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Sixth-order symmetric and symplectic exponentially fitted Runge–Kutta methods of the Gauss type

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Abstract

The construction of exponentially fitted Runge–Kutta (EFRK) methods for the numerical integration of Hamiltonian systems with oscillatory solutions is considered. Based on the symplecticness, symmetry, and exponential fitting properties, two new three-stage RK integrators of the Gauss type with fixed or variable nodes, are obtained. The new exponentially fitted RK Gauss type methods integrate exactly differential systems whose solutions can be expressed as linear combinations of the set of functions $\{\exp(\lambda t), \exp(-\lambda t)\}$, $\lambda \in \mathbb{C}$, and in particular $\{\sin(\omega t), \cos(\omega t)\}$ when $\lambda = \mathrm{i}\omega$, $\omega \in \mathbb{R}$. The algebraic order of the new integrators is also analyzed, obtaining that they are of sixth-order like the classical three-stage RK Gauss method. Some numerical experiments show that the new methods are more efficient than the symplectic RK Gauss methods (either standard or else exponentially fitted) proposed in the scientific literature.

MSC: 65L05; 65L06

Keywords: Exponential fitting; Symplecticness; RK methods; Oscillatory Hamiltonian systems

1. Introduction

The construction of Runge–Kutta (RK) methods for the numerical solution of ODEs which have periodic or oscillating solutions has been considered extensively in the literature (see [2–8,11–13,16–22] and the references therein) with the aim of using the available information on the solutions to derive more accurate and/or efficient algorithms than the general purpose algorithms for such types of problems. A detailed survey including an extensive bibliography on this subject can be found in [10].

An approach to construct EFRK methods is to select the coefficients of the method so that it integrates exactly a set of linearly independent functions which are chosen depending on the nature of the solutions of the differential system to be solved. Some results on the existence of a unique solutions for the coefficients of an EFRK method are obtained in [11,12], and several authors [3,5,7,11,13,19] have derived methods with variable coefficients that are able

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to integrate exactly first or second order differential systems whose solutions belong to the linear space generated by the set of functions $\{1, t, \ldots, t^k, \exp(\pm\lambda t), t\exp(\pm\lambda t), \ldots, t^p\exp(\pm\lambda t)\}$, where $\lambda \in \mathbb{C}$ is a prescribed frequency. It is expected that these methods integrate oscillatory problems more accurately than standard methods based on polynomial functions.

On the other hand, oscillatory problems arise in different fields of applied sciences such as celestial mechanics, astrophysics, chemistry, electronics, molecular dynamics, and in many cases they are Hamiltonian systems [1]. It has been widely recognized by several authors (see [9,14,15,17,22,23]) that symplectic integrators have some advantages for the preservation of qualitative properties of the flow over the standard integrators when they are applied to Hamiltonian systems. For the class of oscillatory Hamiltonian systems, in addition to using EF methods, it may be appropriate to consider symplectic methods that preserve the structure of the original flow. As an example of such methods we mention the paper [22] in which the well known theory of symplectic RK methods is extended to modified EFRK methods, giving sufficient conditions on the coefficients of the method that imply symplecticness for general Hamiltonian systems. In addition, he has derived a two-stage fourth-order symplectic modified EFRK method of Gauss type testing its behaviour for several problems. Recently, the authors [3] have studied the preservation properties of modified EFRK methods for first order differential systems, and they present a family of two-stage fourth-order symmetric and symplectic EFRK Gauss integrators. The construction of EFRK (–Nyström) methods of Gauss type have been analyzed by several authors (see [4,11,21]) and EF methods up to order six have been derived, but unfortunately they are not symplectic. In addition, as it has been pointed out in [9] (see Chap. V and XI), symmetric methods show a better long time behaviour than non symmetric ones when applied to reversible differential systems, as it is the case for conservative mechanical systems. In general, it has been proved that for all differential systems whose flow maps are reversible, the numerical flow of an RK method will be also reversible iff it is symmetric.

Here, we investigate the construction of three-stage sixth-order symmetric and symplectic EFRK methods which integrate exactly first-order differential systems whose solutions can be expressed as linear combinations of the set of functions $\{\exp(\lambda t), \exp(-\lambda t)\}$, $\lambda \in \mathbb{C}$, in particular $\{\sin(\omega t), \cos(\omega t)\}$ when $\lambda = \mathrm{i}\omega$, $\omega \in \mathbb{R}$. Our purpose is to derive accurate and efficient EF geometric integrators based on the combination of the EF approach and symmetry and symplecticness conditions. The paper is organized as follows: In Section 2 we present the notations and definitions to be used in the rest of the paper as well as some previous results on symmetric and symplectic methods. In Section 3 we derive new three-stage symplectic EFRK integrators with fixed nodes and variable nodes and we analyze their algebraic order, obtaining that they are of sixth-order, just as the classical three-stage RK Gauss method. In Section 4 we present some numerical experiments with oscillatory Hamiltonian systems that show the accuracy and efficiency of the new methods when they are compared with other symplectic RK Gauss integrators given in [9,22]. Finally, Section 5 is devoted to conclusions.

2. Basic notations and definitions

We consider initial value problems (IVPs) for first-order differential systems

$$y'(t) = f(y(t)), \qquad y(t_0) = y_0 \in \mathbb{R}^m, \tag{1}$$

where for simplicity $f : \mathbb{R}^m \to \mathbb{R}^m$ is assumed to be sufficiently smooth, so that for all $(t_0, y_0) \in \mathbb{R}\times\mathbb{R}^m$, the IVP (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 case of Hamiltonian systems $m = 2d$; moreover, there exists a scalar Hamiltonian function $H = H(y) : \mathbb{R}^{2d} \to \mathbb{R}$, so that $f(y) = -J\ \nabla_y H(y)$. Here J is the $2d$-dimensional skew symmetric matrix

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

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

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

For each fixed t_0, the flow map of (1) will be denoted by $\phi_{h,f} : \mathbb{R}^m \to \mathbb{R}^m$ so that $\phi_{h,f}(y_0) = y(t_0 + h; t_0, y_0)$. In particular, for the case of Hamiltonian systems (2), $\phi_{h,f}$ is a symplectic map for all h in its domain of definition

(see [9,14,15]), i.e. the Jacobian matrix of $\phi_{h,f}(y_0)$ satisfies

$$\phi'_{h,f}(y_0) J \phi'_{h,f}(y_0)^{\mathrm{T}} = J. \tag{3}$$

A desirable property of a numerical method defined by the flow map ψ_h for the numerical integration of the Hamiltonian system (2), is that in addition to providing an accurate approximation of the exact flow $\phi_{h,f}$ for a reasonable range of step sizes $h \in [0, h_0]$, it preserves the qualitative properties of the original flow $\phi_{h,f}$ such as the symplecticness.

Definition 2.1. A numerical method defined by flow map ψ_h is called symplectic if for all Hamiltonian systems (2) it satisfies the condition

$$\psi'_h(y_0) J \psi'_h(y_0)^{\mathrm{T}} = J. \tag{4}$$

Among the best known examples of symplectic methods are the s-stage RK Gauss methods which possess accuracy of order $2s$. An s-stage RK method for solving the IVP (1) is a one-step method defined by the equations

$$y_1 = \psi_h(y_0) = y_0 + h \sum_{i=1}^{s} b_i f(Y_i), \tag{5}$$

$$Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} f(Y_j), \quad i = 1, \ldots, s, \tag{6}$$

where $y_1 \approx y(t_0 + h)$, $Y_i \approx y(t_0 + c_i h)$, $i = 1, \ldots, s$, and the real parameters c_i and b_i are known as the nodes and the weights of the method. The Eq. (5) will be referred to as the final stage and Eq. (6) as the internal stages of the RK method ψ_h. The s-stage RK method (5) and (6) is also represented by means of its Butcher's tableau

$$\begin{array}{c|c} c & A \\ \hline & b^{\mathrm{T}} \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \tag{7}$$

or equivalently by the triplet (c, A, b). The conditions on the coefficients of an RK method to be symplectic have been obtained independently by several authors (see [9,15] and the references therein) and they are given in the following theorem.

Theorem 2.2. *The RK method (5) and (6) for solving any Hamiltonian system (2) is symplectic if the following conditions are satisfied*

$$m_{ij} \equiv b_i b_j - b_i a_{ij} - b_j a_{ji} = 0, \quad 1 \le i, j \le s. \tag{8}$$

In general, all RK methods (5) and (6) preserve any linear invariant of (1), but if in addition its coefficients satisfy (8), then they also preserve all quadratic invariants [9]. The RK Gauss methods satisfy conditions (8), and therefore they preserve both linear and quadratic invariants.

On the other hand, symmetric numerical methods have many important properties for long term integrations. A key for understanding symmetry is the concept of the adjoint method.

Definition 2.3. The adjoint method ψ_h^* of a numerical method ψ_h is the inverse map of the original method with reversed time step $-h$, i.e., $\psi_h^* := \psi_{-h}^{-1}$. In other words, $y_1 = \psi_h^*(y_0)$ is implicitly defined by $\psi_{-h}(y_1) = y_0$. A method for which $\psi_h^* = \psi_h$ is called symmetric.

One of the properties of a symmetric method $\psi_h^* = \psi_h$ is that its accuracy order is even. In the case of s-stage RK methods (5) and (6), the conditions on their coefficients in order to be symmetric are given by

$$c = e - Sc, \qquad b = Sb, \qquad AS + SA = eb^{\mathrm{T}}, \tag{9}$$

where

$$e = (1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^s \quad \text{and} \quad S = \left(s_{ij}\right) \in \mathbb{R}^{s\times s} \quad \text{with } s_{ij} = \begin{cases} 1, & \text{if } i + j = s + 1, \\ 0, & \text{if } i + j \neq s + 1. \end{cases}$$

We note that the standard RK Gauss methods satisfy conditions (9), and therefore they are also symmetric.

When the coefficients (7) of an RK method are h-dependent, as it is in the case of EF methods [19,21] or adapted methods [16,17], then the conditions in order to be symmetric are given by

$$c(-h) = e - Sc(h), \qquad b(-h) = Sb(h), \qquad A(-h)S + SA(h) = eb^{\mathrm{T}}(h). \tag{10}$$

But for RK methods whose coefficients are even functions of h, as usually occurs in the case of EFRK methods, the conditions (10) reduce to the classical symmetry conditions (9) for standard RK methods.

The idea of constructing RK methods which integrate exactly a set of linearly independent functions different from the polynomials has been proposed by several authors (see for example [4,11–13,19,21]). This idea consists in selecting the available parameters of the method (5) and (6) in order to be exact for a set of linearly independent functions

$$\mathcal{F} = \{u_1(t), u_2(t), \ldots, u_r(t)\}, \quad r \leq s.$$

When $\mathcal{F}$ contains only polynomial functions up to a certain degree ($u_k(t) = t^k$) the corresponding methods are the standard RK collocation methods at the nodes $c_j = \sum_{k=1}^{s} a_{jk}$. If $\mathcal{F}$ contains polynomial functions and exponential or trigonometric functions, the resulting RK methods are called in [4] mixed collocation methods. In the general case, when $\mathcal{F}$ contains arbitrary functions, the resulting methods are called in [11,12] functionally fitted RK methods.

In general, the coefficients of an RK method (5) and (6) so that it integrates exactly the reference set of functions $\mathcal{F}$ are determined by the solution of the following linear systems

$$\sum_{i=1}^{s} b_i\, u_k'(t_0 + c_i\, h) = \frac{u_k(t_0 + h) - u_k(t_0)}{h}, \quad k = 1, \ldots, r, \tag{11}$$

$$\sum_{j=1}^{s} a_{ij}\, u_k'(t_0 + c_j\, h) = \frac{u_k(t_0 + c_i\, h) - u_k(t_0)}{h}, \quad i = 1, \ldots, s, k = 1, \ldots, r. \tag{12}$$

For the case $r = s$, Ozawa [11] has shown that the coefficients defined by the linear systems (11) and (12) are unique for all h and t, if the nodes are different ($c_i \neq c_j,\ i \neq j$) and the Wronskian matrix

$$W(u_1'(t), \ldots, u_s'(t)) = \begin{pmatrix} u_1'(t) & \cdots & u_s'(t) \\ \vdots & \ldots & \vdots \\ u_1^{(s)}(t) & \cdots & u_s^{(s)}(t) \end{pmatrix}, \tag{13}$$

is nonsingular at $t = 0$. In addition, if the functions $u_r(t)$ are analytic, then the coefficients b_i and a_{ij} are also analytic functions.

The most usual case is to consider exponential or trigonometric functions as a reference set of functions: $\mathcal{F}_1 = \{\exp(\lambda t),\ \exp(-\lambda t)\}$ or $\mathcal{F}_2 = \{\sin(\omega t),\ \cos(\omega t)\}$. The trigonometric case $\mathcal{F}_2$ is obtained from $\mathcal{F}_1$ with $\lambda = \mathrm{i}\omega$. For the reference set of functions $\mathcal{F}_1$ the linear systems (11) and (12) reduce to

$$\sum_{i=1}^{s} b_i\, \cosh(c_i z) = \frac{\sinh(z)}{z}, \qquad \sum_{i=1}^{s} b_i\, \sinh(c_i z) = \frac{\cosh(z) - 1}{z}, \tag{14}$$

$$\sum_{j=1}^{s} a_{ij}\, \cosh(c_j z) = \frac{\sinh(c_i z)}{z}, \qquad \sum_{j=1}^{s} a_{ij}\, \sinh(c_j z) = \frac{\cosh(c_i z) - 1}{z}, \quad i = 1, \ldots, s, \tag{15}$$

where $z = \lambda h$, and for $s = 2$ the coefficients b_i and a_{ij} are uniquely determined in terms of the nodes c_i. By choosing symmetric nodes: $c_1 = \frac{1}{2} - \theta$ and $c_2 = \frac{1}{2} + \theta$, and imposing the symplecticness conditions (8), the fourth-order

symplectic EFRK Gauss method given in [3] is obtained. This method is defined by

$$\theta = \frac{\operatorname{arccosh}(\alpha(z))}{z}, \qquad \alpha(z) = \frac{\sqrt{8 + \cosh^2(z/2)} + \cosh(z/2)}{4}, \tag{16}$$

or else

$$\theta = \frac{\sqrt{3}}{6}\left(1 + \frac{z^2}{72} - \frac{z^4}{51840} - \frac{17\,z^6}{2903040} - \frac{61\,z^8}{2508226560} + \frac{15073\,z^{10}}{2708884684800} + \cdots\right), \tag{17}$$

and for $z = 0$ the standard two-stage RK Gauss method is recovered. Until now, the only symplectic EFRK Gauss methods known to us are the two-stage fourth-order integrators given in [3,22], and the procedure presented above is not direct for the case of $s > 2$. In next section we try to extend the construction of symplectic EFRK Gauss methods to case of $s = 3$ stages.

3. Construction of the symplectic EFRK Gauss methods

Now we analyze the construction of symmetric and symplectic EFRK Gauss methods with $s = 3$ stages whose coefficients are even functions of h. These EFRK methods will have the properties of symmetry, symplecticness, accuracy with order $2s$, and preservation of linear and quadratic invariants as the standard RK Gauss methods.

From the symmetry assumption (9) it follows that the nodes $c_j = c_j(h^2)$ and weights $b_j = b_j(h^2)$ satisfy

$$c_1 = \frac{1}{2} - \theta, \qquad c_2 = \frac{1}{2}, \qquad c_3 = \frac{1}{2} + \theta, \qquad b_3 = b_1, \tag{18}$$

θ being a real parameter, and the coefficients $a_{ij} = a_{ij}(h^2)$:

$$\begin{aligned} &a_{22} = b_2/2, \qquad a_{11} + a_{33} = b_3, \qquad a_{12} + a_{32} = b_2,\\ &a_{13} + a_{31} = b_1, \qquad a_{21} + a_{23} = b_3. \end{aligned} \tag{19}$$

The symplecticness conditions (8) are equivalent to

$$\begin{aligned} &a_{jj} = b_j/2, \quad j = 1, 2, 3, \qquad b_1b_2 - b_1a_{12} - b_2a_{21} = 0,\\ &b_1b_3 - b_1a_{13} - b_3a_{31} = 0, \qquad b_2b_3 - b_2a_{23} - b_3a_{32} = 0. \end{aligned} \tag{20}$$

Leaving aside the symmetry conditions on the nodes (18) and taking b_1 and b_2 as parameters, the conditions (19) and (20) hold if and only if the coefficients a_{ij} satisfy

$$\begin{aligned} &a_{13} + a_{31} = b_1, \qquad a_{12} + a_{32} = b_2,\\ &a_{23} + a_{21} = b_1, \qquad b_1\,a_{12} - b_2\,a_{23} = 0,\\ &a_{11} = a_{33} = b_1/2, \qquad a_{22} = b_2/2. \end{aligned} \tag{21}$$

The EF conditions (14) and (15) with $s = 3$ give two conditions for the weights b_j and six conditions for the coefficients a_{ij}, but for the symmetry conditions (18) and (19), they reduce to one condition for the weights

$$b_2 + 2\,b_1\cosh(\theta z) = \frac{\sinh(z/2)}{z/2}, \tag{22}$$

and three conditions for the coefficients a_{ij}

$$\begin{aligned} &(a_{13} - a_{11})\,\sinh(\theta z) = \frac{\cosh(\theta z) - \cosh(z/2)}{z},\\ &a_{12} + (a_{11} + a_{13})\,\cosh(\theta z) = \frac{\sinh(z/2) - \sinh(\theta z)}{z},\\ &(b_1 - 2a_{21})\,\sinh(\theta z) = \frac{1 - \cosh(z/2)}{z}. \end{aligned} \tag{23}$$

3.1. Three-stage EFRK Gauss method with fixed nodes

First we impose that the final stage is also exact for the functions $\{\exp(2\lambda t),\ \exp(-2\lambda t)\}$, i.e., the following conditions are also satisfied

$$\sum_{i=1}^{3} b_i\ \cosh(2c_i z) = \frac{\sinh(2z)}{2z}, \qquad \sum_{i=1}^{3} b_i\ \sinh(2c_i z) = \frac{\cosh(2z)-1}{2z}. \tag{24}$$

By the symmetry conditions on the nodes and weights (18), the conditions (24) reduce to

$$b_2 + 2\,b_1 \cosh(2\theta z) = \frac{\sinh(z)}{z}, \tag{25}$$

and the weights b_1 and b_2 can be computed from Eqs. (22) and (25) obtaining

$$b_1 = \frac{\sinh(z) - 2\,\sinh(z/2)}{2\,z\,(\cosh(\theta z) - \cosh(2\theta z))}, \qquad b_2 = \frac{\cosh(\theta z)\sinh(z) - 2\,\cosh(2\theta z)\sinh(z/2)}{z\,(\cosh(\theta z) - \cosh(2\theta z))}. \tag{26}$$

If now the symplecticness conditions (20) are imposed, the second equation of (23) can be skipped, and introducing the auxiliary parameters $\gamma_1 = b_1 - 2a_{21}$, $\gamma_2 = a_{13} - a_{11}$, the first and third equations of (23) give

$$\gamma_1 = \frac{1-\cosh(z/2)}{z\,\sinh(\theta z)}, \qquad \gamma_2 = \frac{\cosh(\theta z) - \cosh(z/2)}{z\,\sinh(\theta z)}. \tag{27}$$

Hence, taking into account (21), the coefficients of matrix A can be written as

$$A = \begin{pmatrix} \dfrac{b_1}{2} & \dfrac{b_2\,(b_1+\gamma_1)}{2\,b_1} & \dfrac{b_1}{2}+\gamma_2 \\ \dfrac{b_1-\gamma_1}{2} & \dfrac{b_2}{2} & \dfrac{b_1+\gamma_1}{2} \\ \dfrac{b_1}{2}-\gamma_2 & \dfrac{b_2\,(b_1-\gamma_1)}{2\,b_1} & \dfrac{b_1}{2} \end{pmatrix}. \tag{28}$$

The coefficients (18) and (26)–(28) define a family of EFRK methods which are symmetric, symplectic and they preserve linear and quadratic invariants for all $\theta \in \mathbb{R}$. In particular, by choosing the parameter θ such that the nodes c_i are the Gauss nodes: $\theta = \sqrt{15}/10$, we obtain an EF method with fixed nodes which will be denoted as EFGauss3F, and when $z = 0$ it reduces to the standard three-stage RK Gauss method.

We note that the internal stages of the new EFGauss3F method are exact for the basis $\langle 1, \exp(\lambda t),\ \exp(-\lambda t)\rangle$, whereas the final stage is exact for the basis $\langle 1,\ \exp(\lambda t),\ \exp(-\lambda t), \exp(2\lambda t),\ \exp(-2\lambda t)\rangle$. In the trigonometric case, ($\lambda = \mathrm{i}\omega$, $\omega \in \mathbb{R}$) we have $z = \mathrm{i}\nu$ with $\nu = \omega h$, and the coefficients (26) and (27) emerge having in mind the relations $\cosh(\mathrm{i}\nu) = \cos(\nu)$ and $\sinh(\mathrm{i}\nu) = i\sin(\nu)$. In this case, the internal stages are exact for the basis $\langle 1, \cos(\omega t),\ \sin(\omega t)\rangle$, whereas the final stage is exact for the basis $\langle 1,\ \cos(\omega t),\ \sin(\omega t), \cos(2\omega t),\ \sin(2\omega t)\rangle$.

Although the coefficients of the resulting method are analytic in a neighbourhood of $z = 0$, in practical calculations with $|z| < \delta$ (δ being a small value), it is better to change to a series expansion of the coefficients. For practical purposes $\delta = 0.1$ is a suitable value. The series expansions that we are using for such small z-values are given by

$$\begin{aligned}
b_1 &= \frac{5}{18} + \frac{z^4}{14400} - \frac{191\,z^6}{87091200} + \frac{623\,z^8}{8294400000} - \frac{78713\,z^{10}}{30656102400000} + \cdots, \\
b_2 &= \frac{4}{9} - \frac{z^4}{7200} - \frac{241\,z^6}{43545600} + \frac{217\,z^8}{4147200000} - \frac{8147\,z^{10}}{3065610240000} + \cdots, \\
\gamma_1 &= -\frac{\sqrt{15}}{12} + \frac{\sqrt{15}\,z^2}{2880} - \frac{13\sqrt{15}\,z^4}{1728000} + \frac{221\sqrt{15}\,z^6}{1935360000} - \frac{6061\sqrt{15}\,z^8}{3483648000000} + \frac{9733\sqrt{15}\,z^{10}}{367873228800000} + \cdots, \\
\gamma_2 &= -\frac{\sqrt{15}}{30} - \frac{\sqrt{15}\,z^2}{3600} + \frac{\sqrt{15}\,z^4}{540000} - \frac{17\sqrt{15}\,z^6}{604800000} + \frac{23\sqrt{15}\,z^8}{54432000000} - \frac{4603\sqrt{15}\,z^{10}}{718502400000000} + \cdots.
\end{aligned}$$

3.2. Three-stage EFRK Gauss method with variable nodes

Now we impose that the final stage is also exact for the larger reference set of functions $\{\exp(2\lambda t), \exp(-2\lambda t), \exp(3\lambda t), \exp(-3\lambda t)\}$, which implies the following additional conditions on the weights b_j

$$\sum_{i=1}^{3} b_i \cosh(kc_i z) = \frac{\sinh(kz)}{kz}, \qquad \sum_{i=1}^{3} b_i \sinh(kc_i z) = \frac{\cosh(kz)-1}{kz}, \quad k = 2, 3. \tag{29}$$

By the symmetry conditions on the nodes and weights (18), the conditions (29) are equivalent to

$$b_2 + 2\,b_1 \cosh(2\theta z) = \frac{\sinh(z)}{z}, \qquad b_2 + 2\,b_1 \cosh(3\theta z) = \frac{\sinh(3z/2)}{3z/2}, \tag{30}$$

and the weights b_1 and b_2 can be computed from Eqs. (22) and (30). The solution of these equations is given by (26) iff θ satisfies

$$\det \begin{pmatrix} \cosh(\theta z) & 1 & 2\,\sinh(z/2) \\ \cosh(2\theta z) & 1 & \sinh(z) \\ \cosh(3\theta z) & 1 & \dfrac{2}{3}\,\sinh(3z/2) \end{pmatrix} = 0, \tag{31}$$

obtaining

$$\theta = \frac{2\,\mathrm{arccosh}(\beta)}{z}, \quad \text{with } \beta = \frac{\sqrt{5 + 2\,\cosh(\frac{z}{2}) + \sqrt{15 + 8\,\cosh(\frac{z}{2}) + 2\,\cosh(z)}}}{2\sqrt{3}}, \tag{32}$$

or else

$$\theta = \frac{\sqrt{15}}{10}\left(1 + \frac{z^2}{150} - \frac{31\,z^4}{240000} + \frac{89\,z^6}{144000000} + \frac{45539\,z^8}{725760000000} - \frac{3085681\,z^{10}}{145152 \times 10^{10}} + \cdots\right), \tag{33}$$

and the rest of coefficients are given by (18), (27) and (28).

In this case we obtain an EF method with variable nodes which will be denoted here as EFGauss3V. The new method EFGauss3V also is symmetric, symplectic, it preserves linear and quadratic invariants, and when $z = 0$ it reduces to standard three-stage RK Gauss method.

We note that for the method EFGauss3V the final stage is exact for the linear space $\langle 1,\ \exp(\lambda t), \exp(-\lambda t), \exp(2\lambda t),\ \exp(-2\lambda t),\ \exp(3\lambda t),\ \exp(-3\lambda t)\rangle$. In the trigonometric case ($\lambda = \mathrm{i}\omega$, $\omega \in \mathbb{R}$, $z = \mathrm{i}\nu$, $\nu = \omega h$) the coefficients emerge having in mind the relations $\cosh(\mathrm{i}\nu) = \cos(\nu)$ and $\sinh(\mathrm{i}\nu) = \mathrm{i}\sin(\nu)$, and the final stage is exact for the linear space $\langle 1, \cos(\omega t), \sin(\omega t), \cos(2\omega t), \sin(2\omega t), \cos(3\omega t), \sin(3\omega t)\rangle$. In addition, since the final stage of the standard three-stage RK Gauss method is exact for the basis $\langle 1,\ t,\ t^2,\ t^3,\ t^4,\ t^5,\ t^6\rangle$, we feel that the new method EFGauss3V is the natural extension from the polynomial to exponential case.

Again, for small values of z ($|z| < 0.1$) it is better to use a series expansion of the coefficients. In this case, the series expansions that we are using in practical calculations are given by

$$\begin{aligned}
b_1 &= \frac{5}{18} - \frac{z^2}{270} - \frac{23\,z^4}{432000} + \frac{1433\,z^6}{226800000} - \frac{555073\,z^8}{2612736000000} + \frac{24846889\,z^{10}}{14370048000000000} + \cdots, \\
b_2 &= \frac{4}{9} + \frac{z^2}{135} + \frac{23\,z^4}{216000} + \frac{37\,z^6}{7087500} - \frac{216047\,z^8}{1306368000000} + \frac{14276111\,z^{10}}{7185024000000000} + \cdots, \\
\gamma_1 &= -\frac{\sqrt{15}}{12} + \frac{13\sqrt{15}z^2}{14400} + \frac{\sqrt{15}\,z^4}{288000} - \frac{28061\sqrt{15}\,z^6}{48384000000} + \frac{1192963\sqrt{15}\,z^8}{87091200000000} + \frac{1695787\sqrt{15}\,z^{10}}{23950080000000000} + \cdots, \\
\gamma_2 &= -\frac{\sqrt{15}}{30} + \frac{11\sqrt{15}z^2}{18000} - \frac{11\sqrt{15}\,z^4}{1800000} - \frac{6653\sqrt{15}\,z^6}{30240000000} + \frac{107593\sqrt{15}\,z^8}{8709120000000} - \frac{48160367\sqrt{15}\,z^{10}}{239500800000000000} + \cdots.
\end{aligned}$$

3.3. Algebraic order of the symplectic EFRK Gauss methods

The new EFRK Gauss methods previously derived integrate exactly those IVPs whose solutions belong to linear spaces $\langle 1,\ \exp(\lambda t), \exp(-\lambda t)\rangle$ or $\langle 1,\ \cos(\omega t), \sin(\omega t)\rangle$. But for IVPs with general smooth solutions they present local truncation errors. In order to evaluate the magnitude of these errors we use the algebraic order of accuracy in the same way as is used for standard methods. As is usual in the literature an RK method has algebraic order p if, for all sufficiently smooth IVP (1), the numerical solution (5) and (6) satisfies

$$y_1 - y(t_0 + h) = \psi_h(y_0) - \phi_h(y_0) = \mathcal{O}\left(h^{p+1}\right), \quad h \to 0. \tag{34}$$

Since the EFRK methods considered here are formally RK methods with h-dependent coefficients, according to the theory of order for standard RK methods [9] the local error $\psi_h(y_0) - \phi_h(y_0)$ at y_0 with step size h, possesses the power series expansion

$$\psi_h(y_0) - \phi_h(y_0) = \sum_{\tau\in\mathcal{T}} \frac{h^{\rho(\tau)}}{\rho(\tau)!}\left(\gamma(\tau) b(h)^{\mathrm{T}} \Phi_{A(h)}(\tau) - 1\right)\alpha(\tau) F(\tau)(y_0), \tag{35}$$

where $\mathcal{T}$ is the set of rooted trees with order $\rho(\tau) \geq 1$, $F(\tau)(y_0)$ is the elementary differential of f associated to $\tau \in \mathcal{T}$ at y_0, $\alpha(\tau)$ is the number of monotonic labellings of τ and $\Phi = \Phi_{A(h)} : \mathcal{T} \to R^s$ is a vector function depending exclusively on $A(h)$ defined recursively by

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

where $\cdot$ is the componentwise product.

From the independence of the elementary differentials $F(\tau)$, it follows from (35) that an EFRK method (5) and (6) has algebraic order p if this is the largest integer such that

$$b(h)^{\mathrm{T}} \Phi_{A(h)}(\tau) - \frac{1}{\gamma(\tau)} = \mathcal{O}\left(h^{p+1-\rho(\tau)}\right) \tag{36}$$

holds for all $\tau \in \mathcal{T}$ with order $\rho(\tau) \leq p$.

We note that in our EFRK methods, the vector of nodes $c = (c_1, c_2, c_3)^{\mathrm{T}}$ does not satisfy the simplifying assumption $A(h)e = c$, and therefore the 3-dimensional vector function $\Phi_{A(h)}(z)$ must be computed recursively on the order of the rooted trees by using only $A(h)$.

With the help of *Mathematica*, we have computed for our methods EFGauss3F and EFGauss3V the expression $b^{\mathrm{T}}(h)\Phi_{A(h)}(\tau)$ for the 37 elementary differentials with order ≤ 6 and checked the conditions (36) by using their power series expansions in (even) powers of h. It must be noticed that in the case of fixed nodes, i.e. for the EFGauss3F method, the proof that this method has order 6 also follows from the theory developed in [11].

4. Numerical experiments

In this section we present some numerical experiments to test the behaviour of the new EFRK methods derived in Section 3 when they are applied to the numerical solution of several oscillatory Hamiltonian differential systems. The new methods have been compared with a fourth-order symplectic exponentially fitted integrator proposed in [22], denoted here as EFVyver, and with the standard three-stage sixth-order Gauss method given in [9] denoted as Gauss3. We note that all methods employed in our numerical experiments are symplectic and according to [15], the global preservation of symplecticness only holds for a fixed step-size together with a fixed fitting frequency along the integration. In view of this, all numerical experiments have been carried out with fixed h and ω. In this case, one has to evaluate the coefficients of the EF methods one time for all integration and the extra costs in computing the coefficients are negligible. In our numerical experiments we have solved the non-linear equation (6) with a modified Newton's method using finite differences to approximate the Jacobian of $f(y)$ with respect to y, and taking as initial values $Y_i^{(0)} = y_0$, $i = 1, 2, 3$. The iteration is carried out until the difference between the Euclidean norm of two successive iterations attains the round off level.

The criterion used in the numerical comparisons is the usual test based on computing the maximum global error in the solution over the whole integration interval. In Figs. 1–4 we show the decimal logarithm of the maximum

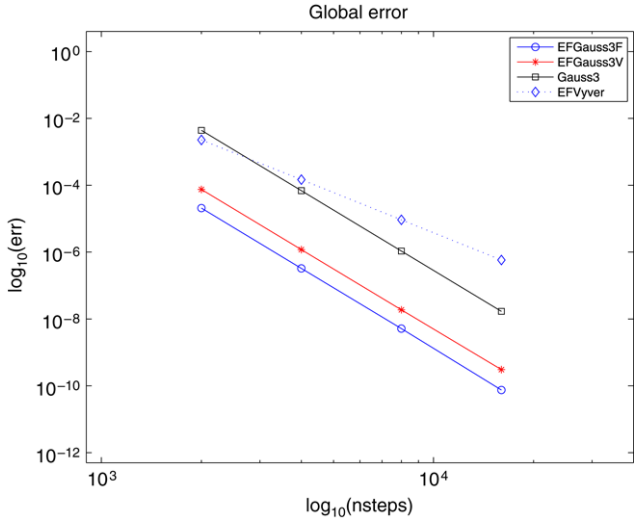

Fig. 1. Maximum global error in the solution for Problem 1.

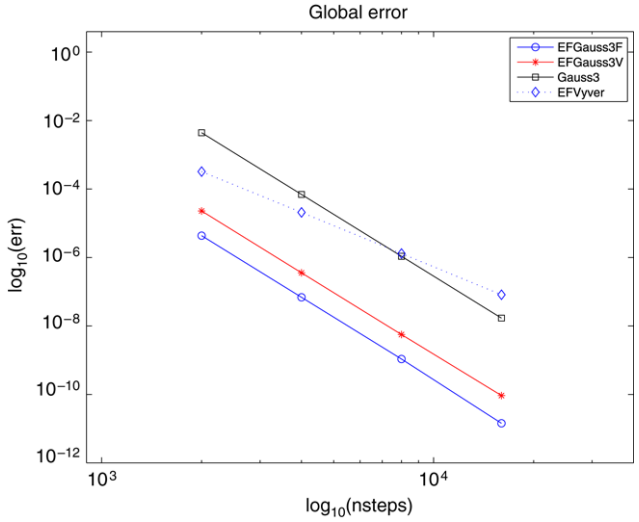

Fig. 2. Maximum global error in the solution for Problem 2.

global error ($\log_{10}$(err)) versus the number of steps required by each code on a logarithmic scale ($\log_{10}$(nsteps)). All computations are carried out in double precision arithmetic (16 significant digits of accuracy), and numerical considerations indicate that series expansions must be used for the coefficients of the new EFRK methods when $|z| < 0.1$.

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

$$H(p,q) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \left(q_1^2 + q_2^2\right)^{-1/2},$$

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 $(0 \le e < 1)$ represents the eccentricity of the elliptic orbit. The exact solution of this IVP is a 2π-periodic elliptic orbit in the (q_1, q_2)-plane with semimajor axis 1, where the starting point is the pericenter of this orbit.

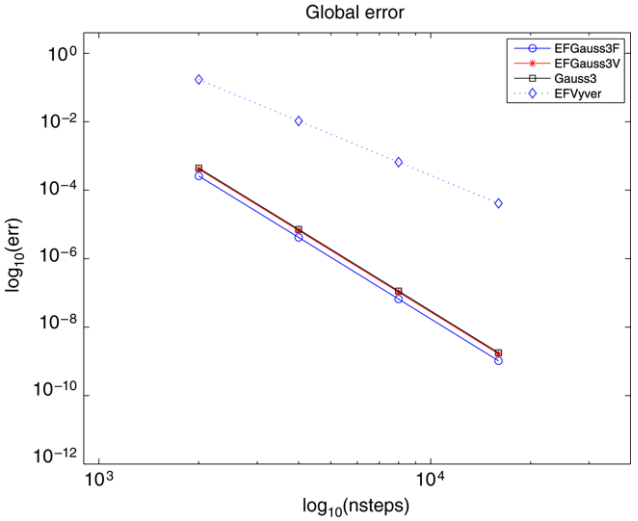

Fig. 3. Maximum global error in the solution for Problem 3.

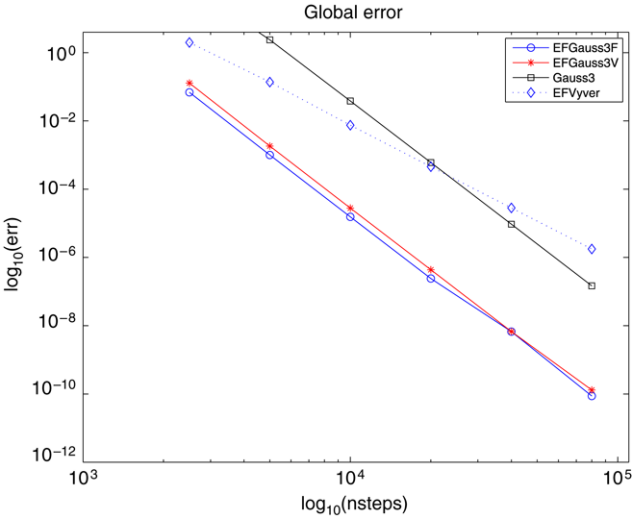

Fig. 4. Maximum global error in the solution for Problem 4.

In the numerical experiments presented here we have chosen the same values as in [22], i.e. $e = 0.001$, $\lambda = \mathrm{i}\omega$ with $\omega = \left(q_1^2 + q_2^2\right)^{-3/2}$, and the integration is carried out on the interval [0, 1000] with the steps $h = 1/2^m$, $m = 1, \ldots, 4$. The numerical behaviour of the global error in the solution is presented in Fig. 1.

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

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

with the initial conditions

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

where ε is a small positive parameter. The exact solution of this IVP is given by

$$q_1(t) = \cos(t + \varepsilon t), \qquad q_2(t) = \sin(t + \varepsilon t), \qquad p_i(t) = q_i'(t), \quad i = 1, 2.$$

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

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

$$\dot{q} = f(q) = ((\alpha - \beta)q_2 q_3,\ (1-\alpha)q_3 q_1,\ (\beta - 1)q_1 q_2)^{\mathrm{T}},$$

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

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

it is periodic with period $T = 7.45056320933095$, and sn, cn, dn stand for the elliptic Jacobi functions. Fig. 3 shows the numerical results obtained for the global error computed with the integration steps $h = 1/2^m$, $m = 1, \ldots, 4$, on the interval $[0, 1000]$, and $\lambda = \mathrm{i}2\pi/T$.

Problem 4. A two dimensional nonlinear oscillatory Hamiltonian system

$$H(p, q) = \frac{1}{2}\left(p_1^2 + p_2^2\right) + \frac{1}{4}\left(\alpha\, q_1^2 + 2\,\beta\, q_1\, q_2 + \alpha\, q_2^2\right) q - \frac{1}{8}\, k^2\, (q_1 - q_2)^4,$$

with the initial conditions

$$q_1(0) = \frac{1}{2}, \qquad q_2(0) = \frac{1}{2}, \qquad p_1(0) = -\frac{1}{\sqrt{2}} - \frac{\omega}{2}, \qquad p_2(0) = \frac{1}{\sqrt{2}} - \frac{\omega}{2},$$

where $\alpha = \omega^2 + k^2 + 1$, $\beta = \omega^2 - k^2 - 1$ and the parameters $\omega > 0$, $0 \le k < 1$. This Hamiltonian problem represents a simple model consisting of two mass points connected with a soft nonlinear spring and a stiff linear spring. The analytic solution is given by

$$q(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos\left(\frac{\pi}{4} + \omega t\right) - \mathrm{sn}(t; k) \\ \cos\left(\frac{\pi}{4} + \omega t\right) + \mathrm{sn}(t; k) \end{pmatrix},$$

and represents a periodic motion in terms of trigonometric and Jacobian elliptic functions.

In our test we chose the parameter values $\omega = 50$, $k = 0.5$, $t_{end} = 100$ and the numerical results presented in Fig. 4 have been computed with the integration steps $h = 1/(2^{m-1}\omega)$, $m \ge 0$, and $\lambda = \mathrm{i}\omega$.

From the numerical experiments carried out, it follows that for the problems under consideration an accurate estimation of the frequency is essential to assessing the accuracy of symplectic integrators based on the fitted methods. This fact was already recognised by Vanden Berghe and coworkers in [20], where some algorithms to estimate the frequency are proposed for problems in which it is not known in advance. So, in Problem 3 in which the frequency used by the EF methods is not accurate, all the sixth-order codes (EFGauss3F, EFGauss3V and Gauss3) show a similar accuracy behaviour whereas the fourth-order code EFVyver gives the poorest results for all the considered stepsizes.

If we focus on oscillatory Hamiltonian systems (Problems 1, 2 and 4), the accuracy of the fitted methods is in general superior to the non fitted ones of the same order. On the other hand, the numerical results show that for high accuracy the non fitted high order code Gauss3 is superior to low order code EFVyver. This fact shows that in addition to symplecticness and exponential fitting, the algebraic order is also a significant factor to be considered in the accurate integration of oscillatory Hamiltonian systems. In general, the method EFGauss3F (fixed nodes) results in being slightly more accurate than the method EFGauss3V (variable nodes), and both are clearly superior to the other methods. This fact has also been observed in [21] and these authors conclude that fixed knot methods are preferred for solving differential systems. An explanation given by them is that each component of the system may have its own fitting frequency and different components could be integrated with different RK formulas. Then the numerical integrator is a partitioned RK method and, although the integrators of all components have the same order p, the order of the whole vector solution can be lower than p.

5. Conclusions

In this paper new three-stage sixth-order EFRK integrators of the Gauss type which are symmetric and symplectic and preserve linear and quadratic invariants have been derived. It is shown that such methods are reliable alternatives to the standard three-stage Gauss integrator and the two-stage EFRK code derived in [22] to describe the evolution of some oscillatory problems. Furthermore, the computational cost of the new EFRK methods is similar to their counterparts the standard RK methods. The investigation of new symplectic EFRK methods with a larger algebraic orders and/or which are exact for other reference sets of functions as well their application to oscillatory problems is now in progress.

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