

CLOSED NEWTON-COTES TRIGONOMETRICALLY-FITTED FORMULAE FOR LONG-TIME INTEGRATION OF ORBITAL PROBLEMS

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RESUMEN

En este trabajo se investiga la conexión entre fórmulas Newton-Cotes, métodos diferenciales por ajustes trigonométricos e integradores simplécticos. Se conoce, a través de la literatura, que varios integradores simplécticos de un paso han sido obtenidos basándose en geometría simpléctica. Sin embargo, la investigación de integradores simplécticos multicapa es muy pobre. Zhu et al. (1996) presentaron los conocidos métodos diferenciales Newton-Cotes abiertos como integradores simplécticos multicapa. También Chiou & Wu (1997) investigaron la construcción de integradores simplécticos multicapa basándose en los métodos de integración abierta Newton-Cotes. En este trabajo investigamos las fórmulas cerradas Newton-Cotes y las escribimos como estructuras simplécticas multicapa. Después de esto, construimos métodos simplécticos por ajustes trigonométricos, los cuales se basan en las fórmulas cerradas Newton-Cotes. Aplicamos los esquemas simplécticos para resolver las ecuaciones de movimiento de Hamilton que son lineales en posición y momento. Observamos que la energía hamiltoniana del sistema permanece casi constante a medida que la integración avanza.

ABSTRACT

The connection between closed Newton-Cotes, trigonometrically-fitted differential methods and symplectic integrators is investigated in this paper. It is known from the literature that several one step symplectic integrators have been obtained based on symplectic geometry. However, the investigation of multistep symplectic integrators is very poor. Zhu et al. (1996) presented the well known open Newton-Cotes differential methods as multilayer symplectic integrators. Also, Chiou & Wu (1997) investigated the construction of multistep symplectic integrators based on the open Newton-Cotes integration methods. In this paper we investigate the closed Newton-Cotes formulae and we write them as symplectic multilayer structures. After this we construct 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 integration proceeds.

Key Words: **CELESTIAL MECHANICS — METHODS: NUMERICAL**

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1. INTRODUCTION

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

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

where m is a constant scalar or matrix. It is well known that the Eq. (1) is an important one in the field of molecular dynamics. In order to preserve the characteristics of the Hamiltonian system in the numerical solution it is necessary to use symplectic integrators. In recent years work has been done mainly in the construction of one step symplectic integrators (see Sanz-Serna & Calvo 1994). In their work Zhu, Zhao, & Tang (1996) and Chiou & Wu (1997) constructed multistep symplectic integrators by writing open Newton-Cotes differential schemes as multilayer symplectic structures.

During the last decades much work has been done on exponential fitting and on the numerical solution of periodic initial value problems (see Anastassi & Simos (2004;2005), Monovasilis, Kalogiratou, & Simos (2004;2005), Psihoyios & Simos (2003;2004a;2004b), Simos (1996;1998a;1998b;2000;2002a;2002b;2003;2004a;2004b;2005), Van Daele, & Vanden Berghe (2004), Vanden Berghe, Van Daele & Vande Vyver (2004), Vlachos & Simos (2004), and references therein).

In this paper first we try to present closed Newton-Cotes differential methods as multilayer symplectic integrators. After this we apply the closed Newton-Cotes methods on the Hamiltonian system (Eq. 1) and we obtain as a result that the Hamiltonian energy of the system remains almost constant as the integration proceeds. After this, trigonometrically-fitted methods are developed. We note that the aim of this paper is to generate methods that can be used for non-linear differential equations as well as linear ones.

In § 2 the results about symplectic matrices and schemes are presented. In § 3 closed Newton-Cotes integral rules and differential methods are described and the new trigonometrically-fitted methods are developed. In § 4 the conversion of the closed Newton-Cotes differential methods into multilayer symplectic structures is presented. Numerical results are presented in § 5.

2. BASIC THEORY ON SYMPLECTIC SCHEMES AND NUMERICAL METHODS

Following Zhu et al. (1996) we have the following basic theory on symplectic numerical schemes and symplectic matrices. The proposed methods can be used for non-linear differential equations as well as linear ones. Dividing an interval $[a, b]$ with N points we have

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

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

The above division leads to the following discrete scheme

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

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 $A^T J A = J$ 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 symplectic. Consequently, the discrete scheme (2) is symplectic if each matrix M_n is symplectic.

3. TRIGONOMETRICALLY-FITTED CLOSED NEWTON-COTES DIFFERENTIAL METHODS

3.1. General Closed Newton-Cotes Formulae

The closed Newton-Cotes integral rules are given by

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

where

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

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

TABLE 1
CLOSED NEWTON-COTES
INTEGRALS RULES

k	z	t_0	t_1	t_2	t_3	t_4
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

From the above table it is easy to see that the coefficients t_i are symmetric i.e., we have the following relation:

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

Closed Newton-Cotes differential methods were produced from the integral rules. For the above table we have the following differential methods:

$$\begin{aligned}
k = 1 \quad y_{n+1} - y_n &= \frac{h}{2}(f_{n+1} + f_n), \\
k = 2 \quad y_{n+1} - y_{n-1} &= \frac{h}{3}(f_{n-1} + 4f_n + f_{n+1}), \\
k = 3 \quad y_{n+1} - y_{n-2} &= \frac{3h}{8}(f_{n-2} + 3f_{n-1} + 3f_n + f_{n+1}), \\
k = 4 \quad y_{n+2} - y_{n-2} &= \frac{2h}{45}(7f_{n-2} + 32f_{n-1} + 12f_n + 32f_{n+1} + 7f_{n+2}).
\end{aligned}$$

In the present paper we will investigate the case $k = 4$ and we will produce trigonometrically-fitted differential methods.

3.2. Trigonometrically-Fitted Closed Newton-Cotes Differential Method

Requiring the differential scheme:

$$y_{n+2} - y_{n-2} = h(a_0 f_{n-2} + a_1 f_{n-1} + a_2 f_n + a_3 f_{n+1} + a_4 f_{n+2}), \quad (4)$$

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

$$\{1, x, x^2, x^3, \cos(\pm wx), \sin(\pm wx)\}, \quad (5)$$

the following set of equations is obtained:

$$\begin{aligned}
a_0 + a_1 + a_2 + a_3 + a_4 &= 4 \\
-4a_0 - 2a_1 + 2a_3 + 4a_4 &= 0 \\
12a_0 + 3a_1 + 3a_3 + 12a_4 &= 16 \\
v \sin(v)(a_1 - a_3 - 2a_4 \cos(v) + 2 \cos(v)a_0) &= 0 \\
4 \cos(v) \sin(v) &= v(-a_0 + a_2 - a_4 + 2a_0 \cos(v)^2 + \\
&\quad + 2a_4 \cos(v)^2 + a_3 \cos(v) + a_1 \cos(v)), \quad (6)
\end{aligned}$$

where $v = wh$. We note that the first equation is produced requiring the scheme (4) to be accurate for $1, x$, while the second and the third equations are obtained requiring the algorithm (4) to be accurate for $\cos(\pm wx), \sin(\pm wx)$. The requirement for the accurate integration of functions (5), helps the method to be accurate for all the problems with solution which has behavior of trigonometric functions.

Solving the above system of equations we obtain:

$$\begin{aligned}
a_0 &= \frac{-3 \sin(2v) - 2v + 8v \cos(v)}{-9v - 3v \cos(2v) + 12v \cos(v)} \\
a_1 &= \frac{12 \sin(2v) - 16v - 8v \cos(2v)}{-9v - 3v \cos(2v) + 12v \cos(v)} \\
a_2 &= \frac{4v \cos(2v) + 32v \cos(v) - 18 \sin(2v)}{-9v - 3v \cos(2v) + 12v \cos(v)} \\
a_3 &= \frac{12 \sin(2v) - 16v - 8v \cos(2v)}{-9v - 3v \cos(2v) + 12v \cos(v)} \\
a_4 &= \frac{-3 \sin(2v) - 2v + 8v \cos(v)}{-9v - 3v \cos(2v) + 12v \cos(v)}. \quad (7)
\end{aligned}$$

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

$$\begin{aligned}
 a_0 &= \frac{14}{45} + \frac{8}{945} v^2 + \frac{1}{4725} v^4 + \frac{1}{311850} v^6 \\
 &\quad - \frac{97}{2043241200} v^8 - \frac{139}{20432412000} v^{10} - \frac{229}{595458864000} v^{12} \\
 &\quad\quad - \frac{285689}{16631166071520000} v^{14} + \dots \\
 a_1 &= \frac{64}{45} - \frac{32}{945} v^2 - \frac{4}{4725} v^4 - \frac{2}{155925} v^6 \\
 &\quad + \frac{97}{510810300} v^8 + \frac{139}{5108103000} v^{10} + \frac{229}{148864716000} v^{12} \\
 &\quad\quad + \frac{285689}{4157791517880000} v^{14} + \dots \\
 a_2 &= \frac{8}{15} + \frac{16}{315} v^2 + \frac{2}{1575} v^4 + \frac{1}{51975} v^6 \\
 &\quad - \frac{97}{340540200} v^8 - \frac{139}{3405402000} v^{10} - \frac{229}{99243144000} v^{12} \\
 &\quad\quad - \frac{285689}{2771861011920000} v^{14} + \dots \\
 a_3 &= \frac{64}{45} - \frac{32}{945} v^2 - \frac{4}{4725} v^4 - \frac{2}{155925} v^6 \\
 &\quad + \frac{97}{510810300} v^8 + \frac{139}{5108103000} v^{10} + \frac{229}{148864716000} v^{12} \\
 &\quad\quad + \frac{285689}{4157791517880000} v^{14} + \dots \\
 a_4 &= \frac{14}{45} + \frac{8}{945} v^2 + \frac{1}{4725} v^4 + \frac{1}{311850} v^6 \\
 &\quad - \frac{97}{2043241200} v^8 - \frac{139}{20432412000} v^{10} - \frac{229}{595458864000} v^{12} \\
 &\quad\quad - \frac{285689}{16631166071520000} v^{14} + \dots
 \end{aligned} \tag{8}$$

The Local Truncation Error for the above differential method is given by:

$$L.T.E(h) = -\frac{8h^7}{945} \left(y_n^{(7)} + w^2 y_n^{(5)} \right). \tag{9}$$

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

4. CLOSED NEWTON-COTES CAN BE EXPRESSED AS SYMPLECTIC INTEGRATORS

Theorem 1. *A discrete scheme of the form:*

$$\begin{pmatrix} b & -a \\ a & b \end{pmatrix} \begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} b & a \\ -a & b \end{pmatrix} \begin{pmatrix} q_n \\ p_n \end{pmatrix}, \tag{10}$$

is symplectic.

Proof. We rewrite (3) as

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} b & -a \\ a & b \end{pmatrix}^{-1} \begin{pmatrix} b & a \\ -a & b \end{pmatrix} \begin{pmatrix} q_n \\ p_n \end{pmatrix}.$$

Define

$$M = \begin{pmatrix} b & -a \\ a & b \end{pmatrix}^{-1} \begin{pmatrix} b & a \\ -a & b \end{pmatrix} = \frac{1}{b^2 + a^2} \begin{pmatrix} b^2 - a^2 & 2ab \\ -2ab & b^2 - a^2 \end{pmatrix},$$

and it can easily be verified that

$$M^T J M = J,$$

thus the matrix M is symplectic.

Zhu et al. (1996) have proved the symplectic structure of the well-known second-order differential scheme (SOD),

$$\begin{aligned} y_{n+1} - y_{n-1} &= 2h f_n, \\ y_{n+2} - y_{n-2} &= 4h f_n. \end{aligned} \quad (11)$$

The above method has been produced by the simplest Open Newton-Cotes integral rule.

Based on the paper by Chiou & Wu (1997) we will try to write Closed Newton-Cotes differential schemes as multilayer symplectic structures.

Application of the Newton-Cotes differential formula for $n = 2$ to the linear Hamiltonian system (1) gives:

$$\begin{aligned} q_{n+2} - q_{n-2} &= s \left(a_0 p_{n-2} + a_1 p_{n-1} + a_2 p_n + a_3 p_{n+1} + a_4 p_{n+2} \right), \\ p_{n+2} - p_{n-2} &= -s \left(a_0 q_{n-2} + a_1 q_{n-1} + a_2 q_n + a_3 q_{n+1} + a_4 q_{n+2} \right), \end{aligned} \quad (12)$$

where $s = mh$, where m is defined in (1).

From (11) we have that:

$$\begin{aligned} q_{n+2} - q_{n-2} &= 4s p_n, \\ p_{n+2} - p_{n-2} &= -4s q_n, \end{aligned} \quad (13)$$

$$\begin{aligned} q_{n+1} - q_{n-1} &= 2s p_n, \\ p_{n+1} - p_{n-1} &= -2s q_n, \end{aligned} \quad (14)$$

$$\begin{aligned} q_{n+\frac{1}{2}} - q_{n-\frac{1}{2}} &= s p_n, \\ p_{n+\frac{1}{2}} - p_{n-\frac{1}{2}} &= -s q_n. \end{aligned} \quad (15)$$

Substitution of the approximation which is based on (15) for $(m+1)$ -step to (13) gives:

$$\begin{aligned} q_{n+1} + q_{n-1} &= \left(q_n + s p_{n+\frac{1}{2}} \right) + \left(q_n - s p_{n-\frac{1}{2}} \right), \\ &= 2q_n + s \left(p_{n+\frac{1}{2}} - p_{n-\frac{1}{2}} \right) = \left(2 - s^2 \right) q_n. \end{aligned} \quad (16)$$

Similarly we have:

$$\begin{aligned}
 p_{n+1} + p_{n-1} &= \left(p_n - s q_{n+\frac{1}{2}} \right) + \left(p_n + s q_{n-\frac{1}{2}} \right), \\
 &= 2p_n - s \left(q_{n+\frac{1}{2}} - q_{n-\frac{1}{2}} \right) = \left(2 - s^2 \right) p_n.
 \end{aligned}
 \tag{17}$$

Substituting (16) and (17) into (12) and considering that $a_0 = a_4$ and $a_1 = a_3$ we have:

$$\begin{aligned}
 q_{n+2} - q_{n-2} &= s \left[a_0 \left(p_{n-2} + p_{n+2} \right) + a_1 \left(2 - s^2 + a_2 \right) p_n \right], \\
 p_{n+2} - p_{n-2} &= -s \left[a_0 \left(q_{n+2} + q_{n-2} \right) + a_1 \left(2 - s^2 + a_2 \right) q_n \right],
 \end{aligned}$$

and with (13) we have:

$$\begin{aligned}
 q_{n+2} - q_{n-2} &= s \left[a_0 \left(p_{n-2} + p_{n+2} \right) + a_1 \left(2 - s^2 + a_2 \right) \frac{q_{n+2} - q_{n-2}}{4s} \right], \\
 p_{n+2} - p_{n-2} &= -s \left[a_0 \left(q_{n+2} + q_{n-2} \right) + a_1 \left(2 - s^2 + a_2 \right) \left[-\frac{q_{n+2} - q_{n-2}}{4s} \right] \right],
 \end{aligned}$$

which gives:

$$\begin{aligned}
 \left(q_{n+2} - q_{n-2} \right) \left[1 - \frac{a_1 \left(2 - s^2 \right) + a_2}{4} \right] &= s a_0 \left(p_{n-2} + p_{n+2} \right), \\
 \left(p_{n+2} - p_{n-2} \right) \left[1 - \frac{a_1 \left(2 - s^2 \right) + a_2}{4} \right] &= -s a_0 \left(q_{n+2} + q_{n-2} \right).
 \end{aligned}$$

The above formula in matrix form can be written as:

$$\begin{pmatrix} T(s) & -s a_0 \\ s a_0 & T(s) \end{pmatrix} \begin{pmatrix} q_{n+2} \\ p_{n+2} \end{pmatrix} = \begin{pmatrix} T(s) & s a_0 \\ -s a_0 & T(s) \end{pmatrix} \begin{pmatrix} q_{n-2} \\ p_{n-2} \end{pmatrix},$$

where

$$T(s) = 1 - \frac{a_1 \left(2 - s^2 \right) + a_2}{4},
 \tag{18}$$

which is a discrete scheme of the form (10) and hence it is symplectic.

We note here than in Chiou & Wu (1997) have re-written Open Newton-Cotes differential schemes as multilayer symplectic structures based on (11).

5. NUMERICAL EXAMPLE

5.1. Harmonic Oscillator

In order to illustrate the performance of open Newton-Cotes differential methods consider the equations of motion of a harmonic oscillator given by the system of equations:

$$\begin{aligned}
 \dot{q} &= p, \\
 \dot{p} &= -q,
 \end{aligned}
 \tag{19}$$

and the initial conditions are given as:

$$q(0) = 1, \quad p(0) = 0.$$

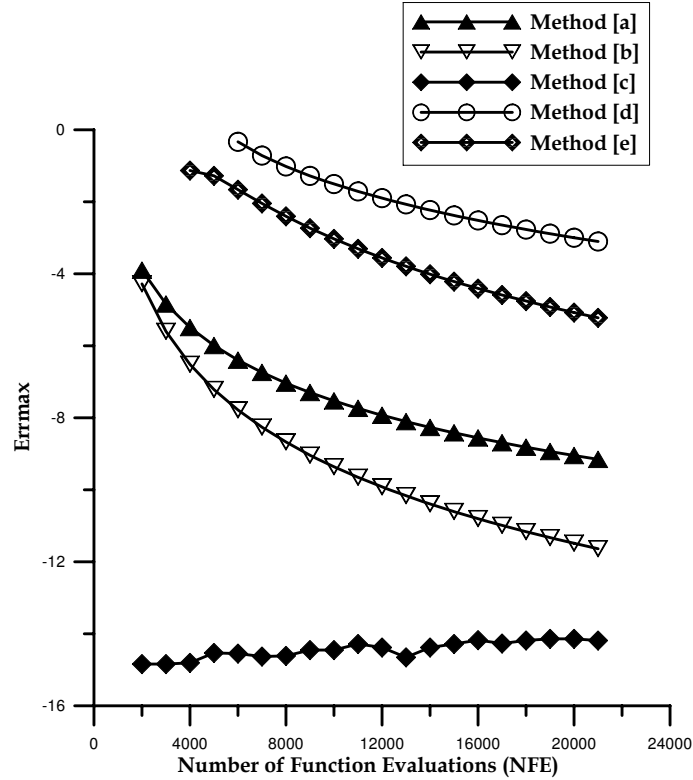


Fig. 1. **Errmax** for several values of **Number of Function Evaluations** for the Hamiltonian for the Harmonic oscillator problem solved by Method [a]-[e].

The Hamiltonian (or energy) of this system is:

$$H(t) = \frac{1}{2} (p^2(t) + q^2(t)) .$$

For comparison purposes we use:

- The classical closed Newton-Cotes differential method of order four (which is indicated as Method [a])².
- The classical closed Newton-Cotes differential method of order six (which is indicated as Method [b]).
- The newly developed trigonometrically-fitted closed Newton-Cotes differential method of order six (which is indicated as Method [c]). For this problem we have $w = 1$.
- The fifth order predictor-corrector Adams-Bashforth-Moulton method (which is indicated as Method [d]).
- The seventh order predictor-corrector Adams-Bashforth-Moulton method (which is indicated as Method [e]).

The integration interval is $[0, 1000]$.

In Figure 1 we present the absolute errors of the Hamiltonian:

$$\text{Errmax} = \log_{10} \left[\max \left(\|H_e(t)_{\text{calculated}} - H_e(t)_{\text{theoretical}}\|, , t \in [0, 1000] \right) \right] , \quad (20)$$

²With the term classical we mean the closed Newton-Cotes differential method with constant coefficients.

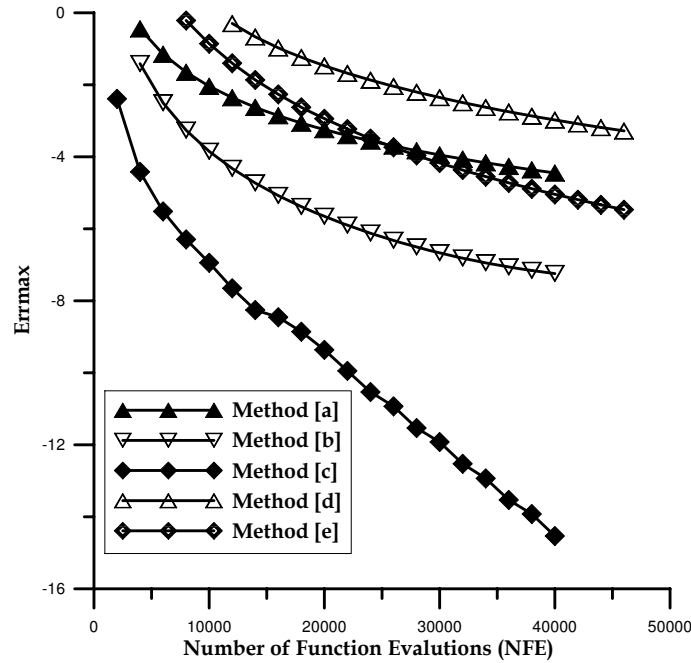


Fig. 2. **Errmax** for several values of **Number of Function Evaluations** for the Methods [a]-[e] for the problem of Stiefel and Bettis. The nonexistence of a value of **Errmax** indicates that for these values **Errmax** is positive

where

$$H_e(t) = H(t) - H(0), \tag{21}$$

for the methods mentioned above and for several values of the Number of Function Evaluations. For Method [c] the absolute error **Errmax** is not actually bounded due to roundoff errors.

5.2. A Problem by Stiefel and Bettis

The “almost” periodic orbit problem studied by Stiefel & Bettis (1969) is the next problem, which is considered.

$$y'' + y = 0.001 e^{ix}, \quad y(0) = 1, \quad y'(0) = 0.9995 i, \quad y \in C, \tag{22}$$

whose equivalent form is:

$$u'' + u = 0.001 \cos(x), \quad u(0) = 1, \quad u'(0) = 0, \tag{23}$$

$$v'' + v = 0.001 \sin(x), \quad v(0) = 0, \quad v'(0) = 0.9995. \tag{24}$$

The analytical solution of the problem (22) is following:

$$y(x) = u(x) + i v(x), \quad u, v \in R, \tag{25}$$

$$u(x) = \cos(x) + 0.0005 x \sin(x), \tag{26}$$

$$v(x) = \sin(x) - 0.0005 x \cos(x). \tag{27}$$

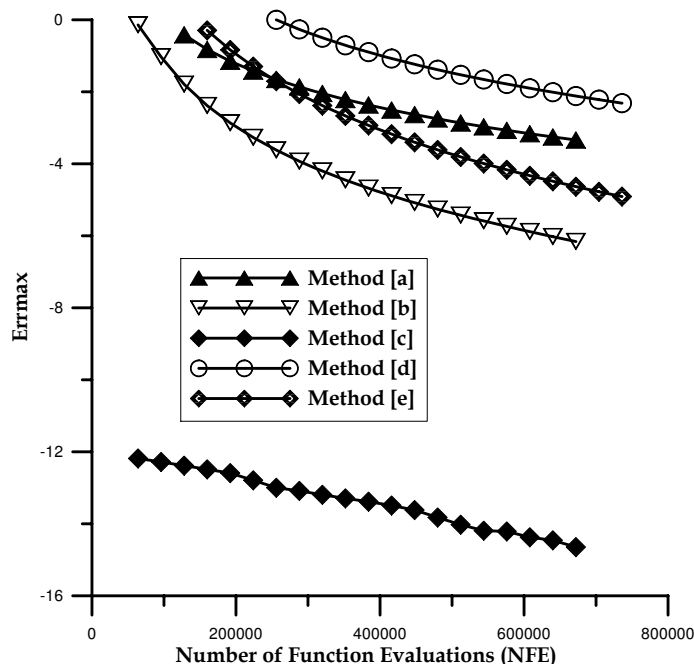


Fig. 3. **Errmax** for several values of **Number of Function Evaluations** for the Methods [a]-[e] for the nonlinear orbit problem. The nonexistence of a value of **Errmax** indicates that for these values **Errmax** is positive

The solution Eqs. (25)-(27) represents motion of a perturbation of a circular orbit in the complex plane.

The system of Eqs. (23) and (24) has been solved for $0 \leq x \leq 1000$ using the five methods mentioned above. For this problem we have also $w = 1$. The numerical results obtained for the five methods mentioned above were compared with the analytical solution. Figure 2 shows the absolute errors.

$$\text{Errmax} = \log_{10} \left[\max \left(\|u(x)_{\text{calculated}} - u(x)_{\text{theoretical}}\|, \|v(x)_{\text{calculated}} - v(x)_{\text{theoretical}}\| \right) \right], \quad x \in [0, 1000], \tag{28}$$

for several values of the Number of Function Evaluations.

5.3. A Nonlinear Orbit Problem

Consider the nonlinear system of equations:

$$u'' + \omega^2 u = \frac{2uv - \sin(2\omega x)}{(u^2 + v^2)^{\frac{3}{2}}}, \quad u(0) = 1, \quad u'(0) = 0, \tag{29}$$

$$v'' + \omega^2 v = \frac{u^2 - v^2 - \cos(2\omega x)}{(u^2 + v^2)^{\frac{3}{2}}}, \quad v(0) = 0, \quad v'(0) = \omega. \tag{30}$$

The analytical solution of the problem (22) is following:

$$u(x) = \cos(\omega x), \quad v(x) = \sin(\omega x). \tag{31}$$

The system of Eqs. (29) and (30) has been solved for $0 \leq x \leq 1000$ and $\omega = 10$ using the five methods mentioned above. For this problem we have $w = 10$. The numerical results obtained for the five methods mentioned above were compared with the analytical solution. Figure 3 shows the absolute errors Err_{max} defined in (28) for several values of the Number of Function Evaluations.

6. CONCLUSIONS

The presentation of the closed Newton-Cotes differential methods as multilayer symplectic integrators and their application on the Hamiltonian system (1) is presented in this paper. The result from the above investigation is that the Hamiltonian energy of the system remains almost constant as the integration proceeds.

We also developed trigonometrically-fitted methods. We applied the newly developed methods to linear and nonlinear problems and we compared them with well known integrators from the literature. Based on these illustrations we conclude that trigonometrically-fitted methods are more efficient than well known methods of the literature.

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REFERENCES

- Anastassi, Z. A., & Simos, T. E. 2004, *NewA*, 10(1), 31
 ————. 2005, *NewA*, 10,(4), 301
 Chiou, J. C., & Wu, S. D. 1997, *J. of Chem. Phys.*, 107, 6894
 Monovasilis, Th., Kalogiratou, Z., & Simos, T. E. 2004, *Appl. Num. Anal. Comp. Math.*, 1(1), 195
 ————. 2005, *Appl. Num. Anal. Comp. Math.*, 2(2), 238
 Psihoyios, G., & Simos, T. E. 2003, *NewA*, 8(7), 679
 ————. 2004a, *Appl. Num. Anal. Comp. Math.*, 1(1), 205
 ————. 2004b, *Appl. Num. Anal. Comp. Math.*, 1(1), 216
 Sanz-Serna, J. M., & Calvo, M. P. 1994, in *Numerical Hamiltonian Problem* (London: Chapman and Hall)
 Simos, T. E. 1996, *International J. of Modern Phys., C*, 7, 825
 ————. 1998a, *International J. of Modern Phys., C*, 9, 1055
 ————. 1998b, *International J. of Modern Phys., C*, 9, 271
 Simos, T. E. 2000, *International J. of Modern Phys., C*, 11, 79
 ————. 2002a, in *Numerical Methods for 1D, 2D, and 3D Differential Equations Arising in Chemical Problems, Chemical Modelling: Applications and Theory* (The Royal Society of Chemistry), 170
 ————. 2002b, *NewA*, 7(1), 1
 ————. 2003, *NewA*, 8(5), 391
 ————. 2004a, *NewA*, 9(6), 409
 ————. 2004b, *NewA*, 9(1), 59
 ————. 2005, *Computing Lett.*, 1(1), 37
 Stiefel, E., & Bettis, D. G. 1969, *Numer. Math.*, 13, 154
 Van Daele, M., & Vanden Berghe, G. 2004, *Appl. Num. Anal. Comp. Math.*, 1(2), 353
 Vanden Berghe, G., Van Daele, M., & Vande Vyver, H. 2004, *Appl. Num. Anal. Comp. Math.*, 1(1), 49
 Vlachos D. S., & Simos, T. E. 2004, *Appl. Num. Anal. Comp. Math.*, 1(2), 540
 Zhu, W., Zhao, X., & Tang, Y. 1996, *J. of Chem. Phys.*, 104, 2275

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