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A fourth-order symplectic exponentially fitted integrator

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Abstract

A numerical method for ordinary differential equations is called symplectic if, when applied to Hamiltonian problems, it preserves the symplectic structure in phase space, thus reproducing the main qualitative property of solutions of Hamiltonian systems. In a previous paper [G. Vanden Berghe, M. Van Daele, H. Van de Vyver, Exponential fitted Runge–Kutta methods of collocation type: fixed or variable knot points?, J. Comput. Appl. Math. 159 (2003) 217–239] some exponentially fitted RK methods of collocation type are proposed. In particular, three different versions of fourth-order exponentially fitted Gauss methods are described. It is well known that classical Gauss methods are symplectic. In contrast, the exponentially fitted versions given in [G. Vanden Berghe, M. Van Daele, H. Van de Vyver, Exponential fitted Runge–Kutta methods of collocation type: fixed or variable knot points?, J. Comput. Appl. Math. 159 (2003) 217–239] do not share this property. This paper deals with the construction of a fourth-order symplectic exponentially fitted modified Gauss method. The RK method is modified in the sense that two free parameters are added to the Buthcher tableau in order to retain symplecticity.

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Keywords: Hamiltonian systems; Symplectic methods; Runge–Kutta methods; Exponential fitting

1. Introduction

In the past decades there has been great research performed in the area of the numerical integration of initial value problems (IVP) related to systems of first-order ordinary differential equations (ODE)

$$y' = f(x, y), \quad y(x_0) = y_0. \tag{1.1}$$

Hamiltonian systems are first-order ODEs that can be expressed as

$$p' = -\frac{\partial H}{\partial q}(p, q), \qquad q' = \frac{\partial H}{\partial p}(p, q), \tag{1.2}$$

whereby $p, q \in \mathbb{R}^d$ and H is a twice continuously differentiable function $H : U \to \mathbb{R}^{2d}$ ($U \subset \mathbb{R}^{2d}$ is an open set). Hamiltonian systems appear frequently in the area of classical mechanics, physics, chemistry and elsewhere. A lot of these problems take the special form

$$p' = f(q), \quad q' = p, \tag{1.3}$$

i.e. second-order systems $q'' = f(q)$. If f is the gradient of a scalar function $-V(q)$, then (1.3) is a Hamiltonian system with

$$H(p, q) = T(p) + V(q), \quad T(p) = \frac{1}{2}p^{\mathrm{T}}p. \tag{1.4}$$

In mechanics, the q variables represent Lagrangian coordinates, the p variables the corresponding momenta, f the forces, T is the kinetic energy, V the potential energy, and H the total energy.

For the numerical solution of Hamiltonian systems much attention has been paid to symplectic integrators which take into account the symplecticity of such systems (see [2,3]). It has been widely recognized that symplectic integrators have the numerical superiority when applied to solving Hamiltonian systems. Quite often the solution of (1.2) exhibits a pronounced oscillatory character. For a Hamiltonian system with oscillating or periodic solutions it should be highly interesting to design a method that pays attention both to the symplecticity and the oscillatory character. As an example of such methods we refer to Vigo-Aguiar et al. [4] where adapted symplectic modified Runge–Kutta–Nyström (RKN) methods are presented. Re-

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cently, Simos and Vigo-Aguiar [5] have constructed a second-order symplectic modified explicit RKN method based on the Runge–Kutta (RK) approach of Simos [6]. For more work in this direction we can refer to Monovasilis et al. [7].

Another efficient approach for developing methods for the numerical solution of ODEs with oscillating or periodic solutions is to use exponential fitting (in short: EF) [8]. A good theoretical foundation for the EF technique was given by Gautschi [9] and Lyche [10]. The study of exponentially fitted Runge–Kutta–(Nyström) (EFRK(N)) methods is a relatively new development and rather limited (for example, see [1,11–15]). Motivated by the results from [4,5] the present author [16] has constructed a second-order symplectic modified explicit EFRKN method. As a follow-up, a fourth-order symplectic modified implicit EFRK method is constructed and discussed in this work. The paper is organized as follows: in Section 2 we present some basic elements and properties of Hamiltonian systems and symplectic one-step methods. In Section 3 we repeat, in short, the main idea for the construction of EFRK methods given in [1]. We conclude that the EF versions of the fourth-order Gauss method from [1] are not symplectic. Based on this observation we introduce modified RK methods and we present the symplecticity conditions for this kind of methods. A combination of these conditions, EF techniques and Gauss nodes will deliver a fourth-order symplectic EF integrator. In Section 4 some numerical illustrations confirm the developed theory and finally, in Section 5 some conclusions are drawn.

2. Symplectic schemes

Definition 1. A differentiable map $g : U \to \mathbb{R}^{2d}$ is called symplectic if the Jacobian matrix $g'(p,q)$ is everywhere symplectic

$$g'(p,q)^{\mathrm{T}} J g'(p,q) = J \quad \text{with } J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{2.1}$$

There is also a geometric interpretation: in the case that $d = 1$ it means that a symplectic transformation preserves the surface. We associate with the Hamiltonian system (1.2) the following flow

$$\psi_x : U \to \mathbb{R}^{2d} : (p_0, q_0) \to \bigl(p(x, p_0, q_0), q(x, p_0, q_0)\bigr),$$

where $(p(x, p_0, q_0), q(x, p_0, q_0))$ is the solution of the system (1.2) corresponding to initial values $p(0) = p_0$, $q(0) = q_0$.

Theorem 1 *(Poincaré 1899). Let $H(p,q)$ be a twice continuously differentiable function on $U \subset \mathbb{R}^{2d}$. Then, for each fixed x, the flow ψ_x is a symplectic transformation wherever it is defined.*

Proof. See [2]. □

Symplecticity is a characteristic property of Hamiltonian systems. Therefore it is natural to search for numerical methods that share this property. We denote a one-step method for (1.1) as $y_{n+1} = \Phi_h(y_n)$ with $y_n = (p_n, q_n)^{\mathrm{T}}$.

Definition 2. A one-step method is called symplectic if the following condition is satisfied

$$\Phi_h'(y_n)^{\mathrm{T}} J \Phi_h'(y_n) = J. \tag{2.2}$$

One of the most well-known examples for (1.3) is the Störmer/Verlet method. A very interesting review on this method and its various interpretations is given in [17]. The method admits the one-step formulation:

$$\begin{aligned} p_{n+1/2} &= p_n + \frac{h}{2} f(q_n), \\ q_{n+1} &= q_n + h\, p_{n+1/2}, \\ p_{n+1} &= p_{n+1/2} + \frac{h}{2} f(q_{n+1}), \end{aligned} \tag{2.3}$$

where $p_{n+1/2}$ has to be interpret as the numerical solution of the p-component at the point $x_n + h/2$. It is a second-order explicit method.

The most studied one-step methods for (1.1) are Runge–Kutta (RK) methods

$$\begin{aligned} Y_i &= y_n + h \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j), \quad i = 1, \dots, s, \\ y_{n+1} &= y_n + h \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i). \end{aligned} \tag{2.4}$$

A RK method is completely determined by means of its Butcher tableau

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array}$$

$$\text{or equivalently by the triplet } (c, A, b), \tag{2.5}$$

where $c, b \in \mathbb{R}^s$, $A \in \mathbb{R}^{s \times s}$ and s denotes the number of stages of the RK method. The following theorem is well known and it was found independently by Lasagni, Sanz-Serna and Suris (see [2,3,18,19] and references therein).

Theorem 2. *The RK method (2.4)–(2.5) is symplectic when the following equalities are satisfied*

$$b_j a_{ji} + b_i a_{ij} - b_i b_j = 0, \quad 1 \leqslant i, j \leqslant s. \tag{2.6}$$

As a classical example we mention the Gauss methods as symplectic RK methods. It should be noted that symplectic RK methods are always implicit.

3. Exponential fitting and symplecticity

The idea of EF has been discussed and applied in detail in [8]. A flow chart has been introduced for the construction of EF algorithms which are exact for a chosen reference set of functions

$$\bigl\{1, x, \dots, x^K, \exp(\mu x), \dots, x^P \exp(\mu x) \mid \mu \in \mathbb{R} \text{ or } \mu \in i\mathbb{R}\bigr\}. \tag{3.1}$$

Vanden Berghe et al. [1] have applied this scheme for the construction of EFRK methods of collocation type. It is known that s-stage RK methods of collocation type integrate exactly a set of $s+1$ linearly independent functions thus we have that $K+2P=s-2$. Following Albrecht's approach [20,21] each internal stage of the RK method (2.4)–(2.5) can be seen as a linear multistep method on a non-equidistant grid and one can associate the following linear functionals:

- for the internal stages

$$\mathcal{L}_i\big[y(x);h;\mathbf{a}\big]=y(x+c_ih)-y(x)-h\sum_{j=1}^{s}a_{ij}y'(x+c_jh),\quad i=1,2,\ldots,s,\tag{3.2}$$

- for the final stage

$$\mathcal{L}\big[y(x);h;\mathbf{b}\big]=y(x+h)-y(x)-h\sum_{i=1}^{s}b_iy'(x+c_ih).\tag{3.3}$$

Demanding that the functionals will vanish for the functions from (3.1) for a prescribed μ will result in systems of linear equations with unknown A- and b-values (for the derivation of these equations see [1] (pp. 218–221)). For example, the two-stage EFGauss method from [1] (case 1: fixed nodes) is capable of integrating exactly the functions from (3.1) with $K=0$ and $P=0$. The method is determined by the following EF equations for the two internal stages ($i=1,2$):

$$\begin{aligned}&\cosh(c_i\nu)-1-\nu\big(a_{i1}\sinh(c_1\nu)+a_{i2}\sinh(c_2\nu)\big)=0,\\&\sinh(c_i\nu)-\nu\big(a_{i1}\cosh(c_1\nu)+a_{i2}\cosh(c_2\nu)\big)=0,\end{aligned}\tag{3.4}$$

and for the final stage:

$$\begin{aligned}&\cosh(\nu)-1-\nu\big(b_1\sinh(c_1\nu)+b_2\sinh(c_2\nu)\big)=0,\\&\sinh(\nu)-\nu\big(b_1\cosh(c_1\nu)+b_2\cosh(c_2\nu)\big)=0,\end{aligned}\tag{3.5}$$

where $\nu=\mu h$. On solving the EF equations (3.4)–(3.5) for the unknown A- and b-values and choosing the Gauss nodes: $c_1=(3-\sqrt{3})/6$, $c_2=1-c_1$ we obtain the fourth-order EFGauss method from [1]. We have that all the A- and b-values are completely determined by the EF equations. It is not surprising that the method does not satisfy the symplecticity conditions (2.6). The same observation is done for the two other fourth-order EFGauss methods from [1] (case 2: frequency-dependent nodes). Our intension in this paper is to make an improvement of these methods in the sense that symplecticity conditions must hold. In order to realize this goal we have to modify the RK method (2.4)–(2.5) by introducing extra γ-parameters in the following way

$$\begin{aligned}&Y_i=\gamma_iy_n+h\sum_{j=1}^{s}a_{ij}f(x_n+c_jh,Y_j),\quad i=1,\ldots,s,\\&y_{n+1}=y_n+h\sum_{i=1}^{s}b_if(x_n+c_ih,Y_i),\end{aligned}\tag{3.6}$$

or in tableau form

$$\begin{array}{c|c|cccc}c_1&\gamma_1&a_{11}&a_{12}&\ldots&a_{1s}\\c_2&\gamma_2&a_{21}&a_{22}&\ldots&a_{2s}\\\vdots&\vdots&\vdots&\vdots&\ddots&\vdots\\c_s&\gamma_s&a_{s1}&a_{s2}&\ldots&a_{ss}\\\hline&&b_1&b_2&\ldots&b_s\end{array}\tag{3.7}$$

Such modification is also used in the context of EF [14] and phase fitting [22] procedures for explicit RK methods. Another related modification is recently proposed by the present author [23]. The symplecticity conditions for the modified RK method (3.6)–(3.7) are presented in the following theorem.

Theorem 3. *The modified RK method (3.6)–(3.7) is symplectic when the following equalities are satisfied*

$$b_j\frac{a_{ji}}{\gamma_j}+b_i\frac{a_{ij}}{\gamma_i}-b_ib_j=0,\quad 1\leqslant i,j\leqslant s.\tag{3.8}$$

The proof is essentially the same as the proof of Theorem 2 given in [3]. The extension of the EF treatment for RK methods to modified RK methods (3.6)–(3.7) is trivial, one can associate the following linear functionals for the internal stages:

$$\mathcal{L}_i\big[y(x);h;\mathbf{a}\big]=y(x+c_ih)-\gamma_iy(x)-h\sum_{j=1}^{s}a_{ij}y'(x+c_jh),\quad i=1,2,\ldots,s.\tag{3.9}$$

Requiring that this functional will vanish for functions from the set (3.1) with $K=0$ and $P=0$ we obtain the following equations for the two internal stages ($i=1,2$):

$$\begin{aligned}&\cosh(c_i\nu)-\gamma_i-\nu\big(a_{i1}\sinh(c_1\nu)+a_{i2}\sinh(c_2\nu)\big)=0,\\&\sinh(c_i\nu)-\nu\big(a_{i1}\cosh(c_1\nu)+a_{i2}\cosh(c_2\nu)\big)=0,\end{aligned}\tag{3.10}$$

where $\nu=\mu h$. The EF equations (3.5) and (3.10) together with the symplecticity conditions (see Theorem 3)

$$\begin{aligned}&b_1\frac{a_{11}}{\gamma_1}+b_1\frac{a_{11}}{\gamma_1}-b_1b_1=0,\qquad b_1\frac{a_{12}}{\gamma_1}+b_2\frac{a_{21}}{\gamma_2}-b_2b_1=0,\\&b_2\frac{a_{22}}{\gamma_2}+b_2\frac{a_{22}}{\gamma_2}-b_2b_2=0,\end{aligned}\tag{3.11}$$

form a consistent non-linear system with unknown A-, b- and γ-values. In order to obtain a fourth-order method we choose the Gauss nodes: $c_1=(3-\sqrt{3})/6$ and $c_2=1-c_1$. We have found the following solution:

$$\begin{aligned}&a_{11}=\frac{(\exp(\nu)-1)(1+E^2)}{\nu(\exp(\nu)+1)(1+E)^2},\\&a_{12}=\frac{2(\exp(\nu)-E^2)}{\nu(\exp(\nu)+1)(1+E)^2},\\&a_{21}=\frac{2(-1+\exp(\nu)E^2)}{\nu(\exp(\nu)+1)(1+E)^2},\qquad a_{22}=a_{11},\\&\gamma_1=\frac{2\exp(\nu/2)(1+E+E^2+E^3)}{\sqrt{E}(1+E)^2(\exp(\nu)+1)},\qquad \gamma_2=\gamma_1,\\&b_1=\frac{\exp(\nu)-1}{\nu\exp(c_1\nu)(1+E)},\qquad b_2=b_1,\\&\text{with } E=\exp(\nu\sqrt{3}/3).\end{aligned}\tag{3.12}$$

Unfortunately the solution is subject to heavy cancellation when evaluated for small values of $|\nu|$. In that case the following series expansions should be preferred:

$$
\begin{aligned}
a_{11} &= \frac{1}{4} - \frac{7}{8640}\nu^4 + \frac{31}{272160}\nu^6 - \frac{167}{13063680}\nu^8 + \cdots,\\
a_{12} &= \frac{1}{4} - \frac{\sqrt{3}}{6} + \frac{\sqrt{3}}{216}\nu^2 - \left(\frac{7}{8640} + \frac{\sqrt{3}}{6480}\right)\nu^4\\
&\quad + \left(\frac{31}{272160} + \frac{17\sqrt{3}}{3265920}\right)\nu^6\\
&\quad - \left(\frac{167}{13063680} + \frac{31\sqrt{3}}{176359680}\right)\nu^8 + \cdots,\\
a_{21} &= \frac{1}{4} + \frac{\sqrt{3}}{6} - \frac{\sqrt{3}}{216}\nu^2 + \left(-\frac{7}{8640} + \frac{\sqrt{3}}{6480}\right)\nu^4\\
&\quad + \left(\frac{31}{272160} - \frac{17\sqrt{3}}{3265920}\right)\nu^6\\
&\quad + \left(-\frac{167}{13063680} + \frac{31\sqrt{3}}{176359680}\right)\nu^8 + \cdots,\\
\gamma_1 &= 1 - \frac{1}{288}\nu^4 + \frac{1}{2160}\nu^6 - \frac{881}{17418240}\nu^8 + \cdots,\\
b_1 &= \frac{1}{2} + \frac{1}{8640}\nu^4 - \frac{1}{272160}\nu^6 + \frac{13}{104509440}\nu^8 + \cdots.
\end{aligned}
\tag{3.13}
$$

It is clear that in the limit $\nu \to 0$ the well known classical fourth-order Gauss method is reproduced. We have implemented an algorithm for the generation of the principal local truncation error (plte) based on the work of Lambert [24] (pp. 150–152). Given an explicit or implicit (modified) RK method the algorithm produces automatically the plte. In order to obtain a compact shape for the plte we have to collect all occurring partial derivatives of $f(x,y)$ from (1.1) with respect to x and y in terms of total derivatives of y. The plte of the new method reads

$$
\begin{aligned}
\text{plte} &= \frac{h^5}{4320}\big((y^{(5)} - \mu^2 y^{(3)}) + \mu^2(y^{(3)} - \mu^2 y')\\
&\quad - 5 f_y (y^{(4)} - \mu^2 y^{(2)})\\
&\quad + 10\big(f_y^2 - (f_{xy} + f_{yy} f)\big)(y^{(3)} - \mu^2 y')\\
&\quad - 15\mu^2 f_y (y^{(2)} - \mu^2 y)\big).
\end{aligned}
\tag{3.14}
$$

The plte (3.14) is slightly different from the plte of the EFGauss method (case 1: fixed knot-points) from [1]:

$$
\text{plte} = \text{plte}\big(\text{EFGauss [1], case 1}\big) - \frac{h^5}{288}\mu^2 f_y (y^{(2)} - \mu^2 y).
\tag{3.15}
$$

Observing the plte it is visible that the new method integrates exactly, without truncation error, every linear combination of functions from the set (3.1) for $K = 0$ and $P = 0$. Although, the non-symplectic and symplectic EFGauss methods achieve a comparable accuracy for small time intervals, in the numerical experiments we will demonstrate that the symplectic method is more suitable for long-time integration of Hamiltonian systems.

4. Numerical examples

For the numerical comparisons we consider the various methods we have discussed in the preceding sections:

- S/V: The standard Störmer/Verlet method (2.3).
- GAUSS4: The classical fourth-order Gauss method (symplectic).
- EFGAUSS4: The non-symplectic fourth-order EFGauss method (case 1: fixed nodes) given in [1].
- EFSGAUSS4: The symplectic fourth-order EFGauss method developed in this paper.

4.1. *The test problems*

The methods are applied to some typical test examples.

Problem 1 (*The two-body problem*). The problem consists of finding the positions and velocities of two massive bodies that attract each other gravitationally, given their masses, positions, and velocities at some initial time. The first body is located in the origin while the second body is located in the plane with Cartesian coordinates (q_1, q_2). The velocity of the second body is given by $(q_1', q_2') = (p_1, p_2)$. The Hamiltonian is given by

$$
H = T + V, \qquad T = \frac{1}{2}\big(p_1^2 + p_2^2\big),
$$
$$
V = -\frac{1}{\sqrt{q_1^2 + q_2^2}}.
$$

The equations of motion are then

$$
\begin{aligned}
p_1' + \frac{q_1}{(q_1^2 + q_2^2)^{3/2}} &= 0, \quad q_1' = p_1,\\
p_2' + \frac{q_2}{(q_1^2 + q_2^2)^{3/2}} &= 0, \quad q_2' = p_2.
\end{aligned}
\tag{4.1}
$$

For problem (4.1) we choose, with $0 \leqslant e < 1$, the initial values

$$
\begin{aligned}
q_1(0) &= 1 - e, \qquad p_1(0) = 0,\\
q_2(0) &= 0, \qquad p_2(0) = \sqrt{\frac{1+e}{1-e}}.
\end{aligned}
\tag{4.2}
$$

The exact solution is

$$
q_1 = \cos(E) - e, \qquad q_2 = \sqrt{1 - e^2}\sin(E),
\tag{4.3}
$$

where e is the eccentricity of the orbit and the eccentric anomaly E is expressed as an implicit function of the independent variable x by Kepler's equation

$$
x = E - e\sin(E).
\tag{4.4}
$$

The system has the energy H and the *angular momentum* $M = q_1 p_2 - q_2 p_1$ as conserved quantities. The initial conditions (4.2) imply

$$
H_0 = -\frac{1}{2}, \qquad M_0 = \sqrt{1 - e^2}.
$$

Further, it is obvious that an acceptable value of the estimated frequency for EF methods is given by $\mu = i\sqrt{1/r^3}$ where $r = \sqrt{q_1^2 + q_2^2}$.

Problem 2 (*A modified two-body problem*). In many applications the potential V has to be corrected in various ways. For instance, the Hamiltonian

$$H = T + V, \qquad T = \frac{p_1^2 + p_2^2}{2},$$
$$V = -\frac{1}{\sqrt{q_1^2 + q_2^2}} - \frac{\epsilon}{2\sqrt{(q_1^2 + q_2^2)^3}}$$

(ϵ is a small *perturbation* parameter) corresponds to the motion in a plane of a particle gravitationally attracted by a slightly oblate sphere (rather than by a point mass). The attracting body is rotationally symmetric with respect to an axis orthogonal to the plane of the particle. Again, the system has the energy H and the angular momentum M as conserved quantities. The initial values are (4.2). We have that

$$H_0 = -\frac{1}{2} - \frac{\epsilon}{2(1-e)^3}, \qquad M_0 = \sqrt{1-e^2}.$$

An estimation of the frequency should be $\mu = i\sqrt{1/r^3 + 3\epsilon/r^5}$ where $r = \sqrt{q_1^2 + q_2^2}$.

Problem 3 (*Standard pendulum problem*). The Hamiltonian is given by

$$H(p,q) = \frac{p^2}{2} - a\cos(q), \quad a > 0.$$

We associate with this Hamiltonian the following problem

$$p' = -a\sin(q), \qquad q' = p,$$
$$p(0) = 1.5, \qquad q(0) = 0. \tag{4.5}$$

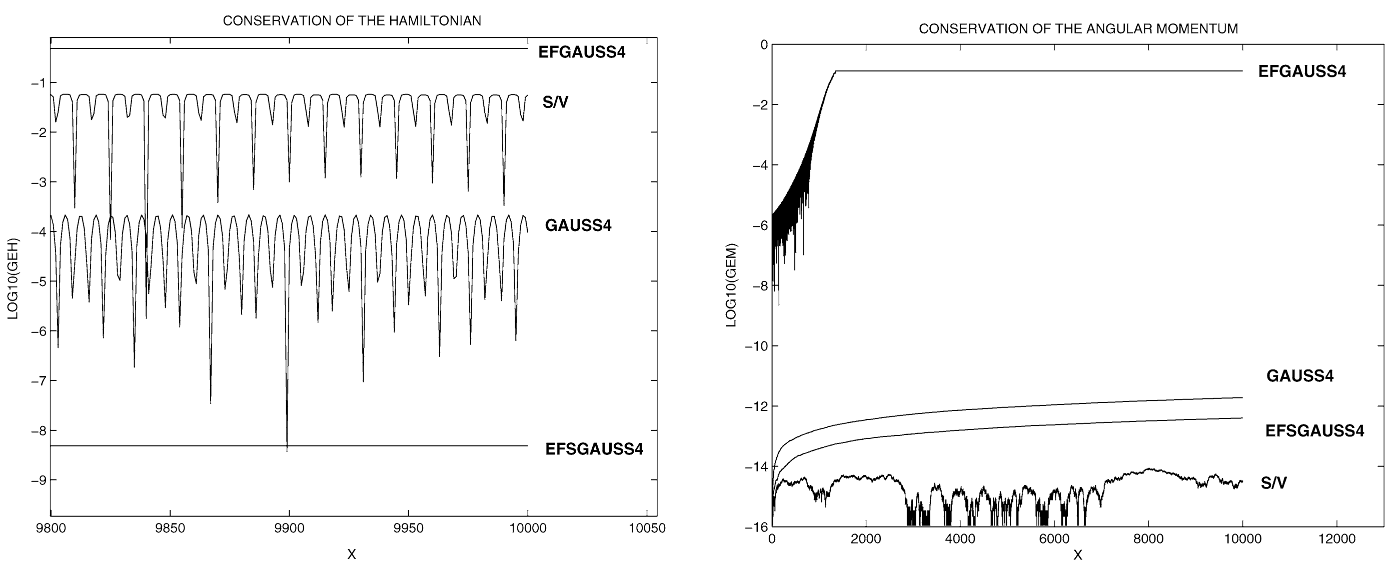

Fig. 1. Conservation of the Hamiltonian and the angular momentum for the two-body with eccentricity $e = 0.0001$. 10000 steps are taken with $h = 1$.

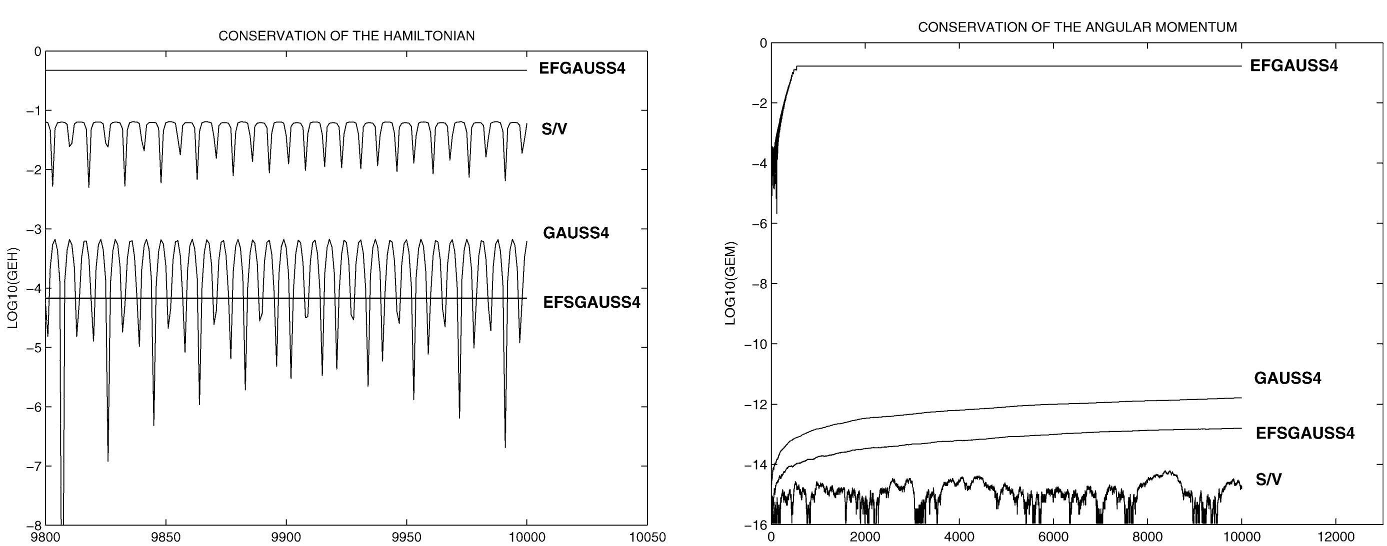

Fig. 2. Conservation of the Hamiltonian and the angular momentum for the modified two-body problem with eccentricity $e = 0.001$ and perturbation $\epsilon = 0.01$. 10000 steps are taken with $h = 1$.

For these initial conditions the constant value of the Hamiltonian is

$$H_0 = \frac{9}{8} - a.$$

Since the first-order system (4.5) is equivalent to the second-order equation

$$q'' = -a\sin(q),$$

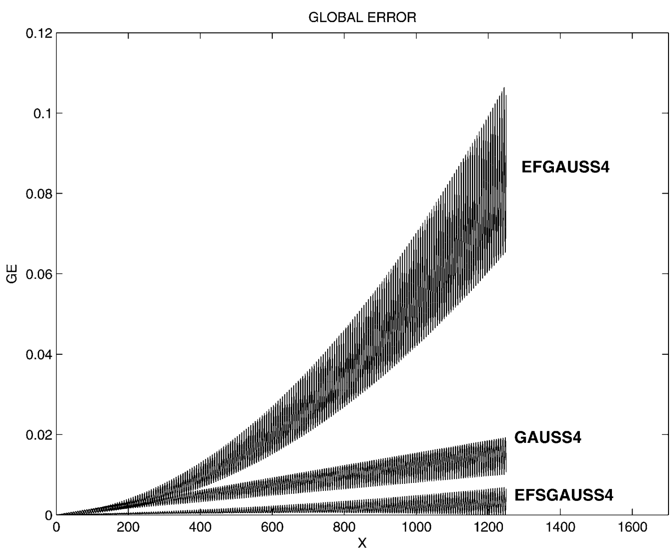

Fig. 3. The global error for the two-body problem with eccentricity $e = 0.2$. 10000 steps are taken with $h = 1/8$.

and for $|q| < 1$ this equation can be expanded as

$$q'' + aq = -a\left(\frac{q^3}{3!} + \frac{q^5}{5!} + \cdots\right),$$

a good choice for the fitted frequency should be $\mu = i\sqrt{a}$.

4.2. Results and discussion

We check the preservation of the Hamiltonian H and the angular momentum M by the methods considered with Problems 1–2. Symplectic methods have to preserve the angular momentum while, in general, the Hamiltonian is not conserved by symplectic methods [3]. In Figs. 1–2 we plot the errors $\mathrm{GEH} = |H_n - H_0|$ and $\mathrm{GEM} = |M_n - M_0|$ where H_n and M_n are the computed values of H and M at each integration point x_n. The conservation of H by symplectic methods is of a higher quality compared to the non-symplectic method EFGAUSS4. M is not conserved in an exact way since numerical methods are using floating-point arithmetic. Round-off error is a particular problem for Hamiltonian systems, because it introduces non-Hamiltonian perturbations despite the use of symplectic integrators. The fact that symplectic methods do produce behavior that looks Hamiltonian shows that the non-Hamiltonian perturbations are much smaller than those introduced by non-symplectic methods.

Fig. 3 illustrates why the role of symplecticity is very crucial for long-time integration. It is remarkable to see that, while symplectic methods exhibit linear error growth, EFGAUSS4 gave a quadratic growth.

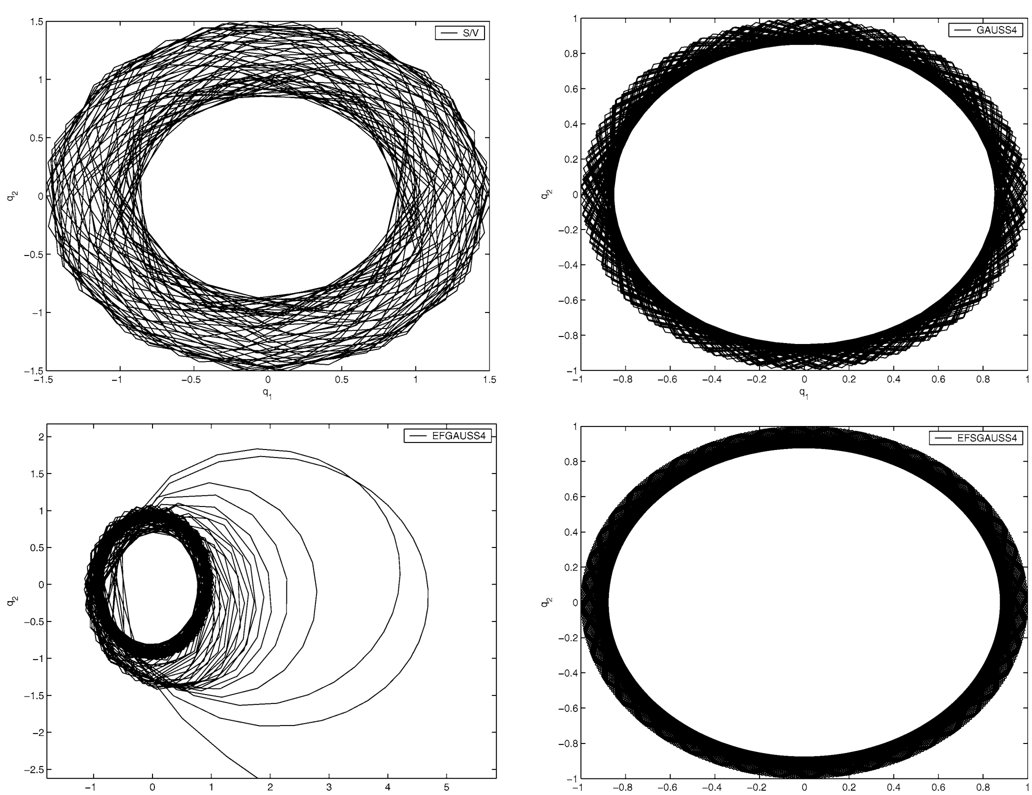

Fig. 4. A (q_1, q_2)-plot of the numerical solution of the two-body problem with eccentricity $e = 0.0001$. 10000 steps are taken with $h = 1$.

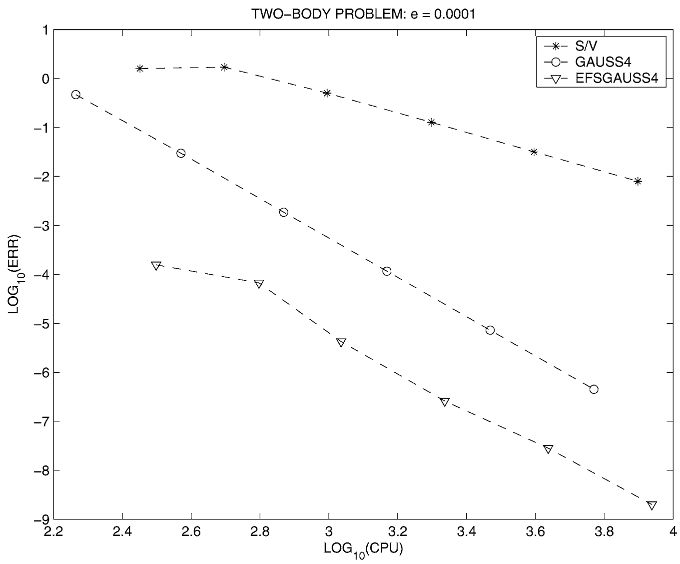

Fig. 5. The global error at the endpoint $x_{\text{end}} = 100\,000$ for the two-body problem with eccentricity $e = 0.0001$. The exact solution can be obtained with (4.3)–(4.4).

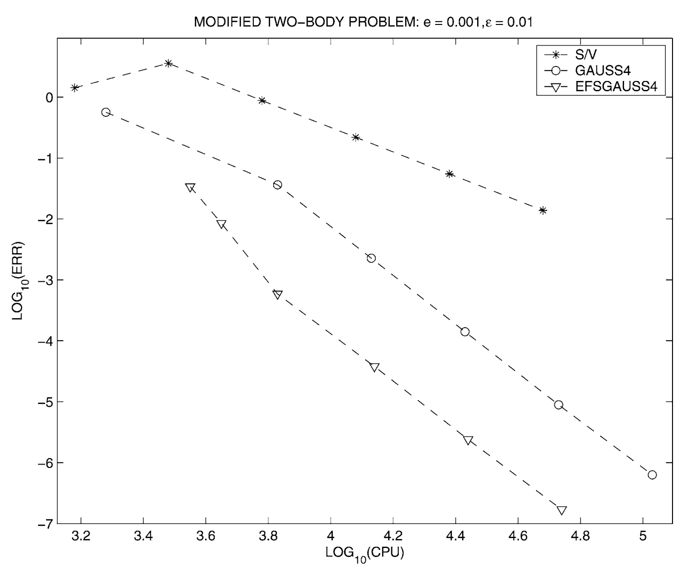

Fig. 6. The global error at the endpoint $x_{\text{end}} = 100\,000$ for the modified two-body problem with eccentricity $e = 0.001$ and perturbation $\epsilon = 0.01$. The exact solution at the endpoint, correct to 8 decimals, is $q_1(x_{\text{end}}) = -0.09382009$ and $q_2(x_{\text{end}}) = -0.99147494$.

As shown in Fig. 4, when plotting the numerical orbit of the two-body problem in the (q_1, q_1)-plane, it is no longer a surprise that the numerical orbits produced by EFGAUSS4 spirals outwards and gives a completely wrong answer.

The efficiency curves of the symplectic methods applied to Problems 1–3 are plotted in Figs. 5–7. The numerical results indicate an excellent long-time behavior of the new method when solving Hamiltonian systems.

5. Conclusions

In this paper we have examined how we can combine symplecticity with the idea of exponential fitting. Motivated by the fact that the EFGauss methods from [1] are not symplectic

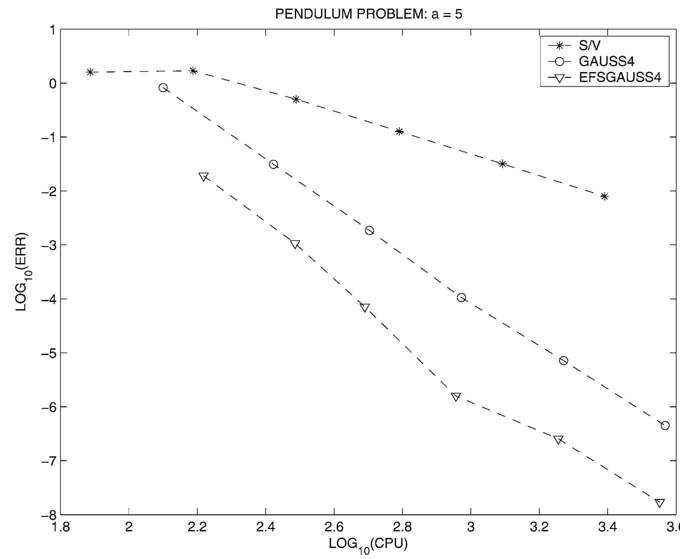

Fig. 7. The global error at the endpoint $x_{\text{end}} = 100\,000$ for the pendulum problem with $a = 5$. The exact solution at the endpoint, correct to 9 decimals, is $q(x_{\text{end}}) = -0.595399559$.

our intension in this paper is to investigate how we can improve these algorithms in order to obtain a symplectic EF based method. A fourth-order symplectic modified EFRK method of Gauss-type is constructed and discussed in this work. The advantages of the new method compared to other (symplectic and non-symplectic) methods are clearly demonstrated. We note that the existence of symplectic EF methods with an order of accuracy higher than four is an open problem. In the future we hope to construct some higher-order symplectic EF methods. We intend to follow this line of research.

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