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Structure preservation of exponentially fitted Runge–Kutta methods☆

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Abstract

The preservation of some structure properties of the flow of differential systems by numerical exponentially fitted Runge–Kutta (EFRK) methods is considered. A complete characterisation of EFRK methods that preserve linear or quadratic invariants is given and, following the approach of Bochev and Scovel [On quadratic invariants and symplectic structure, BIT 34 (1994) 337–345], the sufficient conditions on symplecticity of EFRK methods derived by Van de Vyver [A fourth-order symplectic exponentially fitted integrator, Comput. Phys. Comm. 174 (2006) 255–262] are obtained. Further, a family of symplectic EFRK two-stage methods with order four has been derived. It includes the symplectic EFRK method proposed by Van de Vyver as well as a collocation method at variable nodes that can be considered as the natural collocation extension of the classical RK Gauss method. Finally, the results of some numerical experiments are presented to compare the relative merits of several fitted and nonfitted fourth-order methods in the integration of oscillatory systems.

MSC: 65L06; 65L20

Keywords: Exponential fitting; Runge–Kutta methods; Structure preservation; Symplectic methods

1. Introduction

Exponentially fitted (EF) methods for the numerical solution of ODEs which have periodic or oscillating solutions have been considered by several authors (see e.g., [2,6,8,12,13,15,17]) with the aim to use the available information on the solutions to derive more accurate and/or efficient algorithms than the general purpose algorithms for such a type of problems. After the earlier works of Gautschi [3], there is a well established theory of EF linear multistep methods for first- and second-order differential systems. However, the development of EF Runge–Kutta (Nyström) methods has been more limited mainly due to the nonlinear nature of the Runge–Kutta (RK) methods. A detailed survey including an extensive bibliography on this subject can be found in Ixaru and Vanden Berghe [5].

An approach to derive EF Runge–Kutta (EFRK)-type methods is to select the coefficients of the method so that it integrates exactly all functions of a given linear space that is chosen depending on the nature of the solutions of the

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original problem and also minimising the local error of the numerical solution. Thus, in the papers of Paternoster [6] and Vanden Berghe et al. [12,13,15], by using the linear stage representation of a RK method, they obtain methods with frequency-dependent coefficients that are able to integrate exactly first- (or second-) order differential systems with solutions belonging to the linear space generated by a set of functions of type $\{\sin(\omega t), \cos(\omega t), \sin(2\omega t), \cos(2\omega t), \ldots\}$ where ω is a prescribed frequency. It is expected that including these functions into the space of approximating functions, the numerical method will track $T = 2\pi/w$ periodic solutions more accurately than the standard methods based on polynomial functions.

On the other hand it has been recently recognised by several authors [18,9,16] that adapted and EFRK methods which possess certain additional structure preservation properties can be useful in the numerical integration of special classes of problems. We may consider e.g., the class of Hamiltonian systems which are known to model nondissipative systems and in many cases have periodic or quasi periodic solutions. For these type of problems, in addition to use EF methods, it may be appropriate to consider symplectic methods that preserve the structure of the original flow. So, for the Newtonian equations of motion $q'' = f(q) \equiv -\nabla_q V(q)$ in a conservative field that can be written as a Hamiltonian system with $H(p, q) = (\frac{1}{2})\, p^{\mathrm{T}}\, p + V(q)$, Tocino and Vigo-Aguiar [10] have given conditions on the coefficients of EFRK–Nyström methods that ensure the symplecticness of the numerical flow. More recently Van Daele and Vanden Berghe [11] have presented a detailed study of several EF versions of the well known Störmer–Verlet (S/V) method for the above special second-order equations. They show that, when written the EF S/V method as a one step method, it is a symmetric, symplectic and reversible method and therefore it preserves important properties of the corresponding flows. In addition, some remarks on the choice of the frequency fitting in some practical problems as well as several numerical experiments are presented.

For general Hamiltonian systems, Van de Vyver has extended in [16] the well known theory of symplectic RK methods [7] to EFRK methods, giving sufficient conditions on the coefficients of an EFRK method that ensure the preservation of symplecticness of the flow in general Hamiltonian systems. Further, he has shown that some two-stage EFRK Gauss-type collocation methods with order four proposed in the literature do not satisfy these symplecticness conditions, and he derives an alternative symplectic two-stage fourth-order EFRK method and studies their numerical behaviour for several test problems.

The aim of this paper is to study the preservation of invariants of first-order differential systems by EFRK methods and the derivation of new EF methods with orders $\leqslant 4$ that preserve linear and quadratic invariants and are symplectic. The paper is organised as follows: in Section 2 we introduce the notations and definitions to be used in the rest of the paper as well as previous results on symplectic EFRK methods. Section 3 is concerned with the preservation properties of EFRK methods: firstly, for one-stage EFRK methods necessary and sufficient conditions on the coefficients of the method that ensure the conservation of linear and quadratic invariants and symplecticness are given. These results are partially extended to s-stage methods and a new two-stage Gauss-type symplectic method with order four is derived. It is shown that it is a collocation method with variable nodes with respect to the trigonometrical basis $\{1, \sin(\omega t), \cos(\omega t)\}$. Also, a general family of symplectic two-stage fourth-order EFRK methods is derived. This family includes the method proposed by Van de Vyver [16] as well as our collocation method. In Section 4, the results of some numerical experiments comparing the relative behaviour of fourth-order symplectic fitted and nonfitted methods are presented. The final section is devoted to expose some conclusions.

2. Basic notations and definitions

We consider IVPs for first-order systems of differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t} y(t) = f(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^m, \tag{1}$$

where for simplicity $f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$ is assumed to be sufficiently smooth, so that for all (t_0, y_0) (1) has a unique solution $y(t) = y(t; t_0, y_0)$ defined in some neighbourhood of t_0 with as many derivatives as necessary.

In the case of Hamiltonian systems $m = 2d$ and there exist a scalar Hamiltonian function $H = H(t, y) : \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}$, so that $f(y) = -J\ \nabla_y H(t, y)$. Here J is the $2d$-dimensional skew symmetric matrix

$$J = \begin{pmatrix} 0_d & I_d \\ -I_d & 0_d \end{pmatrix}, \quad J^{-1} = -J,$$

and $\nabla_y H(t, y) = H_y^{\mathrm{T}}(t, y)$ is the column vector of the derivatives of $H(t, y)$ with respect to the components of $y = (y_1, \ldots, y_{2d})^{\mathrm{T}}$. Then the Hamiltonian system can be written as

$$y'(t) = -J\ \nabla_y H(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^{2d}. \tag{2}$$

For each fixed t_0 the flow map of $y' = f(t, y)$ will be denoted by $\phi_{t_0,h} = \phi_h : \mathbb{R}^m \to \mathbb{R}^m$ so that $\phi_h(y_0) = y(t_0 + h; t_0, y_0)$. In particular, for the case of a Hamiltonian system (2), ϕ_h is a symplectic map for all h in its domain of definition (see e.g., [7,4]) i.e., the Jacobian matrix of $\phi_h(y_0)$ satisfies

$$\phi_h'(y_0) J \phi_h'(y_0)^{\mathrm{T}} = J \quad \text{for all } t_0, y_0. \tag{3}$$

We will consider here s-stage EFRK methods that provide an approximation $\psi_h(y_0)$ to $\phi_h(y_0)$ defined by the equations

$$\psi_h(y_0) = \gamma_0 y_0 + h \sum_{j=1}^{s} b_j f(t_{0,j}, Y_j), \tag{4}$$

$$Y_j = \gamma_j y_0 + h \sum_{k=1}^{s} a_{jk} f(t_{0,k}, Y_k), \quad j = 1, \ldots, s, \tag{5}$$

where $t_{0,k} = t_0 + c_k h$ and the real parameters $\gamma_j > 0$, b_j, a_{jk} and c_j are allowed to depend on the step size $h > 0$ and on a given fixed frequency $\omega > 0$ to be chosen by the user. All these parameters will be assumed to be smooth functions of h, ω in some neighbourhood of the origin.

The s-stage EFRK method (4)–(5) is defined by the following vectors and matrix: $\gamma_0 \in \mathbb{R}$, $c = (c_i)$, $b = (b_i)$, $\gamma = (\gamma_i) \in \mathbb{R}^s$, $A = (a_{ij}) \in \mathbb{R}^{s \times s}$ and in the remainder it will be assumed that (5) possesses a unique solution for the range of step sizes under consideration. Note that in standard RK methods all $\gamma_j = 1$ and the remaining parameters are all constants.

As a first remark note that the method ψ_h given by (4)–(5) integrates exactly the constant solutions of (1) if and only if $\psi_h(y_0) = \gamma_0 y_0 = y_0$ for all y_0, i.e., if and only if $\gamma_0 = 1$. In addition, it can be easily verified that unless the coefficients of (4)–(5) satisfy

$$\gamma_0 = 1, \quad \gamma = e \equiv (1, \ldots, 1)^{\mathrm{T}}, \quad b^{\mathrm{T}} e = 1, \quad c = Ae, \tag{6}$$

this method may give different numerical solution for the nonautonomous IVP (1) and for its equivalent autonomous formulation $\widehat{y}' = \widehat{f}(\widehat{y})$, $\widehat{y}(t_0)^{\mathrm{T}} = (t_0, y_0^{\mathrm{T}})^{\mathrm{T}}$, with $\widehat{y} = (t, y^{\mathrm{T}})^{\mathrm{T}}$, $\widehat{f} = (1, f^{\mathrm{T}})^{\mathrm{T}}$. Therefore for EFRK methods that do not satisfy (6) it will be necessary to distinguish between the integration of autonomous and nonautonomous systems.

An approach to construct s-stage EFRK formulas with respect to a given linear space of functions defined by a basis $\mathscr{F}$ is to associate to (4)–(5) the $(s + 1)$ linear functionals

$$L_j[u](t) \equiv u(t + c_j h) - \gamma_j u(t) - h \sum_{k=1}^{s} a_{jk} u'(t + c_k h), \quad j = 0, 1, \ldots, s, \tag{7}$$

where $c_0 = 1$ and $a_{0j} = b_j$, $(j = 1, \ldots, s)$. Then, if we choose the available parameters of the method ψ_h so that all linear functionals L_j vanish for the functions of $\mathscr{F}$, we may ensure that the corresponding method (4)–(5) will integrate exactly all IVPs (1) with solutions belonging to the linear space generated by $\mathscr{F}$. Observe that for a given set of nodes c_j, $j = 1, \ldots, s$ distinct between them and a basis $\mathscr{F}$, the conditions $L_j[u](t) = 0$, $j = 0, \ldots, s$, $u \in \mathscr{F}$, define $a_{jk} = a_{jk}(t, h)$ and $\gamma_j = \gamma_j(t, h)$ and therefore the corresponding method (4)–(5) has coefficients that should be computed, even at fixed step size, at each step because of their dependence of t. Here we will restrict our considerations to basis $\mathscr{F}$ such that the corresponding coefficients of (4)–(5) turn out to be independent of t. Note that for an exponential function $u(t) = \exp(\alpha t)$, $\alpha \in \mathbb{C}$, $L[u](t) = u(t) L[u](0)$ and therefore conditions $L[u](t) = 0$ can be taken at $t = 0$. Further, by linearity $L[\exp(\mathrm{i}\omega t)] = L[\cos(\omega t)] + \mathrm{i} L[\sin(\omega t)]$, and for a trigonometrical basis the parameters may be chosen independent of t.

Finally, let us recall that it has been proved by Van de Vyver [16] that if the coefficients of (4)–(5) with $\gamma_0 = 1$ satisfy

$$\Omega_{ij} \equiv b_j \gamma_j^{-1} a_{ji} + b_i \gamma_i^{-1} a_{ij} - b_i b_j = 0, \quad 1 \leqslant i, j \leqslant s, \tag{8}$$

then the method is symplectic for all Hamiltonian system (2).

3. EFRK methods

3.1. One-stage methods

We start considering the preservation of invariants by EFRK methods (4)–(5) with $s = 1$ with respect to the two-dimensional fitting space $\mathscr{F} = \langle \exp(\pm i\omega t)\rangle = \langle \cos(wt), \sin(\omega t)\rangle$ where the node $c_1 = c_1(h, \omega) \in [0, 1]$. We will restrict our considerations to autonomous systems (1).

According to (7) the available parameters of the method satisfy the complex equations

$$e^{i\omega h} - \gamma_0 - i\omega h b_1 e^{i\omega h c_1} = 0, \quad e^{-i\omega h} - \gamma_0 + i\omega h b_1 e^{-i\omega h c_1} = 0,$$

$$e^{i\omega h c_1} - \gamma_1 - i\omega h a_{11} e^{i\omega h c_1} = 0, \quad e^{-i\omega h c_1} - \gamma_1 + i\omega h a_{11} e^{-i\omega h c_1} = 0.$$

Taking c_1 as free parameter and putting $v = \omega h$, the remaining coefficients of the one-stage formula are given by

$$\gamma_1 = \frac{1}{\cos(vc_1)}, \quad \gamma_0 = \frac{\cos((1 - c_1)v)}{\cos(c_1 v)}, \quad a_{11} = \frac{\tan(vc_1)}{v}, \quad b_1 = \frac{\sin(v)}{v\cos(c_1 v)}. \tag{9}$$

Hence the equations of the method can be written as

$$\begin{cases} \psi_h(y_0) = \gamma_0 y_0 + h b_1 f(Y_1), \\ Y_1 = \mu_0 y_0 + \mu_1 \psi_h(y_0) \equiv (\gamma_1 - \gamma_0 a_{11} b_1^{-1}) y_0 + (a_{11} b_1^{-1}) \psi_h(y_0). \end{cases} \tag{10}$$

First of all, if (1) possesses a linear invariant $G(y) = d^{\mathrm{T}} y$ for some constant vector d, then $d^{\mathrm{T}} f(y) = 0$ for all y and from (10) it follows that $G(\psi_h(y_0)) = \gamma_0 G(y_0)$ which implies that linear invariants are preserved iff $\gamma_0 = 1$.

Now, suppose that (1) possesses a quadratic invariant $Q(y) = y^{\mathrm{T}} S y$ with S symmetric. Then $y^{\mathrm{T}} S f(y) = 0$ for all y and after some calculations we get

$$Q(\psi_h(y_0)) - Q(y_0) = (\gamma_0^2 - 1) y_0^{\mathrm{T}} S y_0 + h^2 b_1 (b_1 - 2\gamma_0 \gamma_1^{-1} a_{11}) f_1^{\mathrm{T}} S f_1,$$

with $f_1 = f(Y_1)$. Then ψ_h preserves all quadratic invariants iff the coefficients of $y_0^{\mathrm{T}} S y_0$ and $f_1^{\mathrm{T}} S f_1$ vanish therefore the conditions

$$\gamma_0 = \pm 1 \quad \text{and} \quad b_1 = 2\gamma_0 \gamma_1^{-1} a_{11}, \tag{11}$$

are necessary and sufficient for the preservation of quadratic invariants. Note that in view of (9) these conditions hold iff $c_1(h, \omega) = \frac{1}{2}$. Thus the EF Midpoint Rule is the only method of the family (9), (10), that preserves quadratic invariants.

In the case of Hamiltonian equations $\psi_h(y_0) = \gamma_0 y_0 - h b_1 J \nabla_y H(Y_1)$, with Y_1 given by the second equation of (10). After some calculations, condition $\psi_h'(y_0) J \psi_h'(y_0) = J$ of symplecticness of the numerical flow is equivalent to

$$(\gamma_0^2 - 1) J + h^2 b_1^2 (\mu_1^2 - \mu_0^2) J H_{yy} J H_{yy} J = 0,$$

with $H_{yy} = H_{yy}(Y_1)$. Now this equation holds for all $H = H(y)$ if and only if $\gamma_0 = \pm 1$ and $\mu_0 = \pm \mu_1$ which are equivalent to (11). Note that the case $\gamma_0 = -1$ is useless because then the RK method is not zero-stable. In conclusion we may state the following:

Theorem 3.1. *A method of the one-stage EFRK family* (10)

(i) *Preserves linear invariants iff* $\gamma_0 = 1$.
(ii) *Preserves quadratic invariants iff conditions* (11) *hold.*
(iii) *Is symplectic iff conditions* (11) *hold. Among the one-stage family* (10) *with the coefficients defined by* (9) *the only symplectic method is the EF Midpoint Rule corresponding to* $c_1 = \frac{1}{2}$. *Further this is the only method that preserves linear invariants.*

3.2. Multistage EFRK methods

For the preservation of linear invariants $G(y) = d^{\mathrm{T}} y$ of autonomous systems we obtain again $G(\psi_h(y_0)) = \gamma_0 G(y_0)$, which gives the same condition that in the case $s = 1$.

For quadratic invariants $G(y) = y^{\mathrm{T}} S y$ after some calculations we obtain

$$G(\psi_h(y_0)) = \gamma_0^2 G(y_0) - h^2 \sum_{i,j=1}^{s} \Omega_{ij}\ f_i^{\mathrm{T}} S f_j, \tag{12}$$

with $f_i = f(Y_i)$ and Ω_{ij} defined by (8). Now $G(\psi_h(y_0)) = G(y_0)$ holds for all smooth $f(y)$ and S symmetric such that $y^{\mathrm{T}} S f(y) = 0$ and $h > 0$ iff

$$\gamma_0 = 1 \quad \text{and} \quad \Omega = (\Omega_{ij}) \equiv 0. \tag{13}$$

To derive conditions on the coefficients of (4)–(5) that imply the symplecticness of ψ_h, we follow the approach of Bochev and Scovel [1] that relates this property with the preservation of quadratic invariants.

We consider the $\widehat{m} = (m + m \times m)$-dimensional IVP given by the equations

$$\begin{cases} y' = f(y), & y(t_0) = y_0 \in \mathbb{R}^m, \\ \Phi' = f_y(y)\ \Phi, & \Phi(t_0) = I \in \mathbb{R}^{m \times m}. \end{cases} \tag{14}$$

Putting together the variables y and Φ into a new variable $U \in \mathbb{R}^{m+m^2}$ we may view (14) as a new IVP

$$U' = \widehat{f}(U)U, \quad U(t_0) = U_0 = (y_0, I) \in \mathbb{R}^{\widehat{m}}. \tag{15}$$

If we apply the method (4)–(5) to (15) (or (14)) we get $U_1 = \psi_{\widehat{f},h}(U_0)$. Since the first m components of (15) (or (14)) are identical to (1) and we apply the same method, the first m components of U_1 will be exactly $y_1 = \psi_{f,h}(y_0)$. For the remaining m^2 variables the equations of the method are

$$\begin{aligned} \Phi_1 &= \gamma_0 I + h \sum_{i=1}^{s} b_i f_y(Y_i) \Phi_{0,i}, \\ \Phi_{0,i} &= \gamma_i I + h \sum_{j=1}^{s} a_{ij} f_y(Y_j) \Phi_{0,j} \quad (i = 1, \ldots, s). \end{aligned} \tag{16}$$

where $\Phi_{0,i},\ i = 1, \ldots, s$ are the internal stages of the Φ-variable.

Now if we calculate the Jacobian $\partial y_1 / \partial y_0 \in \mathbb{R}^{m \times m}$ of the map $\psi_{f,h}(y_0)$ in Eqs. (4)–(5) we get

$$\begin{aligned} \frac{\partial y_1}{\partial y_0} &= \gamma_0 I + h \sum_{i=1}^{s} b_i f_y(Y_i) \frac{\partial Y_i}{\partial y_0}, \\ \frac{\partial Y_i}{\partial y_0} &= \gamma_i I + h \sum_{j=1}^{s} a_{ij} f_y(Y_j) \frac{\partial Y_j}{\partial y_0} \quad (i = 1, \ldots, s). \end{aligned}$$

These equations are identical to (16) if we identify

$$\Phi_1 \to \frac{\partial y_1}{\partial y_0}, \quad \Phi_{0,i} \to \frac{\partial Y_i}{\partial y_0}.$$

Hence assuming that (15) possesses a unique solution for $h \in (0, h_0]$, then the second set of variables of $\psi_{\widehat{f},h}(U_0)$ satisfies

$$\Phi_1 = \frac{\partial y_1}{\partial y_0} = \frac{\partial}{\partial y_0} \psi_{f,h}(y_0) = \psi_h'(y_0). \tag{17}$$

Finally, since for Hamiltonian equations $\Phi^{\mathrm{T}} J \Phi$ is a quadratic invariant of (14) or (15), if the method ψ_h preserves quadratic invariants we have $\Phi_1^{\mathrm{T}} J \Phi_1 = \Phi(t_0)^{\mathrm{T}} J \Phi(t_0) = J$, and in view of (17) the method ψ_h is symplectic

Then we have proved:

Theorem 3.2. *A method of the s-stage family of EFRK methods* (4)–(5)

(i) *Preserves linear invariants iff* $\gamma_0 = 1$.
(ii) *Preserves quadratic invariants iff satisfies* (13).
(iii) *If their coefficients satisfy* (13) *is symplectic*.

Next we construct a symplectic two-stage collocation EFRK Gauss-type method with order four. We start considering two stage methods with (variable) symmetric nodes $c_{2,1} = (\frac{1}{2}) \pm d(h, \omega)$ such that all stage operators $L_j[u]$, $j = 0, 1, 2$ (7) are exact for the trigonometric space generated by $\mathscr{F} = \langle 1, \cos(\omega t), \sin(\omega t)\rangle = \langle 1, \exp(\pm \mathrm{i}\omega t)\rangle$.

First of all $L_j[1] = 0$, $j = 0, 1, 2$ are equivalent to $\gamma_j = 1$, $j = 0, 1, 2$.

Putting $v = \omega h$, $a_0 = \exp(\mathrm{i}v/2)$, $a = \exp(\mathrm{i}vd)$, $L_0[\exp(\pm \mathrm{i}\omega t)] = 0$ iff

$$b_1 = b_2 = \frac{\mathrm{i}a(1 - a_0^2)}{v a_0(1 + a^2)} = \frac{\sin(v/2)}{v \cos(dv)}. \tag{18}$$

Further, $L_j[\exp(\pm \mathrm{i}\omega t)] = 0$, $j = 1, 2$ iff the coefficients a_{ij} satisfy

$$\begin{aligned} a_{11} &= \frac{\mathrm{i}(a - a_0)(a^3 a_0 - 1)}{a_0 v(-1 + a^4)} = \frac{\cos(2vd) - \cos(vd + v/2)}{v \sin(2vd)}, \\ a_{12} &= -\frac{\mathrm{i}a(a - a_0)^2}{v a_0(-1 + a^4)} = \frac{-1 + \cos(v(d - 1/2))}{v \sin(2vd)}, \\ a_{22} &= a_{11}(a \to a^{-1}), \quad a_{21} = a_{12}(a \to a^{-1}). \end{aligned} \tag{19}$$

Since $b_1 = b_2$, the symplecticness conditions (8) become

$$\begin{aligned} \Omega_{11} &= b_1(2a_{11} - b_1) = 0, \\ \Omega_{22} &= b_1(2a_{22} - b_1) = 0, \\ \Omega_{12} &= \Omega_{21} = b_1(b_1 - a_{12} - a_{21}) = 0. \end{aligned} \tag{20}$$

The last condition of (20) is satisfied in view of (18) and (19). The conditions for Ω_{11} and Ω_{22} hold iff

$$(a + a^3)a_0^2 - 2(1 + a^4)a_0 + (a + a^3) = 0, \tag{21}$$

or else

$$\cos(dv) = \frac{\sqrt{8 + \cos^2(v/2)} + \cos(v/2)}{4}. \tag{22}$$

Hence the two-stage method with coefficients given by (18), (19) and $c_j = (\frac{1}{2}) + (-1)^j d$ with $d = d(v)$ given by (22) is a symplectic EFRK method with respect to the fitting space of functions generated by $\mathscr{F}$.

Further (18) and (21) imply that $L_0[\exp(\pm 2\mathrm{i}\omega t)] = 0$, and therefore, operator L_0 is exact for the trigonometrical basis $\{1, \exp(\pm \mathrm{i}\omega t), \exp(\pm 2\mathrm{i}\omega t)\}$.

Remarks. (1) A noncollocation symplectic two-stage EFRK Gauss-type method has been obtained by Van de Vyver in [16] by choosing the fixed Gauss nodes $c_{2,1} = (3 \pm \sqrt{3})/6$ and the variable coefficients $\gamma_1(v) = \gamma_2(v)$ and $\gamma_0 = 1$, so that $L_j[\exp(i\omega t)] = 0$, $j = 0, 1, 2$ and all $\Omega_{ij} = 0$.

(2) In the derivation of the two-stage classical RK Gauss method, L_0 is chosen to be exact for the polynomial basis $\{1, t, t^2, t^3, t^4\}$ and this fact defines uniquely the nodes c_1, c_2 and coefficients b_1, b_2 of L_0. Then the coefficients a_{ij}

are uniquely defined imposing that $L_{1,2}$ are exact for $\{1, t, t^2\}$. Clearly our above approach translates this pattern to the trigonometrical basis $\{1,\ \cos(\omega t),\ \sin(\omega t), \cos(2\omega t), \sin(2\omega t)\}$.

(3) In view of Remark 2 it can be proved that our two-stage RK Gauss method can be considered as a trigonometric collocation method in the following sense: let $T_0(t), t \in [t_0, t_0 + h]$ be the trigonometric polynomial $T_0(t) = \alpha_0 + \alpha_1 \cos(\omega(t - t_0)) + \alpha_2 \sin(\omega(t - t_0))$ that satisfies the collocation conditions

$$T_0(t_0) = y_0, \quad T_0'(t_0 + c_j h) = f(t_0 + c_j h, T_0(t_0 + c_j h)) \quad (j = 1, 2) \tag{23}$$

for some nodes $c_j = c_j(h, \omega) \in [0, 1]$ where $c_1 \neq c_2$. Assuming that there exist a unique T_0 that satisfies (23) for sufficiently small h, the collocation method $\psi_{h,f}$ at this set of nodes may be defined by $\psi_{h,f}(y_0) = T_0(t_0 + h)$.

In fact, denoting by $Z_j = T_0(t_0 + c_j h)$, $j = 0, 1, 2$ with $c_0 = 1$ and $f_j = f(t_0 + c_j h, Z_j)$, $j = 1, 2$ and putting $S_j = \sin(c_j v)$, $C_j = \cos(c_j v)$ it can be seen that

$$Z_j = y_0 + h(\lambda_{j1} f_1 + \lambda_{j2} f_2), \quad j = 0, 1, 2.$$

with

$$\lambda_{j1} = \frac{C_j C_2 + S_j S_2 - C_2}{v(S_2 C_1 - S_1 C_2)}, \quad \lambda_{j2} = \frac{-C_j C_1 - S_j S_1 + C_1}{v(S_2 C_1 - S_1 C_2)}.$$

Hence the collocation method defined by (23) is equivalent to an EFRK method (4)–(5) with $a_{ij} = \lambda_{ij}$, $1 \leqslant i, j \leqslant 2$, $b_j = a_{0j}$, $j = 1, 2$. In particular, for the symmetrical choice of nodes $c_j = (\frac{1}{2}) + (-1)^j d$ with $d = d(v)$ given by (22) we have the coefficients of our symplectic methods (18), (19).

To check the fourth-order of our two-stage symplectic method note that since all $\gamma_j = 1$, Eqs. (4) and (5) that define $\psi_h(y_0)$ are formally identical to a standard two-stage RK method with $A = A(v)$, $b = b(v)$, $c = c(v)$, depending on the parameter v. Moreover, since $c = Ae$ with $e = (1, 1)^{\mathrm{T}}$ is not satisfied, we will restrict our study to autonomous differential systems.

According to the theory of order for standard RK methods [4] the local error $\psi_h(y_0) - \phi_h(y_0)$ at y_0 with step size h, possesses the power series expansion

$$\psi_h(y_0) - \phi_h(y_0) = \sum_{\tau \in \mathscr{T}} \frac{h^{\rho(\tau)}}{\rho(\tau)!} (\gamma(\tau) b(v)^{\mathrm{T}} \Phi_A(\tau) - 1) \alpha(\tau) F(\tau)(y_0), \tag{24}$$

where $\mathscr{T}$ is the set of rooted trees with order $\rho(\tau) \geqslant 1$, $F(\tau)(y_0)$ is the elementary differential of f associated to $\tau \in \mathscr{T}$ at y_0, $\alpha(\tau)$ is the number of monotonic labellings of τ and $\Phi = \Phi_{A(v)} : \mathscr{T} \to R^2$ defined recursively by

$$\Phi(\cdot) = e, \quad \Phi([\tau_1, \ldots, \tau_k]) = A(v)\Phi(\tau_1) \cdot \cdots \cdot A(v)\Phi(\tau_k),$$

where $\cdot$ is the componentwise product.

From the independence of the elementary differentials and the fact that $v = \omega h$, it follows from (24) that the method has order 4 if

$$b(v)^{\mathrm{T}} \Phi_{A(v)}(\tau) - \frac{1}{\gamma(\tau)} = \mathcal{O}(h^{p'}) \quad \text{with} \quad p' \geqslant 5 - \rho(\tau),$$

hold for all $\tau \in \mathscr{T}$ with order $\rho(\tau) \leqslant 4$. An algebraic calculation taking into account the power series expansion of $b = b(v = \omega h)$ and $A = A(v = \omega h)$ shows that the above conditions hold for all trees with order $\leqslant 4$ and then the method has order 4 for autonomous differential systems.

3.3. A family of two-stage symplectic methods

Here we derive a family of fourth-order two-stage EFRK methods (with respect to the basis $\{\cos(\omega t),\ \sin(\omega t)\}$ that preserve linear and quadratic invariants and are symplectic. By imposing the EF conditions: $L_j[\exp(\pm i\omega t)] = 0$,

$j = 0, 1, 2$ with $\gamma_0 = 1$, the coefficients of A and b are given by

$$A = \frac{1}{\Delta}\begin{pmatrix} \gamma_1\cos(c_2 v) - \cos((c_1 - c_2)v) & 1 - \gamma_1\cos(c_1 v) \\ -1 + \gamma_2\cos(c_2 v) & -\gamma_2\cos(c_1 v) + \cos((c_1 - c_2)v) \end{pmatrix},$$

$$b = \frac{2\sin(v/2)}{\Delta}(\sin((1 - 2c_2)v/2),\ -\sin((1 - 2c_1)v/2))^{\mathrm{T}} \tag{25}$$

with $\Delta = v\sin((c_1 - c_2)v)$ and $c_1 \neq c_2$.

In view of (25) the conditions (8) are satisfied iff γ_1, γ_2 are given by

$$\gamma_1 = \frac{\cos((c_1 - c_2)v)}{\cos(v/2)\cos((1 - 2c_2)v/2)}, \quad \gamma_2 = \frac{\cos((c_1 - c_2)v)}{\cos(v/2)\cos((1 - 2c_1)v/2)}. \tag{26}$$

The coefficients (25)–(26) define a two-parameter family of symplectic EFRK methods which preserve linear and quadratic invariants. In addition, they satisfy the conditions:

$$b^{\mathrm{T}}e = 1 + \mathcal{O}(v^2), \quad b^{\mathrm{T}}c = \tfrac{1}{2} + \mathcal{O}(v^2) = b^{\mathrm{T}}Ae, \quad \gamma = e + \mathcal{O}(v^2),$$

which imply algebraic order $\geqslant 2$.

Next we will select the nodes c_1 and c_2 so that the methods possess algebraic order four. We have calculated the h power expansion of the local error $\psi_h(y_0) - \phi_h(y_0)$, obtaining the following fourth-order conditions:

$$\begin{array}{lll} \gamma = e + \mathcal{O}(v^2), & b^{\mathrm{T}}e = 1 + \mathcal{O}(v^4), & b^{\mathrm{T}}\gamma = 1 + \mathcal{O}(v^4), \\ b^{\mathrm{T}}A\gamma = \frac{1}{2} + \mathcal{O}(v^3), & b^{\mathrm{T}}Ae = \frac{1}{2} + \mathcal{O}(v^3), & b^{\mathrm{T}}(\gamma \cdot Ae) = \frac{1}{2} + \mathcal{O}(v^3), \\ b^{\mathrm{T}}A^2e = \frac{1}{6} + \mathcal{O}(v^2), & b^{\mathrm{T}}(Ae)^2 = \frac{1}{3} + \mathcal{O}(v^2), & b^{\mathrm{T}}(Ae)^3 = \frac{1}{4} + \mathcal{O}(v), \\ b^{\mathrm{T}}A^3e = \frac{1}{24} + \mathcal{O}(v), & b^{\mathrm{T}}A(Ae)^2 = \frac{1}{12} + \mathcal{O}(v), & b^{\mathrm{T}}(Ae \cdot A^2e) = \frac{1}{8} + \mathcal{O}(v). \end{array}$$

These fourth-order conditions are satisfied if the nodes have the form

$$c_j(v) = \left(\frac{1}{2} + (-1)^j\frac{\sqrt{3}}{6}\right) + v^2 f_j(v), \quad j = 1, 2, \tag{27}$$

with $f_j(v)$ arbitrary analytical functions.

We note that the symplectic fourth-order two-stage EFRK method derived by Van de Vyver [16] is obtained for $f_1(v) = f_2(v) = 0$, and the method derived in this paper is obtained for $c_j = \frac{1}{2} + (-1)^j d$ with $d = d(v)$ given by (22). Some observations on the choice of fixed or frequency-dependent c_j-values when the differential system is solved in a partitioned mode are carried out in [15].

In conclusion we may establish the following result:

Theorem 3.3. *All the fourth-order two-stage EFRK methods defined by the nodes* (27) *and* A, b, γ *given by* (25), (26) *preserve linear and quadratic invariants and are symplectic.*

4. Numerical experiments

Here we present the results of some numerical experiments comparing the behaviour of three fourth-order fitted and nonfitted methods for several test problems. The methods are: the classical two-stage fourth-order RK method of Gauss (denoted by GAUSS), the symplectic fourth-order EF method given by Hans Van de Vyver in [16] (denoted by HvDV) and the symplectic fourth-order EFGauss method defined by (19) and (22) (denoted by CFMR). The criterion used in the numerical comparisons is the usual test based on computing the maximum global error in the solution and/or in the invariants of the problem over the whole integration interval. All computations were carried out in double precision arithmetic (16 significant digits of accuracy) on a PC computer.

Problem 1. Kepler's problem defined by the Hamiltonian function

$$H = (1/2)(p_1^2 + p_2^2) - (q_1^2 + q_2^2)^{-1/2},$$

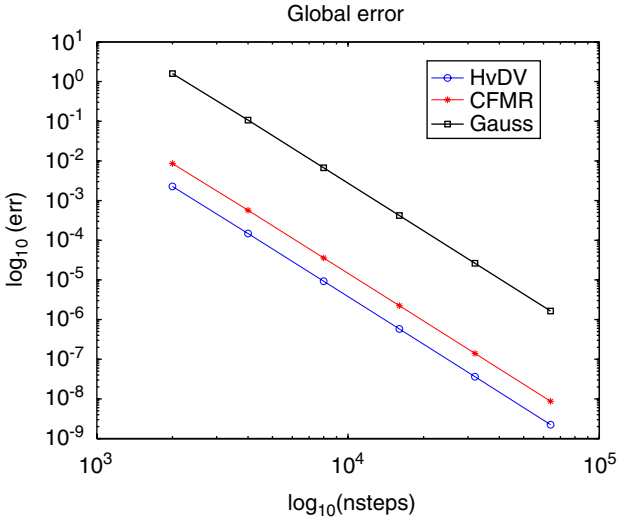

Fig. 1. Maximum global error in the solution for Problem 1.

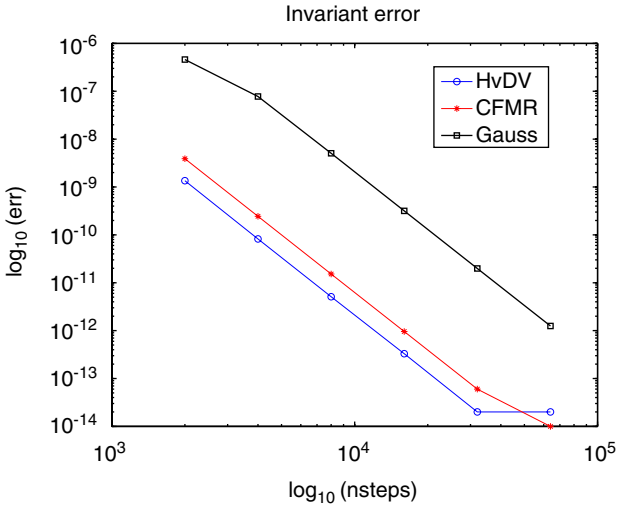

Fig. 2. Maximum global error in the energy H for Problem 1.

with the initial conditions $q_1(0) = 1 - e,\ q_2(0) = 0,\ p_1(0) = 0,\ p_2(0) = ((1+e)/(1-e))^{1/2}$ where $e \in [0, 1)$ is the (constant) eccentricity of the elliptic orbit. The exact solution of this IVP is 2π-periodic and the ellipse in the (q_1, q_2)-plane has semimajor axis 1 and eccentricity e, corresponding the starting point to the pericenter of this orbit.

The system possesses two invariants: the energy $H(p, q)$ and the angular momentum $M(p, q) = q_1 p_2 - q_2 p_1$, that for the above initial conditions have the values $H(p, q) = -\frac{1}{2}$ and $M(p, q) = \sqrt{1 - e^2}$.

In the numerical experiments presented here we have chosen the same values as in [16] i.e., $e = 0.001$, $\omega = (q_1^2 + q_2^2)^{-3/2}$, and the integration is carried out on the interval [0, 1000] with the steps $h = 2^{-i}$, $i = 1, \ldots, 6$. The numerical behaviour of the global error in the solution and in the energy are presented in Figs. 1 and 2.

Problem 2. A perturbed Kepler's problem given by the Hamiltonian function

$$H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{(q_1^2 + q_2^2)^{1/2}} - \frac{2\varepsilon + \varepsilon^2}{3(q_1^2 + q_2^2)^{3/2}},$$

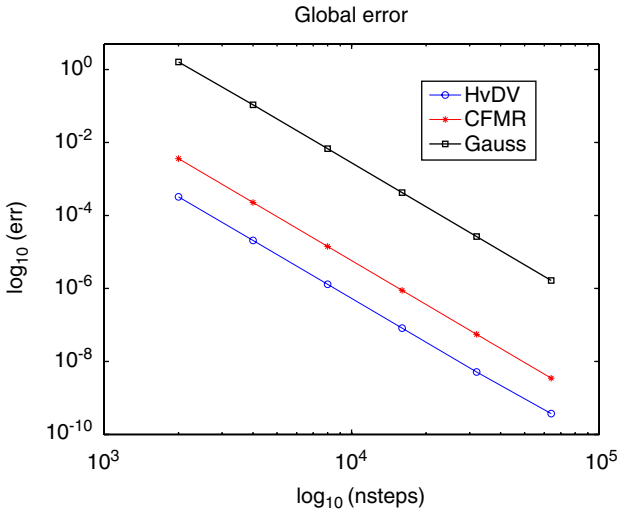

Fig. 3. Maximum global error in the solution for Problem 2.

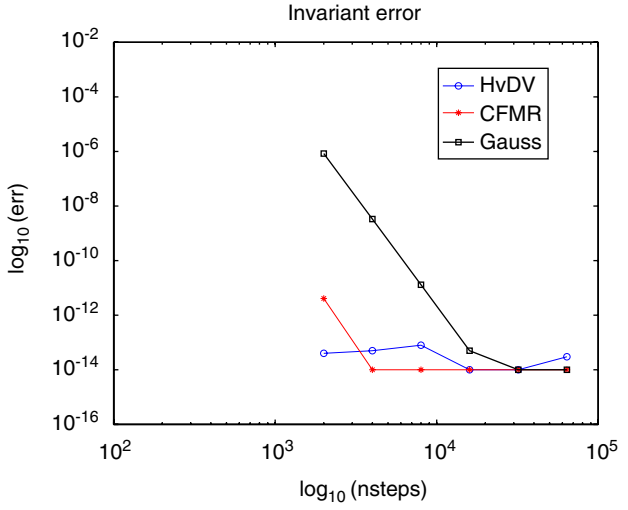

Fig. 4. Maximum global error in the energy H for Problem 2.

where ε is a small positive parameter and with the initial conditions

$$q_1(0) = 1, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = 1 + \varepsilon,$$

whose exact solution is $q_1(t) = \cos(t + \varepsilon t)$, $q_2(t) = \sin(t + \varepsilon t)$, $p_i(t) = q_i'(t)$, $i = 1, 2$, and the Hamiltonian at the initial conditions is $H(p_1(0), p_2(0), q_1(0), q_2(0)) = (\varepsilon + 3)(\varepsilon - 1)/6$.

The numerical results presented in Figs. 3 and 4 have been computed with the integration steps $h = 1/2^m$, $m = 1, \ldots, 6$. We take the parameter values $\varepsilon = 10^{-3}$, $\omega = 1$ and the problem is integrated up to $t_{\text{end}} = 1000$.

Problem 3. Euler's equations, that describe the motion of a rigid body under no forces

$$\dot{q} = f(q) = ((\alpha - \beta)q_2q_3, \ (1 - \alpha)q_3q_1, \ (\beta - 1)q_1q_2)^{\mathrm{T}},$$

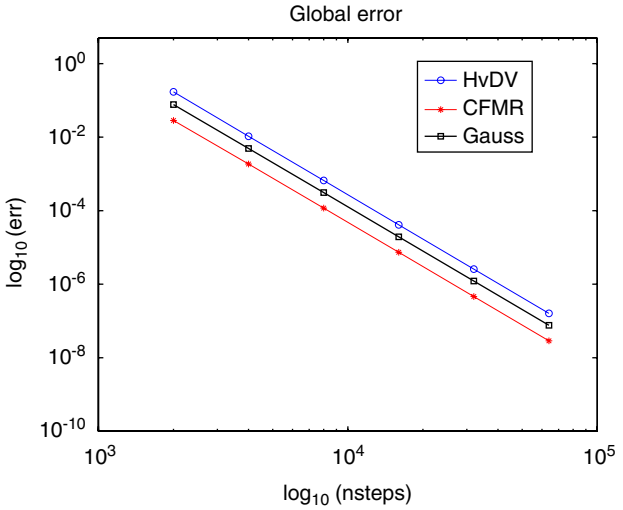

Fig. 5. Maximum global error in the solution for Problem 3.

with the initial values $q(0) = (0, 1, 1)^{\mathrm{T}}$, and the parameter values $\alpha = 1 + (1/\sqrt{1.51})$ and $\beta = 1 - (0.51/\sqrt{1.51})$. The exact solution of this IVP is given by

$$q(t) = (\sqrt{1.51}\,\mathrm{sn}(t, 0.51),\ \mathrm{cn}(t, 0.51),\ \mathrm{dn}(t, 0.51))^{\mathrm{T}},$$

it is periodic with period $T = 7.45056320933095$, and sn, cn, dn stand for the elliptic Jacobi functions. In addition, this problem has the quadratic invariants

$$G_1(q) = q_1^2 + q_2^2 + q_3^2, \qquad G_2(q) = q_1^2 + \beta q_2^2 + \alpha q_3^2.$$

Here we only present results for the global error in the solution (Fig. 5), computed with the integration steps $h = 1/2^m$, $m = 1, \ldots, 6$, on the interval $[0, 1000]$, because for both quadratic invariants the errors for the three methods are near of the roundoff unit.

Problem 4. Duffing's equation $\ddot{q} + (\beta^2 + k^2)q = 2k^2q^3$, where β and k are positive constants. This equation can be written as a 2D Hamiltonian system with

$$H = \tfrac{1}{2}\,[p^2 + (\beta^2 + k^2)q^2 - k^2\,q^4],$$

which is an invariant of this problem. In our numerical experiments we have taken $\beta = 5$, $k = 0.03$ and the initial conditions $q(0) = 0$, $p(0) = \beta$ which correspond to a periodic solution $q(t) = \mathrm{sn}(\beta t, k/\beta)$. In Figs. 6 and 7 we display the global errors and energy errors for step sizes $h = 1/2^i$, $i = 1, \ldots, 5$, and $\omega = 5$ as an estimation of the frequency in the integration interval $[0, 1000]$. Further, in Figs. 8 and 9 the phase space plots obtained with fitted and non fitted methods ($h = \frac{1}{2}$) are presented. Observe that the graph of the exact orbit $H(p, q) = H(p(0), q(0))$ is a closed curve.

From the results of the above numerical experiments it follows that for the problems under consideration an accurate estimation of the frequency is essential to assess the accuracy of symplectic integrators based on fitted methods. This fact was already recognised by Vanden Berghe and coworkers in [14] where some algorithms to estimate the frequency are proposed for problems in which it is not known in advance. Nevertheless the accuracy does not depend only on a good estimate of the frequency. So, in Kepler's problem all orbits are 2π-periodic independently of the eccentricity but, even with the exact frequency, fitted methods may be very inaccurate for higher eccentricities. This can be explained taking into account that the exact solution of this problem can be written as a Fourier series in time with coefficients

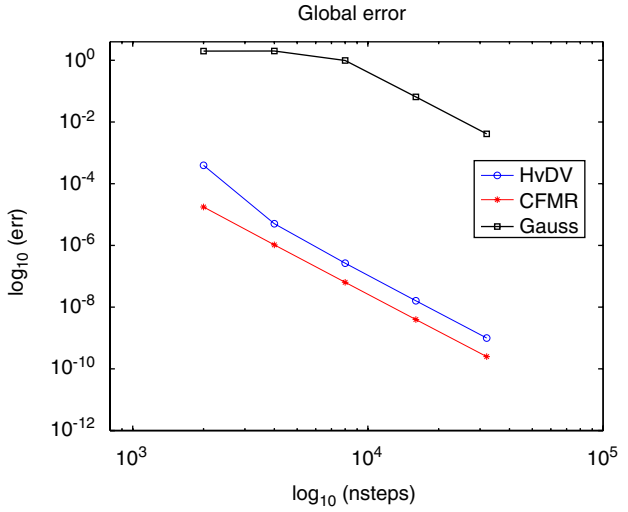

Fig. 6. Maximum global error in the solution for Problem 4.

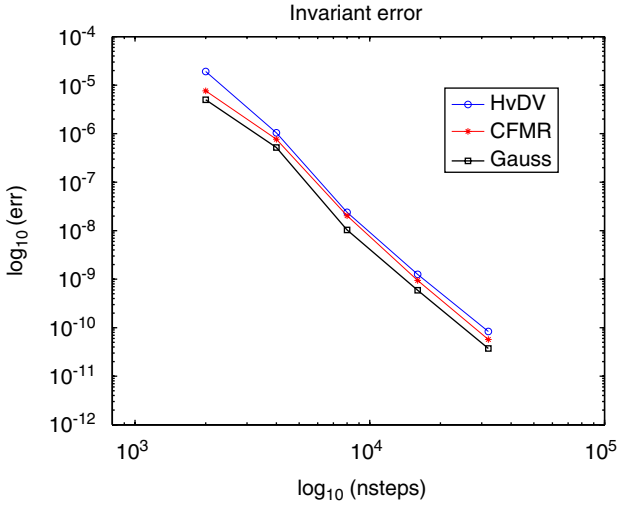

Fig. 7. Maximum global error in the energy H for Problem 4.

that depend on powers of the eccentricity e,

$$q_1(t) = \alpha_0 + \sum_{n \geqslant 1} \alpha_n \cos(nt), \quad q_2(t) = \sqrt{1-e^2} \sum_{n \geqslant 1} \beta_n \sin(nt),$$

where

$$\alpha_0 = -\tfrac{3}{2}\, e, \quad \alpha_1 = 1 - \tfrac{3}{8}\, e^2 + \tfrac{5}{192}\, e^4 - \tfrac{7}{9216}\, e^6 + \cdots,$$
$$\beta_1 = 1 - \tfrac{1}{8}\, e^2 + \tfrac{1}{142}\, e^4 - \tfrac{1}{9216}\, e^6 + \cdots,$$

and α_n and β_n ($n \geqslant 2$) are power series expansions in the eccentricity starting in e^{n-1} terms ($\alpha_n = \mathcal{O}\left(e^{n-1}\right)$ and $\beta_n = \mathcal{O}\left(e^{n-1}\right)$, $n \geqslant 2$). Thus an EF method with respect to the basis $\langle 1, \cos(t), \sin(t)\rangle$ will integrate exactly Kepler's problem for $e = 0$, whereas for $e > 0$ the presence of all integer frequencies in the above expansions imply that such an EF method cannot integrate exactly elliptic Kepler's problem.

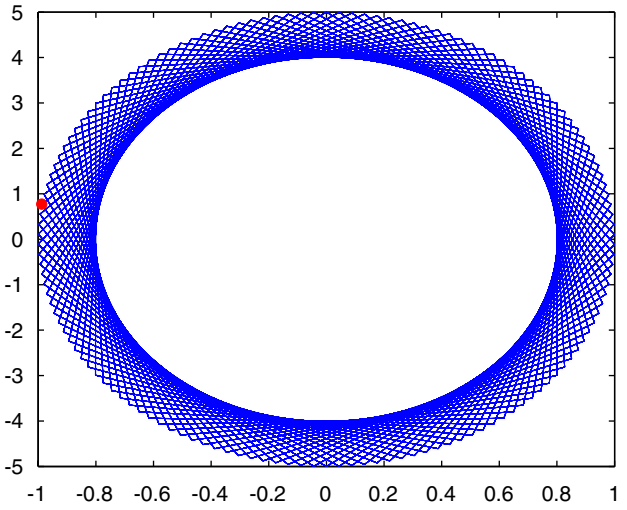

Fig. 8. Phase space for the CFMR code in Problem 4 with $h = \frac{1}{2}$.

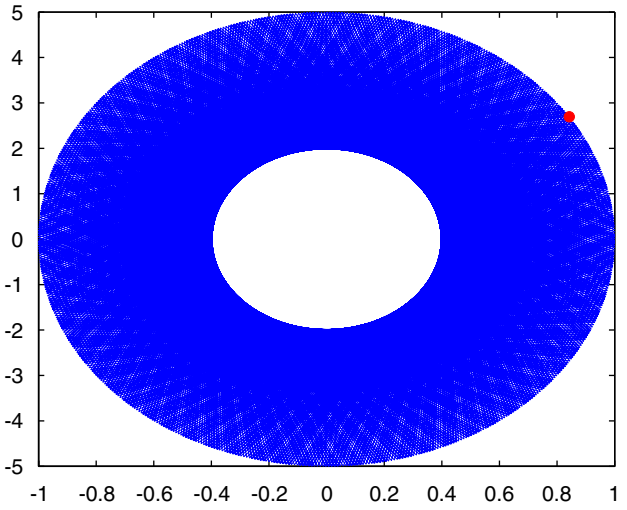

Fig. 9. Phase space for the Gauss code in Problem 4 with $h = \frac{1}{2}$.

If we focus on oscillatory Hamiltonian systems, the accuracy of the fitted methods is in general superior to the nonfitted ones. In some problems the results with HvDV are superior to our CFMR and in others it is the opposite, but in conclusion both show a similar global error behaviour. As far as the preservation of nonquadratic invariants as the energy, EF methods show, in general, a better behaviour. Moreover, a relevant property of classical symplectic methods: the linear error growth of the energy in the integration of periodic orbits has been observed numerically also in EF symplectic methods.

From Figs. 8 and 9 it follows that the qualitative behaviour of our EF integrator is clearly superior to the standard Gauss integrator. In addition, although both methods preserve similarly the energy, the end points (represented by red dots) show a larger global error in the standard Gauss method.

5. Conclusions

In this paper new two-stage fourth-order EFRK integrators that preserve linear and quadratic invariants and are symplectic have been derived. It is shown that such a fitted methods are reliable alternative to the standard two-stage

Gauss integrator to describe the evolution of some oscillatory problems. Furthermore, the computational cost of the fitted methods is similar to their counterparts standard methods. The investigation of new EF methods of high order as well their application to oscillatory problems is now in progress.

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