\frac{4h}{14175}\left(989f_{n-4}+5888f_{n-3}-928f_{n-2}+10496f_{n-1}\right.\\
& \qquad\left.-4540f_n+10496f_{n+1}-928f_{n+2}+5888f_{n+3}+989f_{n+4}\right).
\end{aligned}
\tag{3.4}
$$

In the present paper, we will investigate the case $k = 8$ and we will produce trigonometrically fitted differential methods of order 1.

3.2. Development of Closed Newton-Cotes Differential Schemes

For the development of a Newton-Cotes differential method of the above form, two procedures can be applied.

(i) The procedure which is based on the minimization of the local truncation error. Based on this procedure and for the case $k = 8$, we can produce the well known coefficients: $a_4 = 3956/14175$, $a_3 = 23552/14175$, $a_2 = -3712/14175$, $a_1 = 41984/14175$, and $a_0 = -3632/2835$ (see the closed Newton-Cotes differential scheme for $k = 8$ presented above).

(ii) The procedure which is based on

(1) the minimization of the local truncation error;

(2) the satisfaction of the condition: $2(\sum_{i=1}^{n} |a_i| + |a_0|)/2n = 1$. This condition is produced by application of least squares method to the production of the differential method (see more details in [21] (about stable quadrature rules) and [22]).

The above procedure leads to the following coefficients for the case: $n = 4$: $a_0 = -19672/945 + 70a_4$, $a_1 = 1952/105 - 56a_4$, $a_2 = -848/105 + 28a_4$, $a_3 = 736/189 - 8a_4$ and to the condition $9836/33075 \leq a_4 \leq 244/735$. We choose the value: $a_4 = 3/10$, which satisfies the above condition.

3.3. Exponentially Fitted Closed Newton-Cotes Differential Method

Requiring the differential scheme:

$$\begin{aligned} y_{n+4} - y_{n-4} = h\big(& a_4 f_{n-4} + a_3 f_{n-3} + a_2 f_{n-2} + a_1 f_{n-1} + a_0 f_n \\ & + a_1 f_{n+1} + a_2 f_{n+2} + a_3 f_{n+3} + a_4 f_{n+4}\big) \end{aligned} \tag{3.5}$$

to be accurate for the following set of functions (we note that $f_i = y_i'$, $i = n-1, n, n+1$):

$$\left\{1,\ x,\ x^2,\ x^3,\ x^4,\ x^5,\ x^6,\ \cos(\mathrm{v}x),\ \sin(\mathrm{v}x)\right\}, \tag{3.6}$$

the following set of equations is obtained:

$$\begin{aligned} & 8\cos(w)\sin(w)\left(2(\cos(w))^2 - 1\right) \\ & = w\Big[2a_4 - 2a_2 + a_0 - 6a_3\cos(w) + 4a_2(\cos(w))^2 \\ & \qquad + 2a_1\cos(w) + 8a_3(\cos(w))^3 + 16a_4(\cos(w))^4 - 16a_4(\cos(w))^2\Big] \\ & 2a_4 + 2a_3 + 2a_2 + 2a_1 + a_0 = 8 \\ & 96a_4 + 54a_3 + 24a_2 + 6a_1 = 128 \\ & 2560a_4 + 810a_3 + 160a_2 + 10a_1 = 2048. \end{aligned} \tag{3.7}$$

Requesting that $a_4 = 3/10$ and solving the above system of equations, we obtain

$$a_0 = \frac{1735w\cos(w) + 1353w\cos(3w) + 242w\cos(2w) + 270w\cos(4w) - 900\sin(4w)}{675w\cos(w) + 45w\cos(3w) - 450w - 270w\cos(2w)},$$

$$a_1 = \frac{-1856w\cos(3w) - 1735w - 1404w\cos(2w) - 405w\cos(4w) + 1350\sin(4w)}{1350w\cos(w) + 90w\cos(3w) - 900w - 540w\cos(2w)},$$

$$a_2 = \frac{702w\cos(w) + 418w\cos(3w) - 121w + 81w\cos(4w) - 270\sin(4w)}{675w\cos(w) + 45w\cos(3w) - 450w - 270w\cos(2w)},$$

$$a_3 = \frac{-27w\cos(4w) - 836w\cos(2w) - 1353w + 1856w\cos(w) + 90\sin(4w)}{1350w\cos(w) + 90w\cos(3w) - 900w - 540w\cos(2w)}, \tag{3.8}$$

where $w = \text{v}h$.

For small values of v, the above formulae are subject to heavy cancellations. In this case the following Taylor series expansions must be used:

$$\begin{aligned}
a_0 = {} & \frac{4661}{3780} - \frac{4073}{5670}w^2 + \frac{40193}{249480}w^4 - \frac{6980443}{681080400}w^6 + \frac{9455989}{49037788800}w^8 \\
& - \frac{19551709}{8336424096000}w^{10} + \frac{69457813}{1900704693888000}w^{12} \\
& + \frac{3310479379}{4390627842881280000}w^{14} + \frac{58254816773}{1615751046180311040000}w^{16} \\
& + \frac{97232951747}{7561714896123855667200 0}w^{18} + \cdots, \\
a_1 = {} & \frac{499}{525} + \frac{4073}{7560}w^2 - \frac{40193}{332640}w^4 + \frac{6980443}{908107200}w^6 - \frac{9455989}{65383718400}w^8 \\
& + \frac{19551709}{11115232128000}w^{10} - \frac{69457813}{2534272925184000}w^{12} \\
& - \frac{3310479379}{5854170457175040000}w^{14} - \frac{58254816773}{2154334728240414720000}w^{16} \\
& - \frac{97232951747}{1008228652816514088960 00}w^{18} + \cdots, \\
a_2 = {} & \frac{781}{1050} - \frac{4073}{18900}w^2 + \frac{40193}{831600}w^4 - \frac{6980443}{2270268000}w^6 + \frac{9455989}{163459296000}w^8 \\
& - \frac{19551709}{27788080320000}w^{10} + \frac{69457813}{6335682312960000}w^{12} \\
& + \frac{3310479379}{14635426142937600000}w^{14} + \frac{58254816773}{5385836820601036800000}w^{16} \\
& + \frac{97232951747}{2520571632041285222400 00}w^{18} + \cdots, \\
a_3 = {} & \frac{6493}{4725} + \frac{4073}{113400}w^2 - \frac{40193}{4989600}w^4 + \frac{6980443}{13621608000}w^6 - \frac{9455989}{980755776000}w^8 \\
& + \frac{19551709}{166728481920000}w^{10} - \frac{69457813}{38014093877760000}w^{12}
\end{aligned}$$

$$- \frac{3310479379}{87812556857625600000} w^{14} - \frac{58254816773}{32315020923606220800000} w^{16}$$
$$- \frac{97232951747}{1512342979224771133440000} w^{18} + \cdots . \tag{3.9}$$

The behaviour of the coefficients is given in the following Figure 1.

The local truncation error for the above differential method is given by

$$\text{L.T.E}(h) = -\frac{593h^9}{28350}\left(y_n^{(9)} + \text{v}^2 y_n^{(7)}\right). \tag{3.10}$$

The L.T.E is obtained expanding the terms $y_{n\pm j}$ and $f_{n\pm j}$, $j = 1(1)4$ in (3.5) into Taylor series expansions and substituting the Taylor series expansions of the coefficients of the method.

In Figure 2, we present the behaviour of the quantity $\text{ST} = (2\sum_{i=1}^{n} |a_i| + |a_0|)/2n$ for several values of v.

So, we have the following theorem.

Theorem 3.2. *The method* (3.5) *with coefficients* a_i, $i = 0(1)4$, *obtained by the solution of the system* (3.7) *is accurate for the set of functions* (3.6) *and is of eighth algebraic order.*

4. Closed Newton-Cotes Can Be Expressed as Symplectic Integrators

Let consider Hamilton's equations of motion:

$$\dot{u} = my,$$
$$\dot{y} = -mu, \tag{4.1}$$

where m is a constant scalar or matrix. It is well known that (4.1) is important in the fields of physics, chemistry, material sciences, and so forth.

Theorem 4.1. *A discrete scheme of the form:*

$$\begin{pmatrix} w & -z \\ z & w \end{pmatrix}\begin{pmatrix} u_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} w & z \\ -z & w \end{pmatrix}\begin{pmatrix} u_n \\ y_n \end{pmatrix} \tag{4.2}$$

is symplectic.

Proof. We rewrite (4.2) as

$$\begin{pmatrix} u_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} w & -z \\ z & w \end{pmatrix}^{-1}\begin{pmatrix} w & z \\ -z & w \end{pmatrix}\begin{pmatrix} u_n \\ y_n \end{pmatrix}. \tag{4.3}$$

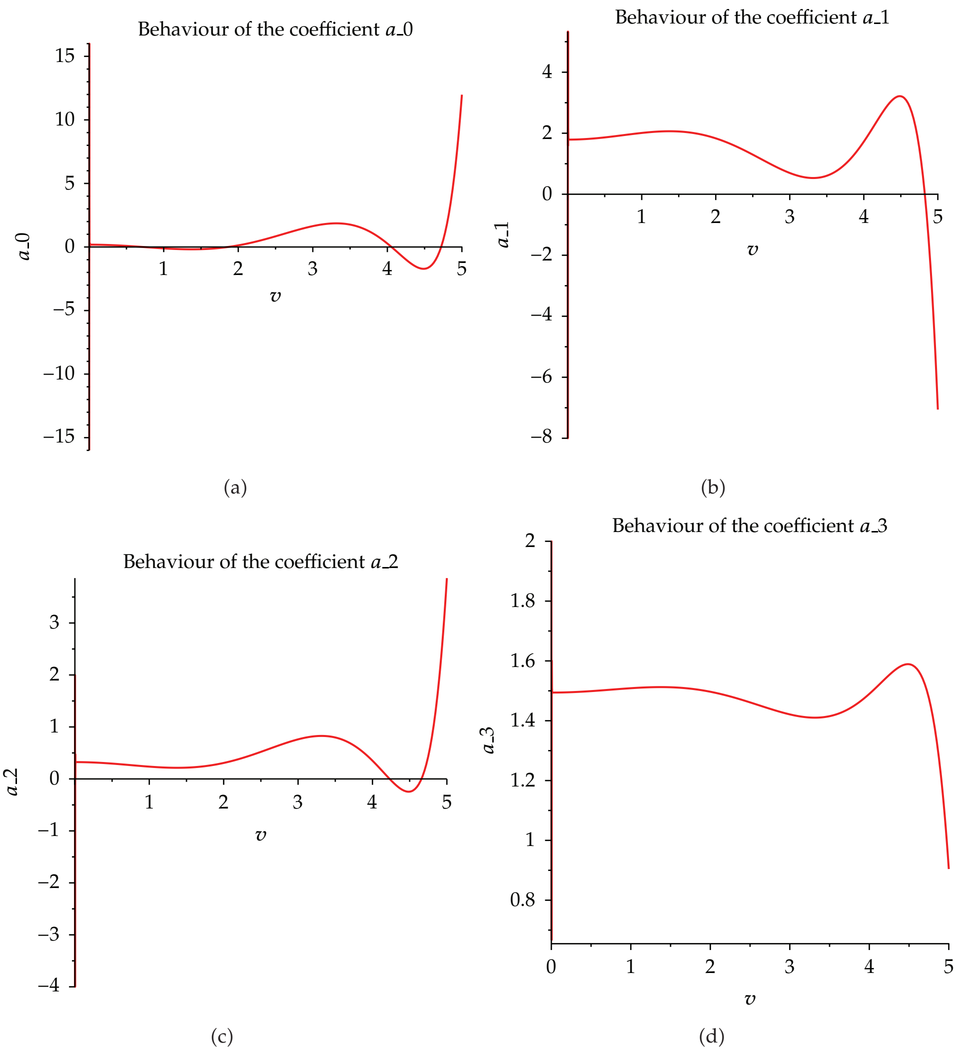

Figure 1: Behavior of the coefficients of the new proposed method given by (3.8) for several values of w.

Defining

$$M = \begin{pmatrix} w & -z \\ z & w \end{pmatrix}^{-1} \begin{pmatrix} w & z \\ -z & w \end{pmatrix} = \frac{1}{w^2 + z^2} \begin{pmatrix} w^2 - z^2 & 2wz \\ -2wz & w^2 - w^2 \end{pmatrix}, \tag{4.4}$$

it can easily be proved that

$$M^T J M = J. \tag{4.5}$$

Thus, the matrix M is symplectic.

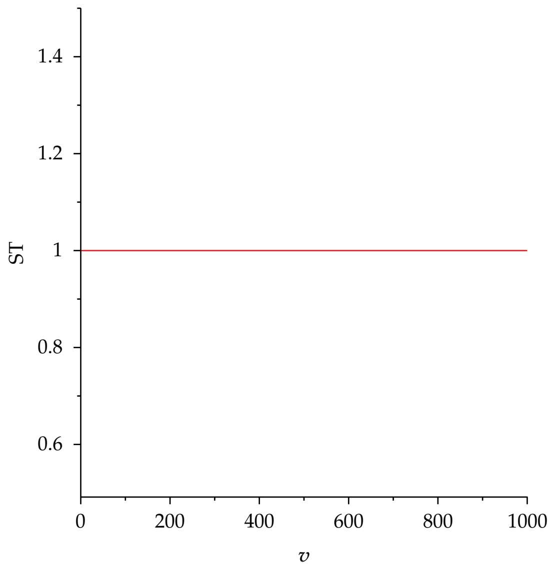

Figure 2: Behaviour of the quantity ST for several values of v.

In [3], Zhu et al. have studied the well-known second-order differential scheme (SOD). They have proved that the scheme:

$$q_{n+i} - q_{n-i} = 2ihf_n, \qquad i = 1(1)4 \tag{4.6}$$

has a symplectic structure.

The above methods have been produced by the simplest Open Newton-Cotes integral formula.

Based on [4, 7], the Closed Newton-Cotes differential schemes will be written as multilayer symplectic structures.

Application of the Newton-Cotes differential formula for $n = 4$ to the linear Hamiltonian system (4.1) gives

$$\begin{aligned} u_{n+4} - u_{n-4} &= s\big(a_0 y_{n-4} + a_1 y_{n-3} + a_2 y_{n-2} + a_3 y_{n-1} + a_4 y_n \\ &\quad + a_5 y_{n+1} + a_6 y_{n+2} + a_7 y_{n+3} + a_8 y_{n+4}\big), \\ y_{n+4} - y_{n-4} &= -s\big(a_0 u_{n-4} + a_1 u_{n-3} + a_2 u_{n-2} + a_3 u_{n-1} + a_4 u_n \\ &\quad + a_5 u_{n+1} + a_6 u_{n+2} + a_7 u_{n+3} + a_8 u_{n+4}\big), \end{aligned} \tag{4.7}$$

where $s = mh$, where m is defined in (4.1).

From (4.6), we have that

$$\begin{aligned} u_{n+i} - u_{n-i} &= 2isy_n, \\ y_{n+i} - y_{n-i} &= -2isu_n, \quad i = 1(1)4 \text{ or } i = \frac{1}{2}(1)\frac{5}{2}. \end{aligned} \tag{4.8}$$

We now consider the approximation based on the first formula of (4.8) for $(n+1)$-step gives (taking into account the second formula of (4.8))

$$\begin{aligned} u_{n+i} + u_{n-i} &= \left(u_n + s y_{n+i-1/2}\right) + \left(u_n - s y_{n-i+1/2}\right) \\ &= u_{n+i-1} + u_{n-i+1} + s\left(y_{n+i-1/2} - y_{n-i+1/2}\right) \\ &= \left(2 - i^2 s^2\right) u_n, \quad i = 1(1)3. \end{aligned} \tag{4.9}$$

Substituting (4.9) into (4.7) and considering that $a_0 = a_8$, $a_1 = a_7$, $a_2 = a_6$, and $a_3 = a_5$, we have:

$$\begin{aligned} u_{n+4} - u_{n-4} &= s\Big[a_0\left(y_{n-4} + y_{n+4}\right) + \Big(a_1\left(2 - 9s^2\right) \\ &\quad +2a_2\left(1 - 2s^2\right) + a_3\left(2 - s^2\right) + a_4\Big) y_n\Big] \\ y_{n+4} - y_{n-4} &= s\Big[a_0\left(u_{n-4} + u_{n+4}\right) + \Big(a_1\left(2 - 9s^2\right) \\ &\quad +2a_2\left(1 - 2s^2\right) + a_3\left(2 - s^2\right) + a_4\Big) u_n\Big], \end{aligned} \tag{4.10}$$

and with (4.8) we have

$$\begin{aligned} u_{n+4} - u_{n-4} &= s\ \Big[a_0\left(y_{n-4} + y_{n+4}\right) + \Big(a_1\left(2 - 9s^2\right) + 2a_2\left(1 - 2s^2\right) \\ &\quad +a_3\left(2 - s^2\right) + a_4\Big) \frac{u_{n+4} - u_{n-4}}{8\ s}\Big], \\ y_{n+4} - y_{n-4} &= s\ \Big[a_0\ \left(u_{n-4} + u_{n+4}\right) + \Big(a_1\left(2 - 9s^2\right) + 2a_2\left(1 - 2s^2\right) \\ &\quad +a_3\ \left(2 - s^2\right) + a_4\Big)\ \left[-\frac{y_{n+4} - y_{n-4}}{8\ s}\right]\Big], \end{aligned} \tag{4.11}$$

which gives:

$$\begin{aligned} \left(u_{n+4} - u_{n-4}\right)\left[1 - \frac{a_1\left(2 - 9s^2\right) + 2a_2\left(1 - 2s^2\right) + a_3\left(2 - s^2\right) + a_4}{8}\right] &= s a_0\left(y_{n+4} + y_{n-4}\right) \\ \left(y_{n+4} - y_{n-4}\right)\left[1 - \frac{a_1\left(2 - 9s^2\right) + 2a_2\left(1 - 2s^2\right) + a_3\left(2 - s^2\right) + a_4}{8}\right] &= -s a_0\left(u_{n+4} + u_{n-4}\right). \end{aligned} \tag{4.12}$$

The above formula in matrix form can be written as

$$\begin{pmatrix} Q(s) & -sa_0 \\ sa_0 & Q(s) \end{pmatrix}\begin{pmatrix} u_{n+4} \\ y_{n+4} \end{pmatrix} = \begin{pmatrix} Q(s) & sa_0 \\ -sa_0 & Q(s) \end{pmatrix}\begin{pmatrix} u_{n-4} \\ y_{n-4} \end{pmatrix}, \tag{4.13}$$

where

$$Q(s) = 1 - \frac{a_1\left(2-9s^2\right) + 2a_2\left(1-2s^2\right) + a_3\left(2-s^2\right) + a_4}{8}, \tag{4.14}$$

which is a discrete scheme of the form (4.2) and hence it is symplectic. □

5. Numerical Example

5.1. A Nonlinear Orbital Problem

Consider the nonlinear system of equations:

$$\begin{aligned} u'' + \omega^2 u &= \frac{2uv - \sin(2\omega x)}{\left(u^2+v^2\right)^{3/2}}, \quad u(0) = 1,\ u'(0) = 0, \\ v'' + \omega^2 v &= \frac{u^2 - v^2 - \cos(2\omega x)}{\left(u^2+v^2\right)^{3/2}}, \quad v(0) = 0,\ v'(0) = \omega. \end{aligned} \tag{5.1}$$

The analytical solution of the problem is the following:

$$u(x) = \cos(\omega x), \qquad v(x) = \sin(\omega x). \tag{5.2}$$

The system of (5.1) has been solved for $0 \le x \le 1000$ and $\omega = 10$ using the methods

(i) The eighth-order multistep method developed by Quinlan and Tremaine [23] (which is indicated as Method I).

(ii) The tenth-order multistep method developed by Quinlan and Tremaine [23] (which is indicated as Method II).

(iii) The twelfth-order multistep method developed by Quinlan and Tremaine [23] (which is indicated as Method III).

(iv) The Newton-Cotes classical tenth-algebraic-order differential method (which is indicated as Method IV), (with the term classical we mean the closed Newton-Cotes differential method with constant coefficients).

(v) The Newton-Cotes eight-algebraic-order differential method with constant coefficient which corresponds to the New Developed Method VII (which is indicated as Method V).

(vi) The Newton-Cotes tenth-algebraic-order differential method developed in [8] (which is indicated as Method VI).

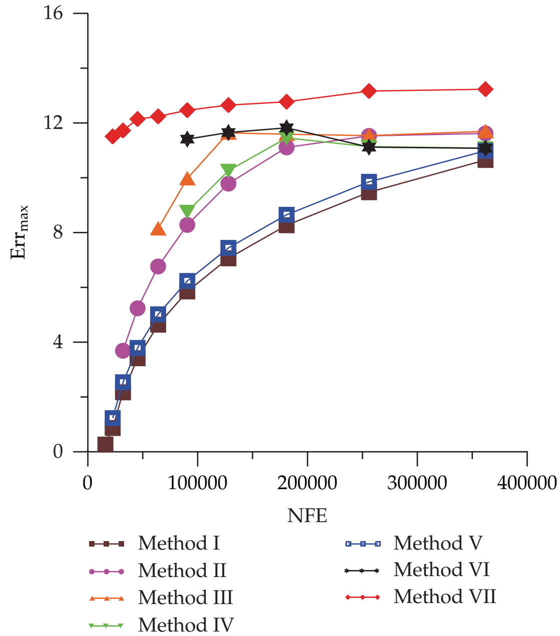

Figure 3: $\text{Err}_{\max}$ for several values of the number of function evaluations (NFE) for the Methods I–VII for the nonlinear orbital problem. The nonexistrnce of a value of $\text{Err}_{\max}$ indicates that for these values $\text{Err}_{\max}$ is negative.

(vii) The stable Newton-Cotes eight-algebraic-order trigonometrically fitted differential method (which is indicated as Method VII).

For this problem, we have $w = 10$. The numerical results obtained for the seven methods mentioned above were compared with the analytical solution. Figure 3 shows the absolute errors $\text{Err}_{\max}$ defined by

$$\text{Err}_{\max} = \left|\log_{10}\left[\max\left(\|u(x)_{\text{calculated}} - u(x)_{\text{theoretical}}\|, \|v(x)_{\text{calculated}} - v(x)_{\text{theoretical}}\|\right)\right]\right|, \quad x \in [0, 1000], \tag{5.3}$$

for several values of the number of function evaluations (NFEs).

5.2. Duffing's Equation

Consider the nonlinear initial value problem:

$$y'' = -y - y^3 + 0.002\cos(1.01t), \qquad y(0) = 0.20042672806, \; u'(0) = 0. \tag{5.4}$$

The analytical solution of the problem is the following:

$$y(t) = 0.200179477536\cos(1.01t) + 2.4694614310^{-4}\cos(3.03t) + 3.0401410^{-7}\cos(5.05t) + 3.74\ 10^{-10}\cos(7.07t). \tag{5.5}$$

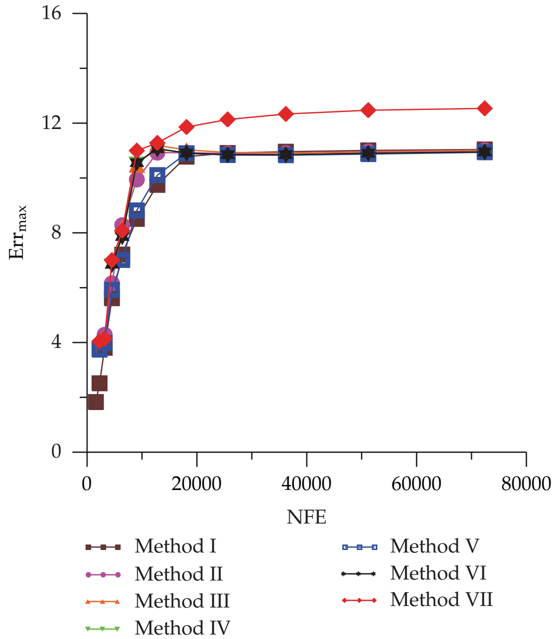

Figure 4: Err_{max} for several values of the number of function evaluations (NFEs) for the Methods I–IV for Duffing's. The nonexistence of a value of Err_{max} indicates that for these values Err_{max} is negative.

The above equation (5.4) has been solved for $0 \le x \le 1000$ using the methods mentioned above.

For this problem, we have $w = 1$. The numerical results obtained for the seven methods mentioned above were compared with the analytical solution. Figure 4 shows the absolute errors Err_{max} defined by

$$Err_{max} = \left|\log_{10}\left[\max\left(\left\|y(x)_{\text{calculated}} - y(x)_{\text{theoretical}}\right\|\right)\right]\right|, \quad x \in [0, 1000], \tag{5.6}$$

for several values of the number of function evaluations (NFEs).

We note here that analogous results for both problems are obtained for interval of integration $[0, 10000]$ or $[0, 1000000]$.

6. Conclusions

In this paper, we have introduced a new procedure for the development of Newton-Cotes differential schemes. The new procedure consists from the following steps:

(i) requirement the Newton-Cotes differential scheme to be accurate for the following set of functions:

$$\left\{1, x, x^2, x^3, \ldots, x^m, \cos(wx), \sin(wx)\right\}; \tag{6.1}$$

(ii) Satisfaction of the condition $2(\sum_{i=1}^{n}|a_i| + |a_0|)/2n = 1$, where $a_i, i = 0(1)n$ are the coefficients of the Newton-Cotes differential scheme;

(iii) Expression of the Newton-Cotes differential scheme as multilayer symplectic integrators.

We applied the new developed methods to several problems. We presented in this paper the application to a nonlinear orbital problem and to Duffing's equation and we compared them with well-known integrators from the literature. Based on these illustrations, we conclude that the new procedure produces much more efficient methods than well-known methods of the literature.

References

[1] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, vol. 31 of *Springer Series in Computational Mathematics*, Springer, Berlin, Germany, 2nd edition, 2006.

[2] J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian Problem*, vol. 7 of *Applied Mathematics and Mathematical Computation*, Chapman & Hall, London, UK, 1994.

[3] W. Zhu, X. Zhao, and Y. Tang, "Numerical methods with a high order of accuracy applied in the quantum system," *Journal of Chemical Physics*, vol. 104, no. 6, pp. 2275–2286, 1996.

[4] J. C. Chiou and S. D. Wu, "Open Newton-Cotes differential methods as multilayer symplectic integrators," *Journal of Chemical Physics*, vol. 107, no. 17, pp. 6894–6898, 1997.

[5] T. E. Simos, "A fourth algebraic order exponentially-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation," *IMA Journal of Numerical Analysis*, vol. 21, no. 4, pp. 919–931, 2001.

[6] T. E. Simos, "Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation," *Acta Applicandae Mathematicae*, vol. 110, no. 3, pp. 1331–1352, 2010.

[7] Z. Kalogiratou and T. E. Simos, "Newton-Cotes formulae for long-time integration," *Journal of Computational and Applied Mathematics*, vol. 158, no. 1, pp. 75–82, 2003.

[8] T. E. Simos, "Closed Newton-Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems," *Applied Mathematics Letters*, vol. 22, no. 10, pp. 1616–1621, 2009.

[9] T. E. Simos, "Exponentially-fitted Runge-Kutta-Nyström method for the numerical solution of initial-value problems with oscillating solutions," *Applied Mathematics Letters*, vol. 15, no. 2, pp. 217–225, 2002.

[10] Ch. Tsitouras and T. E. Simos, "Optimized Runge-Kutta pairs for problems with oscillating solutions," *Journal of Computational and Applied Mathematics*, vol. 147, no. 2, pp. 397–409, 2002.

[11] A. Konguetsof and T. E. Simos, "A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation," *Journal of Computational and Applied Mathematics*, vol. 158, no. 1, pp. 93–106, 2003.

[12] Z. Kalogiratou, T. Monovasilis, and T. E. Simos, "Symplectic integrators for the numerical solution of the Schrödinger equation," *Journal of Computational and Applied Mathematics*, vol. 158, no. 1, pp. 83–92, 2003.

[13] G. Psihoyios and T. E. Simos, "Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions," *Journal of Computational and Applied Mathematics*, vol. 158, no. 1, pp. 135–144, 2003.

[14] T. E. Simos, I. T. Famelis, and C. Tsitouras, "Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions," *Numerical Algorithms*, vol. 34, no. 1, pp. 27–40, 2003.

[15] T. E. Simos, "Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution," *Applied Mathematics Letters*, vol. 17, no. 5, pp. 601–607, 2004.

[16] K. Tselios and T. E. Simos, "Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics," *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 173–181, 2005.

[17] D. P. Sakas and T. E. Simos, "Multiderivative methods of eighth algebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation," *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 161–172, 2005.

[18] G. Psihoyios and T. E. Simos, “A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions,” *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 137–147, 2005.

[19] Z. A. Anastassi and T. E. Simos, “An optimized Runge-Kutta method for the solution of orbital problems,” *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 1–9, 2005.

[20] S. Stavroyiannis and T. E. Simos, “Optimization as a function of the phase-lag order of nonlinear explicit two-step *P*-stable method for linear periodic IVPs,” *Applied Numerical Mathematics. An IMACS Journal*, vol. 59, no. 10, pp. 2467–2474, 2009.

[21] D. Huybrechs, “Stable high-order quadrature rules with equidistant points,” *Journal of Computational and Applied Mathematics*, vol. 231, no. 2, pp. 933–947, 2009.

[22] http://www.holoborodko.com/pavel/numerical-methods/numerical-integration/stable-newton-cotes-formulas/.

[23] G. D. Quinlan and S. Tremaine, “Symmetric multistep methods for the numerical integration of planetary orbits,” *The Astronomical Journal*, vol. 100, no. 5, pp. 1694–1700, 1990.