Available online at www.sciencedirect.com

ScienceDirect

Computer Physics Communications 178 (2008) 732–744

Computer Physics Communications

www.elsevier.com/locate/cpc

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

M. Calvo, J.M. Franco *, J.I. Montijano, L. Rández

Departamento de Matemática Aplicada, Pza. San Francisco s/n., Universidad de Zaragoza, 50009 Zaragoza, Spain

Received 28 September 2007; received in revised form 8 January 2008; accepted 16 January 2008

Available online 2 February 2008

Abstract

The construction of symmetric and symplectic exponentially fitted modified Runge–Kutta (RK) methods for the numerical integration of Hamiltonian systems with oscillatory solutions is considered. In a previous paper [H. Van de Vyver, A fourth order symplectic exponentially fitted integrator, Comput. Phys. Comm. 176 (2006) 255–262] a two-stage fourth-order symplectic exponentially fitted modified RK method has been proposed. Here, two three-stage symmetric and symplectic exponentially fitted integrators of Gauss type, either with fixed nodes or variable nodes, are derived. The algebraic order of the new integrators is also analyzed, obtaining that they possess sixth-order as the classical three-stage RK Gauss method. Numerical experiments with some oscillatory problems are presented to show that the new methods are more efficient than other symplectic RK Gauss codes proposed in the scientific literature.

PACS: 02.60.Lj; 02.70.-c; 02.90.+p

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

1. Introduction

In this paper we deal with the construction of symplectic methods of Runge–Kutta (RK) type for the numerical solution of oscillatory Hamiltonian systems. The oscillatory Hamiltonian systems often arise in different fields of applied sciences such as celestial mechanics, astrophysics, chemistry, electronics, molecular dynamics, and so on (see [1]). In addition, it has been widely recognized by several authors (see [2–7]) that symplectic integrators obtain numerical superiority when they are applied to solving Hamiltonian systems. So, for the class of oscillatory Hamiltonian systems, it may be appropriate to consider symplectic exponentially fitted (EF) methods that preserve the structure of the original flow. As an example of such methods we mention the paper of Van de Vyver [6] 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 their behavior for several problems. Next, the authors [8] have analyzed the preservation properties of modified EFRK methods for first order differential systems, and they present a new two-stage fourth-order symplectic EFRK Gauss integrator.

The construction of RK methods for solving ODEs which have periodic or oscillating solutions has been considered by several authors (see [5–23] and references therein). The aim is to use the available information on the solutions of the corresponding problems to derive more accurate and/or efficient algorithms than the general purpose algorithms for such a type of problems. Some pioneer papers are due to Gautschi [14] and Bettis [9], in which EF linear multistep methods and adapted RK algorithms, respectively, for the integration of ODEs with oscillatory solutions are presented. However, the development of EF Runge–Kutta(–Nyström)

* Corresponding author.
E-mail addresses: calvo@unizar.es (M. Calvo), jmfranco@unizar.es (J.M. Franco), monti@unizar.es (J.I. Montijano), randez@unizar.es (L. Rández).

0010-4655/$ – see front matter
doi:10.1016/j.cpc.2008.01.046

methods has been carried out more recently, mainly due to the nonlinear nature of the RK type methods. A detailed survey including an extensive bibliography on this subject can be found in Ixaru and Vanden Berghe [15]. Usually the construction of EFRK methods lies in selecting 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. So, several authors [8,11,13,16,18,21] have derived methods with frequency-dependent coefficients that are able 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 λ is a prescribed frequency. In particular, the construction of EFRK(–Nyström) methods of Gauss type have been considered in [10,16,23] and EF methods up to order six have been constructed, but unfortunately they are not symplectic.

Here, we investigate the construction of three-stage sixth-order symmetric and symplectic modified EFRK methods which integrate exactly first-order ODEs whose solutions can be expressed as linear combinations of the set of functions $\{\exp(\lambda t), \exp(-\lambda t)\}$, $\lambda \in \mathbb{C}$, or $\{\sin(\omega t), \cos(\omega t)\}$ when $\lambda = i\omega$, $\omega \in \mathbb{R}$. Our purpose is to derive accurate and efficient symplectic 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 basic concepts and results to be used in the rest of the paper. In Section 3 we derive new three-stage symplectic and symmetric modified EFRK integrators with fixed nodes and variable nodes. In Section 4 we analyze the algebraic order of the new EFRK integrators, obtaining that they possess sixth-order as the classical three-stage RK Gauss method. In Section 5 we present some numerical experiments with oscillatory Hamiltonian systems that show the efficiency of the new methods when they are compared with other symplectic RK integrators of Gauss type. Finally, in Section 6 we present some conclusions.

2. Basic concepts and results

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

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

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

In the case of Hamiltonian systems $m = 2d$ and there exists 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

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

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

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

For each fixed t_0 the flow map of (1) will be denoted by $\phi_h : \mathbb{R}^m \to \mathbb{R}^m$ so that $\phi_h(y_0) = y(t_0 + h; t_0, y_0)$. In particular, for the case of Hamiltonian systems (2), ϕ_h is a symplectic map for all h in its domain of definition (see [2–4]), i.e. the Jacobian matrix of $\phi_h(y_0)$ satisfies

$$\phi_h'(y_0) J \phi_h'(y_0)^T = J. \tag{3}$$

A desirable property of a numerical method ψ_h for the numerical integration of the Hamiltonian system (2), in addition to provide an accurate approximation of the exact flow ϕ_h for a reasonable range of step sizes $h \in [0, h_0]$, is to preserve qualitative properties of the original flow ϕ_h such as the symplecticness given by (3).

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

$$\psi_h'(y_0) J \psi_h'(y_0)^T = J. \tag{4}$$

One of the most known examples of symplectic methods is the s-stage RK Gauss methods which possess accuracy of order $2s$. Here we deal with modified RK methods. A s-stage modified RK method for solving the IVP (1) is an one-step method defined by the equations

$$y_1 = \psi_h(y_0) = y_0 + h\sum_{i=1}^{s} b_i f(t_0 + c_i h, Y_i), \tag{5}$$

$$Y_i = \gamma_i y_0 + h\sum_{j=1}^{s} a_{ij} f(t_0 + c_j h, Y_j), \quad i = 1, \ldots, s, \tag{6}$$

where the real parameters c_i and b_i, $i = 1, \ldots, s$, are known as the nodes and the weights of the method. The parameters γ_i are introduced by some authors (see [11,20,21]) in order to obtain explicit EFRK methods. In addition, when $\gamma_i = 1$, $i = 1, \ldots, s$, the algorithm (5)–(6) reduces to a standard RK method. Eq. (5) will be referred to as the final stage and Eqs. (6) as the internal stages of the modified RK method ψ_h. The s-stage modified RK method (5)–(6) is also represented by means of its Butcher's tableau

$$\begin{array}{c|c|c} c & \gamma & A \\ \hline & & b^T \end{array} = \begin{array}{c|c|ccc} c_1 & \gamma_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & \gamma_s & a_{s1} & \cdots & a_{ss} \\ \hline & & b_1 & \cdots & b_s \end{array} \tag{7}$$

or equivalently by the quartet (c, γ, A, b).

Definition 2.2. A modified RK method (5)–(6) has algebraic order p if for all sufficiently smooth IVP (1) it satisfies

$$y_1 - y(t_0 + h) = \psi_h(y_0) - \phi_h(y_0) = \mathcal{O}(h^{p+1}), \quad h \to 0. \tag{8}$$

In addition, it has stage order q if

$$\begin{aligned} &y_1 - y(t_0 + h) = \mathcal{O}(h^{q+1}), \quad h \to 0, \\ &Y_i - y(t_0 + c_i h) = \mathcal{O}(h^{q+1}), \quad i = 1, \ldots, s,\ h \to 0. \end{aligned} \tag{9}$$

The conditions for a modified RK method to be symplectic have been obtained by Van de Vyver [6] and they are given in the following theorem.

Theorem 2.3. *A modified RK method (5)–(6) for solving the Hamiltonian system (2) is symplectic if the following conditions are satisfied*

$$m_{ij} \equiv b_i b_j - \frac{b_i}{\gamma_i} a_{ij} - \frac{b_j}{\gamma_j} a_{ji} = 0, \quad 1 \leqslant i, j \leqslant s. \tag{10}$$

In general, the modified RK methods (5)–(6) preserve linear invariants, but if in addition its coefficients satisfy conditions (10), then they also preserve quadratic invariants [8].

On the other hand, symmetric numerical methods show a better long time behavior than nonsymmetric ones when applied to reversible differential systems, as it is the case of conservative mechanical systems. This fact has been pointed out by Hairer et al. [2] (see Chapters V and XI), and these authors have proved that for all differential system whose flow map is reversible, the numerical flow of a RK method will be also reversible iff it is symmetric. The key for understanding symmetry is the concept of the adjoint method.

Definition 2.4. 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. For s-stage modified RK methods (5)–(6) whose coefficients are h-dependent, as it is the case of EF methods, it is easy to see that the coefficients of ψ_h and ψ_h^* are related by

$$\begin{aligned} &c(h) = e - Sc^*(-h), \qquad b(h) = Sb^*(-h), \\ &\gamma(h) = S\gamma^*(-h), \qquad A(h) = S\gamma^*(-h)b^T(h) - SA(-h)S, \end{aligned} \tag{11}$$

where

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

In the case of modified RK methods (5)–(6) whose coefficients are even functions of h, as usually occurs in the construction of EFRK methods (see, for example, [6,8,21]), the symmetry conditions ($\psi_h^* = \psi_h$) are given by

$$\begin{aligned} &c(h) + Sc(h) = e, \qquad b(h) = Sb(h), \\ &\gamma(h) = S\gamma(h), \qquad SA(h) + A(h)S = \gamma(h)b^T(h). \end{aligned} \tag{12}$$

Here we will restrict our study to symmetric EFRK methods whose coefficients contain only even powers of h. In this case the symmetry conditions can be written in a more convenient form by putting

$$c(h) = \frac{1}{2}e + d(h), \qquad A(h) = \frac{1}{2}\gamma(h)b^T(h) + \Lambda(h), \tag{13}$$

where

$$d(h) = (d_1, \dots, d_s)^T \in \mathbb{R}^s \quad \text{and} \quad \Lambda(h) = (\lambda_{ij}) \in \mathbb{R}^{s\times s}.$$

So, the symmetry conditions (12) reduce to

$$d(h) + Sd(h) = 0, \qquad b(h) = Sb(h), \qquad \gamma(h) = S\gamma(h), \qquad S\Lambda(h) + \Lambda(h)S = 0, \tag{14}$$

where the coefficients $c(h)$ and $A(h)$ are defined by (13).

Therefore, for a symmetric EFRK method (5)–(6) whose coefficients a_{ij} are defined by

$$a_{ij} = \frac{1}{2}\gamma_i b_j + \lambda_{ij}, \quad 1 \leqslant i, j \leqslant s,$$

the symplecticness conditions (10) reduce to

$$\mu_{ij} \equiv \frac{b_i}{\gamma_i}\lambda_{ij} + \frac{b_j}{\gamma_j}\lambda_{ji} = 0, \quad 1 \leqslant i, j \leqslant s, \tag{15}$$

or in matrix form

$$\hat{B}(h)\Lambda(h) + \Lambda(h)\hat{B}(h) = 0, \tag{16}$$

where $\hat{B}(h) = \operatorname{diag}(b_i/\gamma_i)$.

The idea of constructing RK methods which integrate exactly a set of linearly independent functions different of the polynomials has been proposed by several authors (see, for example, [10,16–18,21,23]). This idea consists in to select the available parameters of the method (5)–(6) in order to be exact for a set of linearly independent functions

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

In such case, the coefficients of a modified RK method (5)–(6) are determined by the solution of the following linear systems

$$\sum_{i=1}^{s} b_i u_k'(t_0 + c_i h) = \frac{u_k(t_0 + h) - u_k(t_0)}{h}, \quad k = 1, \dots, r, \tag{17}$$

$$\sum_{j=1}^{s} a_{ij} u_k'(t_0 + c_j h) = \frac{u_k(t_0 + c_i h) - \gamma_i u_k(t_0)}{h}, \quad i = 1, \dots, s,\ k = 1, \dots, r. \tag{18}$$

When $r = s$, the coefficients b_i and a_{ij} defined by the linear systems (17)–(18) are unique for all $h > 0$ and $t \in [t_0, T]$, if the matrix

$$M(t,h) = \begin{pmatrix} u_1'(t + c_1 h) & \cdots & u_1'(t + c_s h) \\ \vdots & \dots & \vdots \\ u_s'(t + c_1 h) & \cdots & u_s'(t + c_s h) \end{pmatrix} \tag{19}$$

is nonsingular. In addition, if the functions $u_k(t)$, $k = 1, \dots, s$, are sufficiently smooth, then

$$u_k'(t + c_i h) = u_k'(t) + c_i h u_k''(t) + \cdots + \frac{(c_i h)^{s-1}}{(s-1)!}u_k^{(s)}(t) + \mathcal{O}(h^s), \tag{20}$$

and the matrix $M(t,h)$ can be expressed by

$$M(t,h) = W^T(t)\begin{pmatrix} 1 & 1 & \cdots & 1 \\ c_1 h & c_2 h & \cdots & c_s h \\ \vdots & \vdots & \dots & \vdots \\ \frac{(c_1 h)^{s-1}}{(s-1)!} & \frac{(c_2 h)^{s-1}}{(s-1)!} & \dots & \frac{(c_s h)^{s-1}}{(s-1)!} \end{pmatrix} + \mathcal{O}(h^s), \tag{21}$$

where $W(t)$ is the Wronskian matrix

$$W(t) \equiv W\big(u_1'(t), \dots, u_s'(t)\big) = \begin{pmatrix} u_1'(t) & \cdots & u_s'(t) \\ \vdots & \dots & \vdots \\ u_1^{(s)}(t) & \cdots & u_s^{(s)}(t) \end{pmatrix}. \tag{22}$$

Therefore, if the nodes are different ($c_i \neq c_j,\ i \neq j$) and the Wronskian matrix $W(t)$ is nonsingular on the interval $[t_0, T]$, then the matrix $M(t,h)$ is also nonsingular and the linear systems (17)–(18) have a unique solution for all $h > 0$ and $t \in [t_0, T]$.

The most usual case is to consider exponential or trigonometric functions as 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 $\lambda = i\omega$. For the reference set of functions $\mathcal{F}_1$ the linear systems (17)–(18) reduce to

$$\sum_{i=1}^{s} b_i \cosh(c_i z) = \frac{\sinh(z)}{z}, \qquad \sum_{i=1}^{s} b_i \sinh(c_i z) = \frac{\cosh(z) - 1}{z}, \tag{23}$$

$$\sum_{j=1}^{s} a_{ij} \cosh(c_j z) = \frac{\sinh(c_i z)}{z}, \qquad \sum_{j=1}^{s} a_{ij} \sinh(c_j z) = \frac{\cosh(c_i z) - \gamma_i}{z}, \quad i = 1, \ldots, s, \tag{24}$$

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 and parameters γ_i. By choosing Gauss nodes: $c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}$ and $c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6}$, and imposing the symplecticness conditions (10), the fourth-order symplectic modified EFRK Gauss integrator given in [6] is obtained. In addition, this integrator reduces to the standard two-stage RK Gauss method when $z = 0$. Until now, the only symplectic modified EFRK Gauss method known to us is the two-stage fourth-order integrator given in [6], and the procedure presented above is not direct for the case of $s > 2$. In the next section, we try to extend the construction of symplectic modified EFRK Gauss methods to the case of $s = 3$ stages.

3. Construction of the symplectic integrators

Here we study the construction of symmetric and symplectic modified EFRK Gauss methods with $s = 3$ stages whose coefficients are even functions of h. Our intention is that the new EF methods should have the properties of symmetry, symplecticness, accuracy order $2s$, and preservation of linear and quadratic invariants as the standard RK Gauss methods.

From the conditions of symmetry (14) and symplecticness (16) it follows that

$$d = \begin{pmatrix} -\theta \\ 0 \\ \theta \end{pmatrix}, \qquad b = \begin{pmatrix} b_1 \\ b_2 \\ b_1 \end{pmatrix}, \qquad \gamma = \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_1 \end{pmatrix}, \qquad \Lambda = \begin{pmatrix} 0 & -\alpha_2 & -\alpha_3 \\ -\alpha_4 & 0 & \alpha_4 \\ \alpha_3 & \alpha_2 & 0 \end{pmatrix}, \tag{25}$$

$$\frac{b_1}{\gamma_1}\alpha_2 + \frac{b_2}{\gamma_2}\alpha_4 = 0, \tag{26}$$

and the three-stage modified RK methods are given by the Butcher's tableau

$$\begin{array}{c|c|ccc} \frac{1}{2} - \theta & \gamma_1 & \frac{\gamma_1 b_1}{2} & \frac{\gamma_1 b_2}{2} - \alpha_2 & \frac{\gamma_1 b_1}{2} - \alpha_3 \\ \frac{1}{2} & \gamma_2 & \frac{\gamma_2 b_1}{2} - \alpha_4 & \frac{\gamma_2 b_2}{2} & \frac{\gamma_2 b_1}{2} + \alpha_4 \\ \frac{1}{2} + \theta & \gamma_1 & \frac{\gamma_1 b_1}{2} + \alpha_3 & \frac{\gamma_1 b_2}{2} + \alpha_2 & \frac{\gamma_3 b_3}{2} \\ \hline & & b_1 & b_2 & b_1 \end{array} \tag{27}$$

The EF conditions (23)–(24) with $s = 3$ give two conditions for the weights b_j and six conditions for the coefficients a_{ij} and γ_i, but for the form of the table of coefficients (27), they reduce to one condition for the weights

$$b_2 + 2b_1 \cosh(\theta z) = \frac{\sinh(z/2)}{z/2}, \tag{28}$$

and three conditions for the rest of the coefficients

$$\begin{aligned} &1 - \gamma_2 \cosh(z/2) - 2z\alpha_4 \sinh(\theta z) = 0, \\ &\cosh(\theta z) - \gamma_1 \cosh(z/2) + z\alpha_3 \sinh(\theta z) = 0, \\ &\sinh(\theta z) - z\alpha_3 \cosh(\theta z) - z\alpha_2 = 0. \end{aligned} \tag{29}$$

3.1. Three-stage EF integrator with fixed nodes

First we impose that the final stage is also exact for the reference set of functions $\{t,\ t^2\}$, i.e., the following conditions are also satisfied

$$\sum_{i=1}^{3} b_i = 1, \qquad \sum_{i=1}^{3} b_i c_i = \frac{1}{2}. \tag{30}$$

By the symmetry of the nodes and weights (27), the conditions (30) reduce to

$$b_2 + 2b_1 = 1, \tag{31}$$

and the weights b_1 and b_2 can be computed from Eqs. (28) and (31) obtaining

$$b_1 = \frac{z - 2\sinh(z/2)}{2z(1-\cosh(\theta z))}, \qquad b_2 = \frac{2\sinh(z/2) - z\cosh(\theta z)}{z(1-\cosh(\theta z))}. \tag{32}$$

From conditions (29) the coefficients α_j can be computed in terms of γ_1 and γ_2 obtaining

$$\begin{aligned}\alpha_2 &= \frac{\cosh(2\theta z) - \gamma_1 \cosh(z/2)\cosh(\theta z)}{z\sinh(\theta z)},\\ \alpha_3 &= \frac{\gamma_1\cosh(z/2) - \cosh(\theta z)}{z\sinh(\theta z)}, \qquad \alpha_4 = \frac{1-\gamma_2\cosh(z/2)}{2z\sinh(\theta z)}.\end{aligned} \tag{33}$$

If now the symplecticness condition (26) is imposed, the parameter γ_1 is determined by

$$\gamma_1 = \frac{\gamma_2(2\sinh(z/2) - z)\cosh(2\theta z)}{2\sinh(z/2) - \gamma_2\sinh(z) + (\gamma_2\sinh(z) - z)\cosh(\theta z)}. \tag{34}$$

The coefficients (32)–(34) define a family of EFRK methods (27) which are symmetric, symplectic and they preserve linear and quadratic invariants for all γ_2 and $\theta \in \mathbb{R}$. In particular, by choosing $\gamma_2 = 1$ and 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 MEFGauss3F, and when $z = 0$ it reduces to standard three-stage RK Gauss method.

We note that the internal stages of the new MEFGauss3F integrator are exact for the basis $\langle \exp(\lambda t), \exp(-\lambda t)\rangle$, whereas the final stage is exact for the basis $\langle 1, t, t^2, \exp(\lambda t), \exp(-\lambda t)\rangle$. In the trigonometric case ($\lambda = i\omega$, $\omega \in \mathbb{R}$) we have $z = i\nu$ with $\nu = \omega h$, and the coefficients (32)–(34) emerge having in mind the relations $\cosh(i\nu) = \cos(\nu)$ and $\sinh(i\nu) = i\sin(\nu)$. In this case, the internal stages are exact for the basis $\langle \cos(\omega t), \sin(\omega t)\rangle$, whereas the final stage is exact for the basis $\langle 1, t, t^2, \cos(\omega t), \sin(\omega t)\rangle$.

For small values of $|z|$ the above formulas are subject to heavy cancellations, and series expansions for the coefficients must be used. So, when $|z| < 0.1$, the following coefficients should be used

$$\begin{aligned}
b_1 &= \frac{5}{18} + \frac{z^4}{302400} - \frac{z^6}{62208000} + \frac{17z^8}{212889600000} - \frac{15641z^{10}}{41845579776000000} + \cdots,\\
b_2 &= \frac{4}{9} - \frac{z^4}{151200} + \frac{z^6}{31104000} - \frac{17z^8}{106444800000} + \frac{15641z^{10}}{20922789888000000} + \cdots,\\
\gamma_1 &= 1 - \frac{3z^6}{56000} + \frac{649z^8}{44800000} - \frac{983177z^{10}}{275968000000} + \frac{2248000621z^{12}}{2583060480000000} + \cdots,\\
\alpha_2 &= \frac{\sqrt{15}}{15} - \frac{\sqrt{15}z^2}{3600} + \frac{\sqrt{15}z^4}{236250} - \frac{4411\sqrt{15}z^6}{1209600000} + \frac{13168313\sqrt{15}z^8}{13412044800000} - \frac{252934109479\sqrt{15}z^{10}}{1046139494400000000} + \cdots,\\
\alpha_3 &= \frac{\sqrt{15}}{30} + \frac{\sqrt{15}z^2}{3600} - \frac{71\sqrt{15}z^4}{1890000} + \frac{1849\sqrt{15}z^6}{302400000} - \frac{47169209\sqrt{15}z^8}{33530112000000} + \frac{178746672227\sqrt{15}z^{10}}{523069747200000000} + \cdots,\\
\alpha_4 &= -\frac{\sqrt{15}}{24} + \frac{\sqrt{15}z^2}{5760} - \frac{13\sqrt{15}z^4}{3456000} + \frac{221\sqrt{15}z^6}{3870720000} - \frac{6061\sqrt{15}z^8}{6967296000000} + \frac{9733\sqrt{15}z^{10}}{735746457600000} + \cdots.
\end{aligned}$$

Finally, we check some conditions satisfied by the new integrator which will be necessary for the study of its algebraic order (see Section 4).

$$\gamma - e = \begin{pmatrix} -\frac{3}{56000} \\ 0 \\ -\frac{3}{56000} \end{pmatrix} z^6 + \mathcal{O}(z^8), \qquad b^T(\gamma - e) = -\frac{z^6}{33600} + \mathcal{O}(z^8), \tag{35}$$

$$Ae - c = \begin{pmatrix} \frac{1}{2000\sqrt{15}} \\ 0 \\ -\frac{1}{2000\sqrt{15}} \end{pmatrix} z^4 + \mathcal{O}(z^6), \qquad b^T e - 1 = 0, \tag{36}$$

$$Ac - \frac{c^2}{2} = \begin{pmatrix} -\frac{1}{2400} \\ \frac{1}{1920} \\ -\frac{1}{2400} \end{pmatrix} z^2 + \mathcal{O}(z^4), \qquad b^T c - \frac{1}{2} = 0, \tag{37}$$

$$Ac^2 - \frac{c^3}{3} = \begin{pmatrix} \frac{-10-\sqrt{15}}{24000} \\ \frac{1}{1920} \\ \frac{-10+\sqrt{15}}{24000} \end{pmatrix} z^2 + \mathcal{O}(z^4), \qquad b^T c^2 - \frac{1}{3} = \mathcal{O}(z^4), \tag{38}$$

$$b^T c^3 - \frac{1}{4} = \mathcal{O}(z^4), \qquad b^T c^4 - \frac{1}{5} = \mathcal{O}(z^4), \qquad b^T c^5 - \frac{1}{6} = \mathcal{O}(z^4), \tag{39}$$

$$\begin{aligned} & b^T(Ae - c) = -\frac{z^6}{67200} + \mathcal{O}(z^7), \qquad b^T\left(Ac - \frac{c^2}{2}\right) = \frac{53z^4}{2016000} + \mathcal{O}(z^5), \\ & b^T\left(Ac^2 - \frac{c^3}{3}\right) = \frac{3z^4}{112000} + \mathcal{O}(z^5), \qquad b^T\left(Ac^3 - \frac{c^4}{4}\right) = \frac{219z^4}{8960000} + \mathcal{O}(z^5), \\ & b^T\left(Ac^4 - \frac{c^5}{5}\right) = \frac{221z^4}{10080000} + \mathcal{O}(z^5). \end{aligned} \tag{40}$$

3.2. Three-stage EF integrator with variable nodes

Now we consider the case of three-stage RK methods (27) such that their internal stages are also exact for the function $y(x) = 1$ which implies $\gamma = e = (1, 1, 1)^T$. These EF methods result to be more accurate than the EF methods which are exact for the basis without $y(x) = 1$ when they are applied to oscillatory problems in which the linear terms are dominant over the remaining terms of the differential system (see the numerical results obtained in Problem 4). In this case, the EF conditions (28)–(29) and (31) give the coefficients (32)–(33) with $\gamma_1 = \gamma_2 = 1$. If in addition the symplecticness condition (26) is imposed, the parameter θ is determined by

$$\theta = \frac{\operatorname{arccosh}(\beta)}{z}, \qquad \beta = \frac{z - 4\sinh(z/2) + \sinh(z)}{4\sinh(z/2) - 2z}. \tag{41}$$

So, we have obtained a EFRK integrator with variable nodes which will be denoted as MEFGauss3V. The new integrator is also symmetric, symplectic, it preserves linear and quadratic invariants, and when $z = 0$ it reduces to the standard three-stage RK Gauss method.

We note that the internal stages of the new MEFGauss3V integrator are exact for the basis $\langle 1, \exp(\lambda t), \exp(-\lambda t)\rangle$. In the trigonometric case ($\lambda = i\omega$, $\omega \in \mathbb{R}$, $z = i\nu$, $\nu = \omega h$) the coefficients of the method emerge having in mind the relations $\cosh(i\nu) = \cos(\nu)$ and $\sinh(i\nu) = i\sin(\nu)$, and the internal stages are exact for the basis $\langle 1, \cos(\omega t), \sin(\omega t)\rangle$.

For small values of z ($|z| < 0.1$) the coefficients suffer heavy cancellations, and the following series expansions should be used

$$\begin{aligned} b_1 &= \frac{5}{18} - \frac{z^2}{756} + \frac{z^4}{282240} + \frac{31z^6}{1564738560} - \frac{1187z^8}{3728060743680} + \frac{2533z^{10}}{1275825232281600} + \cdots, \\ b_2 &= \frac{4}{9} + \frac{z^2}{378} - \frac{z^4}{141120} - \frac{31z^6}{782369280} + \frac{1187z^8}{1864030371840} - \frac{2533z^{10}}{637912616140800} + \cdots, \\ \alpha_2 &= \frac{\sqrt{15}}{15} + \frac{\sqrt{15}z^2}{3600} - \frac{37\sqrt{15}z^4}{14112000} + \frac{61\sqrt{15}z^6}{1358280000} - \frac{10800253\sqrt{15}z^8}{17086945075200000} + \frac{3362441\sqrt{15}z^{10}}{683477803008000000} + \cdots, \\ \alpha_3 &= \frac{\sqrt{15}}{30} - \frac{\sqrt{15}z^2}{25200} - \frac{11\sqrt{15}z^4}{3528000} + \frac{17\sqrt{15}z^6}{248371200} - \frac{3051109\sqrt{15}z^8}{3417389015040000} + \frac{559337\sqrt{15}z^{10}}{85434725376000000} + \cdots, \\ \alpha_4 &= -\frac{\sqrt{15}}{24} + \frac{11\sqrt{15}z^2}{40320} - \frac{\sqrt{15}z^4}{2822400} - \frac{5329\sqrt{15}z^6}{139087872000} + \frac{348151\sqrt{15}z^8}{390558744576000} - \frac{1641379\sqrt{15}z^{10}}{136695560601600000} + \cdots, \\ \theta &= \frac{\sqrt{15}}{10} + \frac{\sqrt{15}z^2}{4200} - \frac{17\sqrt{15}z^4}{7840000} + \frac{769\sqrt{15}z^6}{43464960000} - \frac{280393\sqrt{15}z^8}{2847824179200000} - \frac{7963\sqrt{15}z^{10}}{25313992704000000} + \cdots. \end{aligned}$$

Finally, we check some conditions satisfied by the new method which will be necessary for the study of its algebraic order (see Section 4).

$$\gamma - e = 0, \qquad b^T(\gamma - e) = 0, \tag{42}$$

$$Ae - c = \begin{pmatrix} \frac{\sqrt{15}}{280000} \\ 0 \\ -\frac{\sqrt{15}}{280000} \end{pmatrix} z^4 + \mathcal{O}(z^6), \qquad b^T e - 1 = 0, \tag{43}$$

$$Ac - \frac{c^2}{2} = \begin{pmatrix} -\frac{1}{2400} \\ \frac{1}{1920} \\ -\frac{1}{2400} \end{pmatrix} z^2 + \mathcal{O}(z^4), \qquad b^T c - \frac{1}{2} = 0, \tag{44}$$

$$Ac^2 - \frac{c^3}{3} = \begin{pmatrix} \frac{-70+3\sqrt{15}}{168000} \\ \frac{1}{1920} \\ \frac{-703\sqrt{15}}{168000} \end{pmatrix} z^2 + \mathcal{O}(z^4), \qquad b^T c^2 - \frac{1}{3} = \mathcal{O}(z^4), \tag{45}$$

$$b^T c^3 - \frac{1}{4} = \mathcal{O}(z^4), \qquad b^T c^4 - \frac{1}{5} = \mathcal{O}(z^2), \qquad b^T c^5 - \frac{1}{6} = \mathcal{O}(z^2), \tag{46}$$

$$b^T(Ae - c) = 0, \qquad b^T\left(Ac - \frac{c^2}{2}\right) = \frac{z^4}{112000} + \mathcal{O}(z^5),$$
$$b^T\left(Ac^2 - \frac{c^3}{3}\right) = \frac{z^4}{144000} + \mathcal{O}(z^5), \qquad b^T\left(Ac^3 - \frac{c^4}{4}\right) = -\frac{z^2}{13440} + \mathcal{O}(z^3),$$
$$b^T\left(Ac^4 - \frac{c^5}{5}\right) = -\frac{z^2}{8400} + \mathcal{O}(z^3). \tag{47}$$

4. Algebraic order of the EF integrators

In this section we study the algebraic order of accuracy reached by the new modified EFRK Gauss methods derived in previous section. These methods integrate exactly IVPs whose solutions belong to the linear space generated by the basis $\langle \exp(\lambda t), \exp(-\lambda t)\rangle$ or $\langle \cos(\omega t), \sin(\omega t)\rangle$, but for IVPs with more general solutions they present local truncation errors.

Having in mind that the coefficients of an EFRK method vary as functions of the step-size h, we introduce the following quantities typical in standard RK methods

$$B_k = b^T c^{k-1} - \frac{1}{k}, \qquad C_k = Ac^{k-1} - \frac{c^k}{k}, \quad k \geqslant 1, \tag{48}$$

and we express the errors at the internal stages and the final stage in terms of them.

Given a modified RK method (5)–(6), the exact solution $y(t)$ of the IVP (1) satisfies

$$y(t_0 + h) = \phi_h(y_0) = y(t_0) + h\sum_{i=1}^{s} b_i y'(t_0 + c_i h) - r(h), \tag{49}$$

$$y(t_0 + c_i h) = \gamma_i y(t_0) + h\sum_{j=1}^{s} a_{ij} y'(t_0 + c_j h) - R_i(h), \quad i = 1, \dots, s, \tag{50}$$

where the residuals are defined by

$$r(h) = \sum_{k\geqslant 1} \frac{h^k B_k}{(k-1)!}\, y^{(k)}(t_0), \tag{51}$$

$$R(h) = \begin{pmatrix} R_1(h) \\ \vdots \\ R_s(h) \end{pmatrix} = (\gamma - e)\otimes y(t_0) + \sum_{k\geqslant 1} \frac{h^k C_k}{(k-1)!} \otimes y^{(k)}(t_0). \tag{52}$$

So, the local truncation errors at the internal stages and the final stage are given by

$$\tau_i(h) = Y_i - y(t_0 + c_i h) = h\sum_{j=1}^{s} a_{ij}\big[f(t_0 + c_j h, Y_j) - f\big(t_0 + c_j h, y(t_0 + c_j h)\big)\big] + R_i(h), \quad i = 1, \dots, s, \tag{53}$$

$$\tau(h) = \psi_h(y_0) - \phi_h(y_0) = h\sum_{i=1}^{s} b_i\big[f(t_0 + c_i h, Y_i) - f\big(t_0 + c_i h, y(t_0 + c_i h)\big)\big] + r(h), \tag{54}$$

and the following result can be written

Theorem 4.1. *If the following conditions are satisfied*

$$\gamma - e = \mathcal{O}(h^{q+1}), \qquad B_k = \mathcal{O}(h^{q+1-k}), \qquad C_k = \mathcal{O}(h^{q+1-k}), \quad k = 1, \dots, q, \tag{55}$$

then the EFRK method possesses stage order q.

Proof. The conditions (55) imply that $h^k B_k = \mathcal{O}(h^{q+1})$ and $h^k C_k = \mathcal{O}(h^{q+1})$, and therefore the residuals $r(h) = \mathcal{O}(h^{q+1})$ and $R(h) = \mathcal{O}(h^{q+1})$.

On the other hand, by using the notation

$$E = \big(\tau_1(h), \dots, \tau_s(h)\big)^T, \qquad Y = (Y_1, \dots, Y_s)^T, \qquad F(Y) = \big(f(t_0 + c_1 h, Y_1), \dots, f(t_0 + c_s h, Y_s)\big)^T,$$

Eq. (53) can be written as

$$E = hA \otimes \big[F(Y) - F\big(y(et_0 + ch)\big)\big] + R(h),$$

and Lipschitz continuity of f implies that

$$\|E\| \leqslant \big(1 - hL\|A\|\big)^{-1}\big\|R(h)\big\| = \mathcal{O}(h^{q+1}).$$

From (54) and the smoothness of f we have

$$\tau(h) = h\sum_{i=1}^{s} b_i\big(J_f(t_0 + c_i h)\tau_i(h) + \mathcal{O}\big(\tau_i^2(h)\big)\big) + r(h),$$

where $J_f(t_0 + c_i h) = D_y f(t_0 + c_i h, y(t_0 + c_i h))$, and then

$$\tau(h) = \mathcal{O}(h^{q+1}). \qquad \square$$

In view of (35)–(38) and (42)–(45), the methods MEFGauss3F and MEFGauss3V satisfy conditions (55) with $q = 3$ and the following result can be written.

Corollary 4.2. *The methods MEFGauss3F and MEFGauss3V possess stage order* $q = 3$.

Now we analyze the possibility of superconvergence (i.e., the algebraic order is greater than the stage order q) for the methods MEFGauss3F and MEFGauss3V. Assuming that conditions (55) are satisfied and $E = \mathcal{O}(h^{q+1})$, the local truncation error for the final stage can be written as

$$\tau(h) = h\sum_{i=1}^{s} b_i J_f(t_0 + c_i h)\tau_i(h) + r(h) + \mathcal{O}(h^{2q+3}). \tag{56}$$

From (53) and the smoothness of f

$$\tau_i(h) = h\sum_{j=1}^{s} a_{ij} J_f(t_0 + c_j h)\tau_j(h) + R_i(h) + \mathcal{O}(h^{2q+3}), \quad i = 1, \dots, s,$$

and taking into account that $J_f(t_0 + c_j h) = J_f(t_0) + \mathcal{O}(h)$, Eq. (56) can be written as

$$\tau(h) = h^2\big(J_f(t_0)\big)^2(b^T A \otimes E) + hJ_f(t_0)T(h) + r(h) + \mathcal{O}(h^{q+3}), \tag{57}$$

where

$$T(h) = b^T \otimes R(h) = b^T(\gamma - e) \otimes y(t_0) + \sum_{k\geqslant 1}\frac{h^k b^T C_k}{(k-1)!} \otimes y^{(k)}(t_0).$$

On the other hand, the behavior of the terms $T(h)$ and $r(h)$ depends on the coefficients $b^T(\gamma - e)$, $b^T C_k$ and B_k, i.e.,

$$T(h) = \mathcal{O}(h^{r+1}) \quad \text{iff} \quad b^T(\gamma - e) = \mathcal{O}(h^{r+1}), \qquad b^T C_k = \mathcal{O}(h^{r+1-k}), \quad k = 1, \dots, r, \tag{58}$$

$$r(h) = \mathcal{O}(h^{\rho+1}) \quad \text{iff} \quad B_k = \mathcal{O}(h^{\rho+1-k}), \quad k = 1, \dots, \rho. \tag{59}$$

Thus, we have that the local truncation error for the final stage behaves as

$$\tau(h) = \mathcal{O}(h^{p+1}),$$

where

$$p = \min\{q + 2, r + 1, \rho\}. \tag{60}$$

In view of (35)–(40) and (42)–(47), the methods MEFGauss3F and MEFGauss3V satisfy (60) with $q = 3$, $r = 5$ and $\rho = 6$, and therefore both methods possess at least order $p = 5$. But both methods are symmetric by construction, and therefore both methods have algebraic order 6.

In conclusion we may write the following result:

Theorem 4.3. *The new symplectic methods MEFGauss3F and MEFGauss3V have stage order* 3 *and algebraic order* 6 *as the standard three-stage RK Gauss method.*

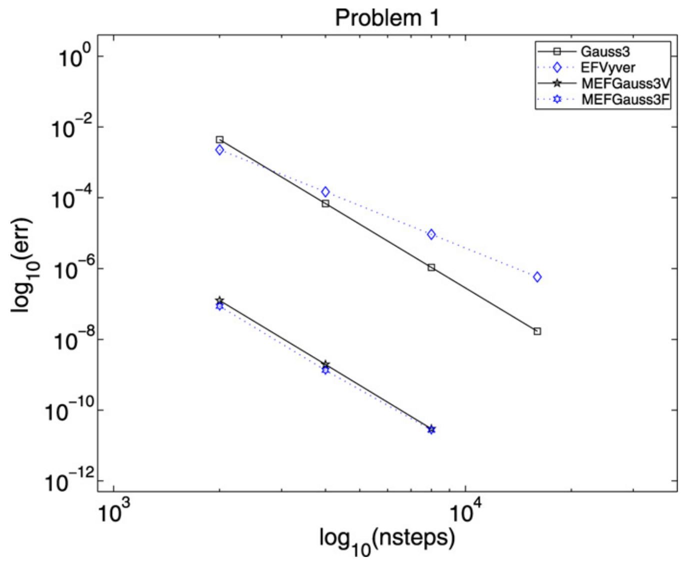

Fig. 1. Maximum global error in the solution for Problem 1.

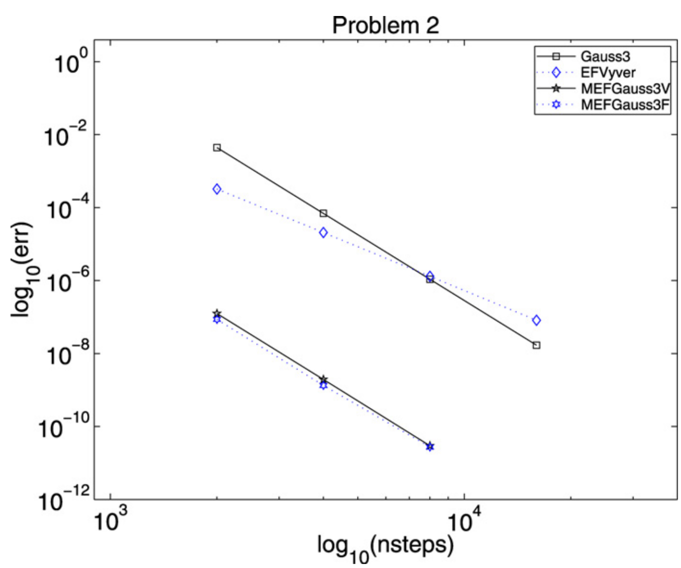

Fig. 2. Maximum global error in the solution for Problem 2.

5. Numerical experiments

In this section we present some numerical experiments to test the effectiveness of the new modified EFRK methods derived in Section 3 when they are applied to the numerical solution of several oscillatory differential systems. The new methods have been compared with a fourth-order symplectic exponentially fitted integrator proposed in [6] denoted here as EFVyver, and with the standard three-stage sixth-order Gauss method given in [2] denoted as Gauss3. We note that all the codes used in the numerical experiments have the same qualitative properties for Hamiltonian systems. 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 global error ($\log_{10}(\text{err})$) versus the number of steps required by each code in logarithmic scale ($\log_{10}(\text{nsteps})$). 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

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

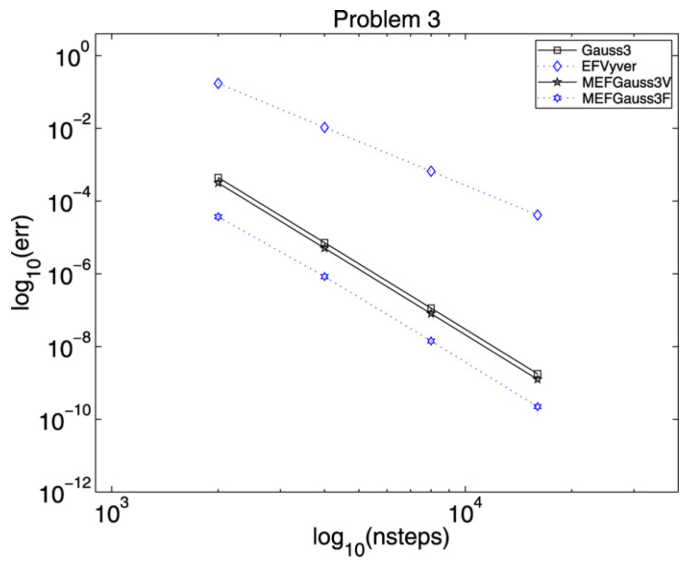

Fig. 3. Maximum global error in the solution for Problem 3.

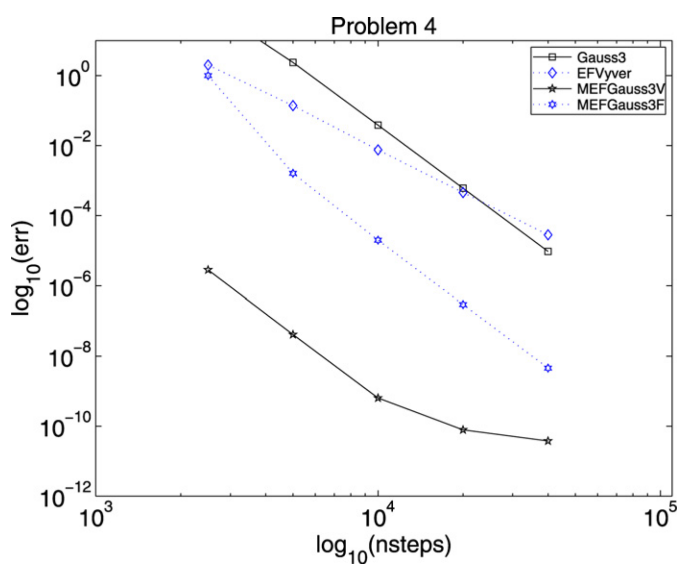

Fig. 4. Maximum global error in the solution for Problem 4.

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 $(0 \leqslant e < 1)$ 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, corresponding the starting point to the pericenter of this orbit.

In the numerical experiments presented here we have chosen the same values as in [6], i.e. $e = 0.001$, $\lambda = i\omega$ with $\omega = (q_1^2 + q_2^2)^{-3/2}$, and the integration is carried out on the interval [0, 1000] with the steps $h = 1/2^m$, $m = 1, \ldots, 4$. The numerical behavior of the global error in the solution is presented in Fig. 1.

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

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

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 $\varepsilon = 10^{-3}$, $\lambda = i\omega$ with $\omega = 1$ 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

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

with the initial values $q(0) = (0, 1, 1)^T$, 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

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

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 $\lambda = i2\pi/T$.

Problem 4. A two dimensional nonlinear oscillatory Hamiltonian system

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

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 $\omega > 0$, $0 \leqslant k < 1$. 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

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

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

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

From the numerical experiments carried out it follows that for the problems under consideration an accurate estimation of the frequency is essential to assess the accuracy of symplectic integrators based on exponentially fitted methods. This fact has been already pointed out by Vanden Berghe and coworkers [22] who propose some algorithms to estimate the frequency of 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, the sixth-order codes show a similar accuracy behavior with the code MEFGauss3F (fixed nodes) being the most accurate 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 exponentially fitted methods is in general superior to the standard ones of the same order (see the results obtained with the codes MEFGauss3F, MEFGauss3V and Gauss3). Moreover, the numerical results show that for high accuracy the standard sixth-order code Gauss3 is superior to fourth-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 new methods MEFGauss3F and MEFGauss3V are clearly superior to the other methods and both show a similar global error behavior. So, the method EFGauss3F (fixed nodes) results to be slightly more accurate than the method EFGauss3V (variable nodes) in Problems 1 and 2 whereas in Problem 4 the method EFGauss3V results to be the most accurate. This fact shows that for oscillatory problems in which the linear terms are dominant over the remaining terms of the differential system (as occurs in Problem 4), the EF methods which are exact for the basis $\langle 1,\ \exp(\lambda t), \exp(-\lambda t)\rangle$ or $\langle 1,\ \cos(\omega t), \sin(\omega t)\rangle$ result to be more accurate than the EF methods which are exact for the basis $\langle \exp(\lambda t), \exp(-\lambda t)\rangle$ or $\langle \cos(\omega t), \sin(\omega t)\rangle$.

6. Conclusions

In this paper a new approach for constructing symplectic exponentially fitted methods of RK type is presented. This approach is based on the combination of the symmetry, symplecticness and exponential fitting properties previously derived for a class of modified RK methods with variable coefficients. Two new three-stage sixth-order modified EFRK integrators of Gauss type which are symmetric and symplectic and preserve linear and quadratic invariants have been derived. When the frequency used in the exponential fitting process is $\lambda = 0$ ($z = 0$), the new integrators reduce to standard three-stage Gauss integrator. It is shown that such fitted methods are reliable alternatives to the standard three-stage Gauss integrator and the two-stage EFRK code derived in [6] to describe the evolution of some oscillatory problems. Furthermore, the computational cost of the new modified EFRK methods is similar to their counterparts standard RK methods. The numerical experiments carried out with some oscillatory problems show that the new methods improve the results obtained with other (standard or exponentially fitted) symplectic integrators. The investigation of new symmetric and symplectic EF methods of RK type with a larger algebraic order and/or which are exact for other reference set of functions as well their application to oscillatory problems is now in progress.

Acknowledgements

This research has been partially supported by Project MTM2004-06466-C02-01 of the Dirección General de Investigación (Ministerio de Educación, Cultura y Deporte).

References

[1] V.I. Arnold, Mathematical Methods of Classical Mechanics, Springer-Verlag, New York, 1989.
[2] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration: Structure Preserving Algorithms for Ordinary Differential Equations, Springer-Verlag, Berlin, 2002.
[3] J.M. Sanz-Serna, Symplectic integrators for Hamiltonian problems: an overview, Acta Numer. 1 (1992) 243–286.
[4] J.M. Sanz-Serna, M.P. Calvo, Numerical Hamiltonian Problems, Chapman and Hall, London, 1994.
[5] T.E. Simos, J. Vigo-Aguiar, Exponentially fitted symplectic integrator, Phys. Rev. E 67 (2003) 1–7.
[6] H. Van de Vyver, A fourth order symplectic exponentially fitted integrator, Comput. Phys. Comm. 176 (2006) 255–262.
[7] J. Vigo-Aguiar, T.E. Simos, A. Tocino, An adapted symplectic integrator for Hamiltonian systems, Int. J. Modern Phys. C 12 (2001) 225–234.
[8] M. Calvo, J.M. Franco, J.I. Montijano, L. Rández, Structure preservation of Exponentially Fitted Runge–Kutta methods, J. Comput. Appl. Math. (2008), doi:10.1016/j.cam.2008.01.026.
[9] D.G. Bettis, Runge–Kutta algorithms for oscillatory problems, J. Appl. Math. Phys. (ZAMP) 30 (1979) 699–704.
[10] J.P. Coleman, S.C. Duxbury, Mixed collocation methods for $y'' = f(x, y)$, J. Comput. Appl. Math. 126 (2000) 47–75.
[11] J.M. Franco, An embedded pair of exponentially fitted explicit Runge–Kutta methods, J. Comput. Appl. Math. 149 (2002) 407–414.
[12] J.M. Franco, Runge–Kutta methods adapted to the numerical integration of oscillatory problems, Appl. Numer. Math. 50 (2004) 427–443.
[13] J.M. Franco, Exponentially fitted explicit Runge–Kutta–Nyström methods, J. Comput. Appl. Math. 167 (2004) 1–19.
[14] W. Gautschi, Numerical integration of ordinary differential equations based on trigonometric polynomials, Numer. Math. 3 (1961) 381–397.
[15] L.Gr. Ixaru, G. Vanden Berghe, Exponential Fitting, Kluwer Academic Publishers, 2004.
[16] K. Ozawa, A functional fitting Runge–Kutta method with variable coefficients, Japan J. Indust. Appl. Math. 18 (2001) 107–130.
[17] K. Ozawa, A functionally fitted three-stage explicit singly diagonally implicit Runge–Kutta method, Japan J. Indust. Appl. Math. 22 (2005) 403–427.
[18] B. Paternoster, Runge–Kutta(–Nyström) methods for ODEs with periodic solutions based on trigonometric polynomials, Appl. Numer. Math. 28 (1998) 401–412.
[19] T.E. Simos, An exponentially-fitted Runge–Kutta method for the numerical integration of initial-value problems with periodic or oscillating solutions, Comput. Phys. Comm. 115 (1998) 1–8.
[20] G. Vanden Berghe, H. De Meyer, M. Van Daele, T. Van Hecke, Exponentially-fitted explicit Runge–Kutta methods, Comput. Phys. Comm. 123 (1999) 7–15.
[21] G. Vanden Berghe, H. De Meyer, M. Van Daele, T. Van Hecke, Exponentially fitted Runge–Kutta methods, J. Comput. Appl. Math. 125 (2000) 107–115.
[22] G. Vanden Berghe, L.Gr. Ixaru, H. De Meyer, Frequency determination and step-length control for exponentially fitted Runge–Kutta methods, J. Comput. Appl. Math. 132 (2001) 95–105.
[23] G. Vanden Berghe, M. Van Daele, H. Van de Vyver, Exponentially-fitted Runge–Kutta methods of collocation type: fixed or variable knot points? J. Comput. Appl. Math. 159 (2003) 217–239.