Symmetric and symplectic exponentially fitted Runge–Kutta methods of high order

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The construction of high order symmetric, symplectic and exponentially fitted Runge–Kutta (RK) methods for the numerical integration of Hamiltonian systems with oscillatory solutions is analyzed. Based on the symplecticness, symmetry, and exponential fitting properties, three new four-stage RK integrators, either with fixed- or variable-nodes, are constructed. The algebraic order of the new integrators is also studied, showing that they possess eighth-order of accuracy as the classical four-stage RK Gauss method. Numerical experiments with some oscillatory test problems are presented to show that the new methods are more efficient than other symplectic four-stage eighth-order RK Gauss codes proposed in the scientific literature.

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1. Introduction

In this paper we consider the construction of high order symmetric and symplectic exponentially fitted Runge–Kutta (EFRK) methods 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. Therefore, 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. Examples of such methods can be found in [6,8–10] in which symplectic EFRK methods with two and three-stage and algebraic orders four and six have been derived. In addition, in [6] the well known theory of symplectic RK methods is extended to modified EFRK methods, obtaining sufficient conditions on the coefficients of these methods that imply symplecticness for general Hamiltonian systems, and in [8] the preservation properties of modified EFRK methods for first order differential systems have been analyzed.

The design and construction of numerical methods for solving ODEs which have periodic or oscillating solutions has been considered by several authors (see [5–26] and references therein). The aim of these methods 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. We mention the pioneer papers of Gautschi [16] and Bettis [11], in which EF linear multistep methods and adapted RK algorithms, respectively, were introduced for solving differential systems with oscillatory solutions. However, the development of EF Runge–Kutta (-Nyström) methods has been carried out more recently. A detailed survey including an extensive bibliography on this subject can be found in Ixaru and Vanden Berghhe [18]. Usually, 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 solution for the coefficients of an EFRK method are obtained by Ozawa [19,20], and several authors [8,13,15,17,19,21,24] have derived methods with variable 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 \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.

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The aim of this paper is the construction of four-stage eighth-order symmetric and symplectic 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}. The paper is organized as follows: Section 2 is devoted to present the basic concepts and results on symmetry and symplecticness as well as the notation to be used in the rest of the paper. In Section 3 we present the derivation of some new four-stage symmetric and symplectic EFRK integrators, either with fixed nodes or variable nodes. In Section 4 we analyze the algebraic order of accuracy of the new EFRK integrators, obtaining that they possess eighth-order as the classical four-stage RK Gauss method. In Section 5 we present some numerical experiments with oscillatory Hamiltonian systems that show the efficiency of the new EFRK integrators when they are compared with the standard symplectic four-stage eighth-order RK Gauss method, and with a symplectic and symmetric trigonometrically fitted four-stage eighth-order integrator. Finally, Section 6 is devoted to present some conclusions.

2. EFRK methods: symmetry and symplecticness

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

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

where for simplicity \( f: \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m \) 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 smooth solution \( y(t) = y(t; t_0, y_0) \).

An s-stage (modified) RK method for solving the IVP (1) is an one-step method defined by the equations

\[
y_1 = \psi_h(y_0) = y_0 + h \sum_{i=1}^{s} b_i f(t_0 + c_i h, Y_i), \quad Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} f(t_0 + c_j h, Y_j), \quad i = 1, \ldots, s, \tag{2}
\]

where the real parameters \( c_i \) and \( b_i, \ i = 1, \ldots, s, \) are known as the nodes and the weights of the method. In standard RK methods all \( y_1 = 1 \), but in EF methods the real parameters \( y_1 \) introduced by some authors (see [13, 23, 24]) allow us to satisfy some fitting requirements.

In general, the coefficients \( y_1, b_i \) and \( a_{ij} \) of an EFRK method may depend not only on the fitting functions but also on the step-size \( h \). Eq. (2) will be referred to as the final stage and Eqs. (3) as the internal stages of the RK method defined by the numerical flow map \( \psi_h \). Note that the final stage of this method is exact for constant functions \( u_0(t) = k \) that are critical points of (1). The s-stage RK method (2)–(3) is also specified by means of its Butcher’s tableau

\[
\begin{bmatrix}
1 & y_1 & a_{11} & \cdots & a_{1s} \\
0 & 0 & a_{21} & \cdots & a_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & a_{s1} & a_{s2} & \cdots & a_{ss}
\end{bmatrix}
\begin{bmatrix}
c \\
b^T
\end{bmatrix}
= \begin{bmatrix}
c_1 \\
\vdots \\
c_s
\end{bmatrix}
\]

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

A collocation approach for 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 [12, 19–21, 26]). This idea consists in to select the available parameters of the method (2)–(3) in order to be exact for a set of linearly independent scalar functions in \([t_0, t_0 + h]\)

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

and these methods are called in [19, 20] functionally fitted RK methods (FFRK methods). In the particular case in which \( \mathcal{F} \) contains exponential functions, these methods are called EFRK methods. The coefficients of an FFRK method (2)–(3) are determined by the solution of the following linear systems

\[
b^T u_0(t_0 e + hc) = h^{-1} (u_k(t_0 + h) - u_k(t_0)), \quad k = 1, \ldots, r, \tag{5}
\]

\[
A u_0^T (t_0 e + hc) = h^{-1} (u_k(t_0 e + hc) - y u_k(t_0)), \quad k = 1, \ldots, r, \tag{6}
\]

where \( e = (1, \ldots , 1)^T \in \mathbb{R}^r \), and for a vector \( v = (v_1, \ldots , v_r)^T \in \mathbb{R}^r \) and for an scalar function \( g \) we denote by \( g(v) \) the s-dimensional real vector \((g(v_1), \ldots , g(v_r))^T\).

In general, the coefficients \( b = (b_i) \) and \( A = (a_{ij}) \) defined by the linear systems (5)–(6) may depend on \( t_0, h \) and the basis \( \mathcal{F} \) but under some usual requirements on \( \mathcal{F} \) they are independent of \( t_0 \). In the following we will consider only class of functions \( \mathcal{F} \) such as the coefficients are independent of \( t_0 \).

In particular, when \( r = s \) the coefficients \( b = (b_i) \) and \( A = (a_{ij}) \) defined by the linear systems (5)–(6) are uniquely determined for all \( h > 0 \), if det \( u'_{k}(t_0 + c_i h)_{j=1}^{r} \neq 0, \) and these coefficients are \( h \)-dependent. As it has been proved by Ozawa [19], for any set of nonconfluent fixed nodes \( (c_i \neq c_j, i \neq j) \) this condition holds for \( h \) sufficiently small if the Wronskian matrix \( W(u'_1(t_0), \ldots , u'_r(t_0)) \) is nonsingular. Weaker requirements for det \( u'_{k}(t_0 + c_i h)_{j=1}^{r} \neq 0 \) have been given in [17].

In the most usual case exponential or trigonometric functions are considered 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 (5)–(6) reduce to

\[
b^T \cosh(cz) = \frac{\sinh(z)}{z}, \quad b^T \sinh(cz) = \frac{\cosh(z) - 1}{z}, \tag{7}
\]

\[
A \cosh(cz) = \frac{\sinh(cz)}{z}, \quad A \sinh(cz) = \frac{\cosh(cz) - y}{z}, \tag{8}
\]
Theorem 2.2. The coefficients of the exact flow map \( \psi \) are symmetric. The key for understanding symmetry is the concept of the adjoint method. In Hamiltonian systems \((m = 2d)\) the vector field \( f(t, y) \) is defined by means of a scalar function (Hamiltonian function) \( H = H(t, y) : \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R} \), so that \( f(t, y) = -J \nabla_y H(t, y) \). 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 \( \nabla_y H(t, y) \) 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
\[
y'(t) = -J \nabla_y H(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^{2d}.
\]
For each fixed \( t_0 \) the flow map of a Hamiltonian system (9) will be denoted by \( \phi_h : \mathbb{R}^d \to \mathbb{R}^d \) so that \( \phi_h(y_0) = y(t_0 + h; t_0, y_0) \) and it 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
\[
\phi_h'(y_0) J \phi_h'(y_0)^T = J, \quad \forall t_0 \in \mathbb{R} \text{ and } y_0 \in \mathbb{R}^{2d}.
\]

A desirable property of a numerical method \( \psi_h \) for solving the Hamiltonian system (9), in addition to providing an accurate approximation of the exact flow \( \phi_h \) for a reasonable range of step sizes \( h \in [0, h_0] \), is to preserve some qualitative properties of the original flow \( \phi_h \) such as the symplecticness given by (10).

**Definition 2.1.** A numerical method defined by the flow map \( \psi_h \) is called symplectic if for all Hamiltonian systems (9) it satisfies the condition
\[
\psi_h(y_0) J \psi_h'(y_0)^T = J, \quad \forall t_0 \in \mathbb{R}, \forall y_0 \text{ and } f = -J \nabla_y H \in \mathbb{R}^{2d}.
\]

One of the most known examples of symplectic methods is the \( s \)-stage RK Gauss methods which possess accuracy of order \( 2s \). The conditions for an RK method (2)–(3) to be symplectic have been obtained by Van de Vyver [6] and they are given in the following theorem.

**Theorem 2.2.** An RK method (2)–(3) for solving the Hamiltonian system (9) is symplectic if the following conditions are satisfied
\[
\bar{M} = b b^T - B A - A^T \bar{B} = 0, \quad \text{(12)}
\]
where \( \bar{B} = \text{diag}(b_i/\gamma_i) \in \mathbb{R}^{s \times s} \).

Note that all RK methods (2)–(3) preserve linear invariants but if in addition its coefficients satisfy conditions (12), then they also preserve quadratic invariants [8].

Other structural properties of the original flow \( \phi_h \) can also be preserved. For example, the original flow of the IVP (1) satisfies
\[
\phi_{-h} \circ \phi_h(y_0) = y_0, \quad \forall y_0 \in \mathbb{R}^m.
\]

and when the numerical flow \( \psi_h \) also satisfies the condition (13), the one-step method is called symmetric. In general, 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 Chap. 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 if it is symmetric. The key for understanding symplecticity is the concept of the adjoint method.

**Definition 2.3.** The adjoint method \( \psi_h^* \) of a numerical method \( \psi_h \) 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 RK methods (2)–(3) whose coefficients are \( h \)-dependent, as it is the case of FR methods, it is easy to see that the coefficients of \( \psi_h \) and \( \psi_h^* \) are related by
\[
c(h) = e - Sc^*(-h), \quad b(h) = Sh^*(-h),
\]
\[
y'(h) = Sy^*(-h), \quad A(h) = Sy^*(-h) b^T(h) - SA(-h) S.
\]

where \( S = (s_{ij}) \in \mathbb{R}^{s \times s} \) with \( s_{ij} = \begin{cases} 1, & \text{if } i + j = s + 1, \\ 0, & \text{otherwise}. \end{cases} \)

In the case of RK methods (2)–(3) whose coefficients are even functions of \( h \), as usually occurs in the construction of EFRK methods (see for example [6,8,24]), the symmetry conditions \( \psi_h^* = \psi_h \) are
\[
c(h) + Sc(h) = e, \quad b(h) = Sh(h),
\]
\[
y'(h) = Sy(h), \quad SA(h) + A(h) S = y(h) b^T(h).
\]
Here we will restrict our study to symmetric FFRK methods whose coefficients contain only even powers of $h$. In this case the symmetry conditions can be written in a more convenient form by

$$c(h) = \frac{1}{2} e - d(h), \quad A(h) = \frac{1}{2} \gamma(h)b^T(h) + A(h),$$  

where $d(h) = (d_1, \ldots, d_s)^T \in \mathbb{R}^s$ and $A(h) = (\lambda_{ij}) \in \mathbb{R}^{s \times s}$.

Now, the symmetry conditions (15) reduce to

$$d(h) + Sd(h) = 0, \quad b(h) = Sb(h), \quad \gamma(h) = Sy(h), \quad SA(h) + A(h)S = 0,$$  

with $c(h)$ and $A(h)$ defined by (16).

Therefore, for a symmetric FFRK method (2)–(3) whose coefficients are defined by (16), the symplecticness conditions (12) reduce to

$$\tilde{N}(h) \equiv \tilde{B}(h)A(h) + A(h)^T \tilde{B}(h) = 0,$$  

where $\tilde{N}(h) = (\tilde{\mu}_{ij}) \in \mathbb{R}^{s \times s}$ is a symmetric matrix.

In the case of symmetric FFRK methods whose coefficients $c(h)$ and $A(h)$ are defined by (16), the fitting conditions (5)–(6) with the change of variable $\tau = x - h/2$ can be written as

$$b^T u'_k (x_0 e - h d) = h^{-1} (u_k (x_0 + h/2) - u_k (x_0 - h/2)), \quad k = 1, \ldots, r,$$  

$$A u'_k (x_0 e - h d) = h^{-1} \left( u_k (x_0 + h/2) + u_k (x_0 - h/2) \right), \quad k = 1, \ldots, r,$$  

and for the reference set of functions $\mathcal{F}$, the fitting conditions (7)–(8) reduce to

$$\sum_{i=1}^k b_i \cosh(d_i z) = \frac{\sinh(z/2)}{z} \quad \text{if } s = 2k, \quad \sum_{i=1}^k b_i \cosh(d_i z) + \frac{b_{k+1}}{2} = \frac{\sinh(z/2)}{z} \quad \text{if } s = 2k + 1,$$  

$$A \cosh(dz) = -z^{-1} (\gamma \cosh(z/2) - \cosh(dz)).$$  

In general, the coefficients of an $s$-stage symmetric and symplectic FFRK method satisfying (17) and (18) are defined by the parameters

$$d = \begin{pmatrix} \theta_1 \\ \vdots \\ -\theta_2 \\ -\theta_1 \end{pmatrix}, \quad b = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_1 \end{pmatrix}, \quad \gamma = \begin{pmatrix} \gamma_1 \\ \vdots \\ \gamma_2 \\ \gamma_1 \end{pmatrix}, \quad A = \begin{pmatrix} 0 & \lambda_{12} & \lambda_{13} & \ldots & \lambda_{1s} \\ \lambda_{21} & 0 & \lambda_{23} & \ldots & \lambda_{2s} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ -\lambda_{s2s} & \ldots & -\lambda_{s23} & 0 & -\lambda_{s21} \end{pmatrix},$$  

together with the $s(s+1)/2$ symplecticness constraints

$$\tilde{\mu}_{ij} \equiv \frac{b_j}{y_i} \lambda_{ij} + \frac{b_i}{y_j} \lambda_{ji} = 0, \quad 1 \leq i \leq j \leq s.$$  

But for the centre-antisymmetry of the matrix $A$ (the coefficients $\lambda_{ij}$ are antisymmetric with respect to the centre of the matrix $A$), the coefficients $\tilde{\mu}_{ij}$ of the matrix $\tilde{N}(h)$ satisfy

$$\tilde{\mu}_{ii} = \tilde{\mu}_{i,s+1-\imath} = 0, \quad \tilde{\mu}_{ij} = -\tilde{\mu}_{s+1-\imath,s+1-\imath}, \quad 1 \leq i \neq j \leq s,$$  

and the symplecticness constraints (24) reduce to the \((\frac{s+1}{2})^2\) conditions:

$$\frac{b_i}{y_i} \lambda_{\imath j} + \frac{b_j}{y_j} \lambda_{\imath j} = 0, \quad i = 1, \ldots, \left\lfloor \frac{s+1}{2} \right\rfloor + 1, \quad j = \imath + 1, \ldots, s - \imath,$$  

where $[x]$ is the integer part of $x \in \mathbb{R}$. Taking into account that the matrix $A$ and the vector $\gamma$ defined in (23) have $s(s-1)/2$ and $\left\lfloor \frac{s+1}{2} \right\rfloor$ free parameters, respectively, then an $s$-stage symmetric and symplectic FFRK method has $\left\lfloor \frac{s+1}{2} \right\rfloor^2$ free parameters in order to fitting the internal stages. In addition, $b$ and $d$ have $\left\lfloor \frac{s+1}{2} \right\rfloor$ free parameters each vector in order to fitting the final stage.

On the other hand, for an $s$-stage symmetric FFRK method the fitting conditions (19)–(20) are equivalent to

$$\hat{L}_i [u(x_0)] = 0, \quad i = 0, 1, \ldots, s,$$  

for all $u \in \mathcal{F}$, where the linear operators $\hat{L}_i$ are defined by

$$\hat{L}_0 [u(x_0)] = u(x_0 + h/2) - u(x_0 - h/2) - h \sum_{i=1}^s b_i u'(x_0 - d_i h),$$  

$$\hat{L}_i [u(x_0)] = u(x_0 - d_i h) - \frac{\gamma_i}{2} \left( u(x_0 + h/2) + u(x_0 - h/2) \right) - h \sum_{j=1}^s \frac{\lambda_{ij}}{2} u'(x_0 - d_i h), \quad i = 1, \ldots, s.$$  

Considering the functional spaces
\[ \mathcal{H}_1 = \{ u : \mathbb{R} \to \mathbb{R} \text{ sufficiently smooth | } u \text{ is odd and } u' \text{ is even} \}, \]
\[ \mathcal{H}_2 = \{ u : \mathbb{R} \to \mathbb{R} \text{ sufficiently smooth | } u \text{ is even and } u' \text{ is odd} \}, \]
and \( x_0 = 0 \) for simplicity, we may write the following results:

**Lemma 2.4.** The linear operators \( \hat{L}_i, i = 1, \ldots, s \), associated to the internal stages of a symmetric FFRK method satisfy
\[ \hat{L}_i[u(0)] = (-1)^q \hat{L}_{s+1-i}[u(0)], \quad \text{if } u \in \mathcal{H}_q, \quad q = 1, 2, \quad i = 1, \ldots, [s/2]. \]  
(32)

In addition, if the number of stages is odd \( (s = 2k + 1) \), the central operator satisfies
\[ \hat{L}_{k+1}[u(0)] = \begin{cases} 0, & \text{if } u \in \mathcal{H}_1, \\ u(0) - \gamma_{k+1} u'(0) + 2h \sum_{j=1}^{k} \lambda_{ij} u'(\theta_j h), & \text{if } u \in \mathcal{H}_2. \end{cases} \]
(33)

**Proof.** According to the coefficients (23) of a symmetric FFRK method the linear operators \( \hat{L}_i[u(0)] \) and \( \hat{L}_{s+1-i}[u(0)] \) can be written as \( (k = [s/2]) \)
\[ \hat{L}_i[u(0)] = u(-\theta h) - \frac{\gamma_i}{2} (u(h/2) + u(-h/2)) - h \left( \sum_{j=1}^{k} \lambda_{ij} u'(-\theta_j h) + \lambda_{i,k+1} u'(0) + \sum_{j=1}^{k} \lambda_{i,s+1-j} u'(-\theta_j h) \right), \]
\[ \hat{L}_{s+1-i}[u(0)] = u(\theta h) - \frac{\gamma_i}{2} (u(h/2) + u(-h/2)) + h \left( \sum_{j=1}^{k} \lambda_{ij} u'(\theta_j h) + \lambda_{i,k+1} u'(0) + \sum_{j=1}^{k} \lambda_{i,s+1-j} u'(\theta_j h) \right), \]
where \( \lambda_{i,k+1} = 0 \) if \( s \) is even.

Clearly if \( u \in \mathcal{H}_q \) \( (q = 1, 2) \), then \( \hat{L}_i[u(0)] = (-1)^q \hat{L}_{s+1-i}[u(0)] \), \( i = 1, \ldots, [s/2] \).

When the number of stages \( s \) is odd \( (s = 2k + 1) \), the central operator can be written as
\[ \hat{L}_{k+1}[u(0)] = u(0) - \frac{\gamma_{k+1}}{2} (u(h/2) + u(-h/2)) - h \sum_{j=1}^{k} \lambda_{ij} (u'(-\theta_j h) - u'(\theta_j h)). \]

If \( u \in \mathcal{H}_1 \), then \( \hat{L}_{k+1}[u(0)] = 0. \)
If \( u \in \mathcal{H}_2 \), then \( \hat{L}_{k+1}[u(0)] = u(0) - \gamma_{k+1} u'(0) + 2h \sum_{j=1}^{k} \lambda_{ij} u'(\theta_j h). \)
\( \square \)

**Lemma 2.5.** The final stage of a symmetric FFRK method is exact for all function \( u \in \mathcal{H}_2 \), whereas it is exact for all function \( u \in \mathcal{H}_1 \), \( \hat{L}_0[u(0)] = 0 \), if the following condition is satisfied
\[ \sum_{l=1}^{[s/2]} b_l u'(\theta_l h) + \frac{b_{[s/2]+1}}{2} u'(0) = \frac{u(h/2)}{h}, \]
(34)
where \( b_{[s/2]+1} = 0 \) when \( s \) is even.

**Proof.** The linear operator \( \hat{L}_0 \) associated to the final stage of a symmetric FFRK method can be written as \( (k = [s/2]) \)
\[ \hat{L}_0[u(0)] = u(h/2) - u(-h/2) - h \left( \sum_{i=1}^{k} b_i (u'(\theta_i h) + u'(-\theta_i h)) + b_{k+1} u'(0) \right), \]
where \( b_{k+1} = 0 \) if \( s \) is even.

If \( u \in \mathcal{H}_2 \), then \( \hat{L}_0[u(0)] = 0. \)
If \( u \in \mathcal{H}_1 \), then \( \hat{L}_0[u(0)] = 2u(h/2) - 2h \sum_{l=1}^{k} b_l u'(\theta_l h) + \frac{b_{k+1}}{2} u'(0) \), and the condition (34) follows from \( \hat{L}_0[u(0)] = 0. \)
\( \square \)

**Remarks.** (i) In the construction of most FF methods the basis of the linear fitting space \( \mathcal{F} \) is constituted mainly by functions of the types
\[ t^l, \quad \cos(j \omega t), \quad \sin(j \omega t), \quad \cosh(j \lambda t), \quad \sinh(j \lambda t), \quad j = 1, \ldots, k, \]
and products of them, and all these functions are included in the functional space \( \mathcal{H}_1 \cup \mathcal{H}_2 \). Note that these functions are the basis of solutions of a linear differential equation of the form
\[ L[y(t)] = \left( D^k \sum_{j=1}^{r} (D^2 + \alpha_j D + \beta_j) \right) y(t) = 0. \]
(ii) In the case of analytic functions \( u(x) \), if \( u(x) \) is odd we have
\[ u(x) = \sum_{n \geq 0} c_n x^{2n+1} \quad \Rightarrow \quad u'(x) = \sum_{n \geq 0} (2n+1) c_n x^{2n}, \]
Corollary 2.6. For an s-stage symmetric FFRK method fitted to a linear space $F \subset \mathcal{H}_1 \cup \mathcal{H}_2$, the fitting conditions (27) reduce to

$$\begin{align*}
\hat{L}_0[u(0)] &= 0, \quad \text{if } u \in \mathcal{H}_1 \cap F, \\
\hat{L}_i[u(0)] &= 0, \quad i = 1, \ldots, [s/2], \quad \forall u \in F, \\
\hat{L}_{[s/2]+1}[u(0)] &= 0, \quad \text{if } u \in \mathcal{H}_2 \cap F \text{ and } s \text{ odd}.
\end{align*}$$

Proof. The conclusion follows from Lemmas 2.4 and 2.5. ☐

Until now, symmetric and symplectic EFRK methods with two and three stages and orders four and six have been constructed by several authors (see [6,8–10]). In the next section we try to extend the construction of symmetric and symplectic EFRK methods (SEFRK methods) to the case of four stages and high order of accuracy.

3. Construction of the SEFRK integrators

Here we study the construction of symmetric and symplectic EFRK methods (SEFRK methods) with $s = 4$ stages whose coefficients are even functions of $h$. Our intention is that the new SE 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 symmetry of the coefficients (23) and the symplecticness constraints (26) it follows that

$$d = \begin{pmatrix} \theta_1 \\ \theta_2 \\ -\theta_2 \\ -\theta_1 \end{pmatrix}, \quad b = \begin{pmatrix} b_1 \\ b_2 \\ b_2 \\ b_1 \end{pmatrix}, \quad \gamma = \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_2 \\ \gamma_1 \end{pmatrix}, \quad A = \begin{pmatrix} 0 & \alpha_2 & \alpha_3 & \alpha_4 \\ \beta_1 & 0 & \beta_3 & \beta_4 \\ -\beta_4 & -\beta_3 & 0 & -\beta_1 \\ -\alpha_4 & -\alpha_3 & -\alpha_2 & 0 \end{pmatrix}.$$

and the four-stage RK methods are defined by the Butcher’s tableau

$$\begin{array}{c|cccc}
1/2 - \theta_1 & \gamma_1 & \gamma_1 b_1/2 & \gamma_1 b_2/2 + \alpha_2 & \gamma_1 b_1/2 + \alpha_4 \\
1/2 - \theta_2 & \gamma_2 & \gamma_2 b_1/2 + \beta_1 & \gamma_2 b_2/2 + \beta_3 & \gamma_2 b_1/2 + \beta_4 \\
1/2 + \theta_2 & \gamma_2 & \gamma_2 b_1/2 - \beta_4 & \gamma_2 b_2/2 - \beta_3 & \gamma_2 b_1/2 - \beta_1 \\
1/2 + \theta_1 & \gamma_1 & \gamma_1 b_1/2 - \alpha_4 & \gamma_1 b_2/2 - \alpha_3 & \gamma_1 b_1/2 - \alpha_2 \\
\hline
& b_1 & b_2 & b_2 & b_1
\end{array}$$

The EF conditions (21)–(22) with $s = 4$ give one condition for the weights $b_j$

$$b_1 \cosh(\theta_1 z) + b_2 \cosh(\theta_2 z) = \frac{\sinh(z/2)}{z},$$

and eight conditions for the rest of the coefficients, but for the conditions (36) of Corollary 2.6, they reduce to four conditions

$$\begin{align*}
\alpha_4 \cosh(\theta_1 z) + (\alpha_2 + \alpha_3) \cosh(\theta_2 z) &= -\frac{\sinh(\theta_1 z)}{z}, \\
\alpha_4 \sinh(\theta_1 z) + (\alpha_1 - \alpha_2) \sinh(\theta_2 z) &= \frac{\cosh(\theta_1 z) - \gamma_1 \cosh(z/2)}{z}, \\
(\beta_1 + \beta_4) \cosh(\theta_1 z) + \beta_3 \cosh(\theta_2 z) &= -\frac{\sinh(\theta_2 z)}{z}, \\
(\beta_4 - \beta_1) \sinh(\theta_1 z) + \beta_3 \sinh(\theta_2 z) &= \frac{\cosh(\theta_2 z) - \gamma_2 \cosh(z/2)}{z}.
\end{align*}$$

and the coefficients $\alpha_2$, $\alpha_4$, $\beta_1$ and $\beta_3$ can be computed in terms of the rest of the coefficients obtaining

$$\begin{align*}
\alpha_2 &= \frac{\gamma_1 \cosh(z/2) \cosh(\theta_1 z) - \cosh(2\theta_1 z) + z\alpha_3 \sinh((\theta_2 - \theta_1) z)}{z \sinh((\theta_1 + \theta_2) z)}, \\
\alpha_4 &= \frac{\cosh((\theta_1 - \theta_2) z) - \cosh(\theta_2 z)(\gamma_1 \cosh(z/2) + 2z\alpha_3 \sinh(\theta_2 z))}{z \sinh((\theta_1 + \theta_2) z)}.
\end{align*}$$
\[ \begin{align*}
\beta_1 &= \frac{y_2 \cosh(z/2) \cosh(\theta_2 z) + z\beta_4 \sinh((\theta_1 - \theta_2)z) - \cosh(2\theta_2 z)}{z \sinh((\theta_1 + \theta_2)z)}, \\
\beta_3 &= \frac{\cosh((\theta_1 - \theta_2)z) - z\beta_4 \sinh(2\theta_1 z) - y_2 \cosh(z/2) \cosh(\theta_1 z)}{z \sinh((\theta_1 + \theta_2)z)}.
\end{align*} \tag{43} \]

3.1. SEFRK integrator 1 (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

\[ b^T e = 1, \quad b^T c = \frac{1}{2}, \tag{44} \]

but for Lemma 2.5, they reduce to

\[ b_1 + b_2 = \frac{1}{2}, \tag{45} \]

and the weights \( b_1 \) and \( b_2 \) can be computed from Eqs. (41) and (45) obtaining

\[ b_1 = \frac{-z \cosh(\theta_2 z) - 2 \sinh(z/2)}{2z(\cosh(\theta_1 z) - \cosh(\theta_2 z))}, \quad b_2 = \frac{z \cosh(\theta_2 z) - 2 \sinh(z/2)}{2z(\cosh(\theta_1 z) - \cosh(\theta_2 z))}. \tag{46} \]

If the symplecticness conditions (39) are imposed, the parameters \( \gamma_1 \) and \( \beta_4 \) are determined by

\[ \begin{align*}
\gamma_1 &= \frac{\gamma_2 \cosh(2\theta_1 z)(z \cosh(\theta_2 z) - 2 \sinh(z/2))}{(z \sinh(\theta_1 z) - \cosh(\theta_1 z))}, \\
\beta_4 &= \frac{\alpha_2 \gamma_2(z \cosh(\theta_2 z) - 2 \sinh(z/2))}{\gamma_1 (z \sinh(z/2) - z \cosh(\theta_1 z)).}
\end{align*} \tag{47} \]

The coefficients (43), (46) and (47) define a family of EFRK methods (40) which are symmetric, symplectic and they preserve linear and quadratic invariants for all \( \gamma_2, \alpha_3, \theta_1 \) and \( \theta_2 \in \mathbb{R} \). In particular, by choosing \( \gamma_2 = 1 \), the parameters \( \theta_i \) such that the nodes \( c_i \) are the Gauss nodes:

\[ \theta_1 = \frac{1}{2} \sqrt{15 + 2\sqrt{30}}, \quad \theta_2 = \frac{1}{2} \sqrt{15 - 2\sqrt{30}}, \]

and the parameter \( \alpha_3 \) such that \( \alpha_{13} = \gamma_1 \theta_2/2 + \alpha_3 \) is the coefficient of the standard four-stage RK Gauss method:

\[ \alpha_{13} = \frac{30\sqrt{90} - 12\sqrt{30} + 108\sqrt{75} - 10\sqrt{30} - 5(12\sqrt{75} + 10\sqrt{30} - 6\sqrt{90} + 12\sqrt{30} + 7(9\sqrt{2} + 3\sqrt{7} + \sqrt{75} - \sqrt{210}))}{360(-\sqrt{2} - 4\sqrt{7} + \sqrt{210})}, \]

we obtain an SEFRK method with fixed nodes which will be denoted as SEFRK1(F), and when \( z = 0 \) it reduces to the standard four-stage RK Gauss method.

We note that the internal stages of the new SEFRK1(F) integrator are exact for the basis \( \exp(\lambda t), \exp(-\lambda t) \), whereas the final stage is exact for the basis \( \{1, t, t^2\} \). In the trigonometric case \( \lambda = \omega \in \mathbb{R} \) we have \( z = iv \) with \( v = oh \), and the coefficients (43), (46) and (47) emerge having in mind the relations \( \cosh(iv) = \cos(v) \) and \( \sinh(iv) = i \sin(v) \). In this case, the internal stages are exact for the basis \( \{\cos(\omega t), \sin(\omega t)\} \), whereas the final stage is exact for the basis \( \{1, t, t^2, \cos(\omega t), \sin(\omega t)\} \).

3.2. SEFRK integrator 2 (variable nodes)

Next we consider the case of four-stage SEFRK methods (40) such that their internal stages are also exact for the function \( u_0(t) = 1 \) which implies \( \gamma = e = (1, 1, 1, 1)^T \). In this case, the EF conditions (41)-(42) and (45) give the coefficients (43) and (46) with \( \gamma_1 = \gamma_2 = 1 \). If in addition the symplecticness conditions (39) are imposed, the parameters \( \beta_4 \) and \( \theta_1 \) are determined by

\[ \begin{align*}
\theta_1 &= \frac{1}{z} \arccosh \left( \frac{z - 4 \cosh(\theta_2 z) \sinh(z/2) + \sinh(z)}{-2z \cosh(\theta_2 z) + 4 \sinh(z/2)} \right), \\
\beta_4 &= \frac{\alpha_3 (z \cosh(\theta_2 z) - 2 \sinh(z/2))}{(2 \sinh(z/2) - z \cosh(\theta_1 z))}. \tag{48} \end{align*} \]

So, we have obtained a family of SEFRK integrators with variable nodes for all \( \alpha_3 \) and \( \theta_2 \in \mathbb{R} \). In particular, by choosing

\[ \theta_2 = \frac{1}{2} \sqrt{15 - 2\sqrt{30}}, \]

and the parameter \( \alpha_3 \) as in the method SEFRK1(F) (such that \( \alpha_{13} \) is the coefficient of the standard four-stage RK Gauss method) we obtain an integrator with variable nodes which will be denoted as SEFRK2(V). The new integrator is also symmetric, symplectic, it preserves linear and quadratic invariants, and when \( z = 0 \) it reduces to the standard four-stage RK Gauss method.

We note that the internal stages of the new SEFRK2(V) integrator are exact for the basis \( \{1, \exp(\lambda t), \exp(-\lambda t)\} \). In the trigonometric case \( \lambda = \omega \in \mathbb{R}, z = iv, v = oh \) the coefficients of the method emerge having in mind the relations \( \cosh(iv) = \cos(v) \) and \( \sinh(iv) = i \sin(v) \), and the internal stages are exact for the basis \( \{1, \cos(\omega t), \sin(\omega t)\} \).
3.3. SEFRK integrator 3 (fixed nodes)

Finally we consider the case of four-stage SEFRK methods (40) such that their internal stages are also exact for the function $u_0(t) = 1$, i.e. $y = e = (1, 1, 1, 1)^T$, and the final stage is also exact for the reference set of functions $\{\exp(2\lambda t), \exp(-2\lambda t)\}$, i.e., the following conditions are also satisfied

$$b^T \cosh(2cz) = \frac{\sinh(2z)}{2z}, \quad b^T \sinh(2cz) = \frac{\cosh(2z) - 1}{2z}. \quad (49)$$

By Lemma 2.5, the conditions (49) reduce to

$$b_1 \cosh(2\theta_1 z) + b_2 \cosh(2\theta_2 z) = \frac{\sinh(z)}{2z}, \quad (50)$$

and the weights $b_1$ and $b_2$ can be computed from Eqs. (41) and (50) obtaining

$$b_1 = \frac{2 \cosh(2\theta_1 z) \sinh(z/2) - \cosh(\theta_2 z) \sinh(\theta_1 z)}{2z \left( \cosh(2\theta_1 z) \sinh(\theta_2 z) - \cosh(\theta_1 z) \cosh(2\theta_2 z) \right)},$$

$$b_2 = \frac{2 \cosh(2\theta_1 z) \sinh(\theta_2 z) - \cosh(\theta_1 z) \cosh(2\theta_2 z)}{2z \left( \cosh(2\theta_1 z) \sinh(\theta_2 z) - \cosh(\theta_1 z) \cosh(2\theta_2 z) \right)}. \quad (51)$$

In this case the two symplecticness conditions (39) reduce to one condition and the parameter $\beta_4$ is determined by

$$\beta_4 = \frac{\alpha_3 (\cosh(\theta_2 z) \sinh(\theta_1 z) - 2 \cosh(2\theta_2 z) \sinh(z/2))}{2 \cosh(2\theta_1 z) \sinh(z/2) - \cosh(\theta_1 z) \sinh(\theta_2 z)}. \quad (52)$$

So, we have obtained a family of SEFRK integrators for all $\alpha_3$, $\theta_1$ and $\theta_2 \in \mathbb{R}$. In particular, by choosing

$$\theta_1 = \frac{1}{2} \sqrt{15 + 2\sqrt{30}}/35, \quad \theta_2 = \frac{1}{2} \sqrt{15 - 2\sqrt{30}}/35,$$

and the parameter $\alpha_3$ as in the previous methods (such that $\alpha_{13}$ is the coefficient of the standard four-stage RK Gauss method) we obtain an integrator with fixed nodes which will be denoted as SEFRK3(F). The new integrator is also symmetric, symplectic, it preserves linear and quadratic invariants, and when $z = 0$ it reduces to the standard four-stage RK Gauss method.

We note that the internal stages of the new SEFRK3(F) integrator are exact for the basis $(1, \exp(\lambda t), \exp(-\lambda t))$, whereas the final stage is exact for the basis $(1, \exp(\lambda t), \exp(-\lambda t), \exp(2\lambda t), \exp(-2\lambda t))$. In the trigonometric case $(\lambda = \omega t, \omega \in \mathbb{R}, z = iv, \nu = \omega \nu)$ the coefficients (43), (51) and (52) emerge having in mind the relations $\cosh(iv) = \cos(\nu)$ and $\sinh(iv) = i \sin(\nu)$. In this case, the internal stages are exact for the basis $(1, \cos(\omega t), \sin(\omega t))$, whereas the final stage is exact for the basis $(1, \cos(\omega t), \sin(\omega t), \cos(2\omega t), \sin(2\omega t))$.

We also note that the new methods SEFRK1(F), SEFRK2(V) and SEFRK3(F) are not collocation methods, in sharp contrast with their classical companion (the standard four-stage RK Gauss method). Moreover, for small values of $|z|$ the above formulas for the coefficients of the methods SEFRK1(F), SEFRK2(V) and SEFRK3(F) are subject to heavy cancellations, and when $|z| < 0.1$ series expansions for these coefficients must be used.

Finally, taking into account the power series expansion of the coefficients $c$, $y$, $b$ and $A$ we check some conditions satisfied by the new methods SEFRK1(F), SEFRK2(V) and SEFRK3(F) which will be necessary for the study of their algebraic order (see Section 4).

$$y - e = O(z^8), \quad b^T (y - e) = O(z^8), \quad b^T A(y - e) = O(z^8), \quad (53)$$

$$A e - c = O(z^4), \quad b^T e - 1 = O(z^4), \quad b^T c - \frac{1}{2} = O(z^4), \quad (54)$$

$$\begin{align*}
A c - \frac{1}{2} c^2 &= O(z^4), \\
b^T c^2 - \frac{1}{3} &= O(z^6), \\
b^T c^3 - \frac{1}{4} &= O(z^6), \\
A c^2 - \frac{1}{3} c^3 &= O(z^4), \\
b^T c^4 - \frac{1}{5} &= O(z^4), \\
b^T c^5 - \frac{1}{6} &= O(z^4), \\
A c^3 - \frac{1}{4} c^4 &= O(z^4), \\
b^T c^6 - \frac{1}{7} &= O(z^4), \\
b^T c^7 - \frac{1}{8} &= O(z^4).
\end{align*} \quad (55)$$

$$\begin{align*}
b^T (A e - c) &= O(z^8), \\
b^T \left( A e - \frac{1}{2} c^2 \right) &= O(z^8), \\
b^T \left( A c - \frac{1}{2} c^2 \right) &= O(z^8), \\
b^T A (A e - c) &= O(z^8), \\
b^T A \left( A e - \frac{1}{2} c^2 \right) &= O(z^8).
\end{align*} \quad (56)$$
4. Algebraic order of the SEFRK integrators

In this section we study the algebraic order of accuracy of the new SEFRK methods derived in previous section. We start with the standard definition of order:

**Definition 4.1.** A modified RK method (2)–(3) has algebraic order \( p \) if for all sufficiently smooth IVP (1) it satisfies

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

(57)

In addition, (2)–(3) has stage order \( q \) if

\[
y_1 - y(t_0 + h) = O(h^{q+1}), \quad Y - y(\text{et}_0 + ch) = O(h^{q+1}), \quad h \to 0,
\]

(58)

where \( Y = (Y_1, \ldots, Y_s)^T \).

Having in mind that the coefficients of an EFRK method may depend on the step-size \( h \), we introduce the quantities \( B_k \in \mathbb{R} \) and \( C_k \in \mathbb{R}^s \) typical in standard RK methods

\[
B_k = b^T e^{k-1} - \frac{1}{k}, \quad C_k = A e^{k-1} - \frac{1}{k}e^k, \quad k \geq 1,
\]

(59)

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

For an RK method (2)–(3), the exact solution of the IVP (1) satisfies

\[
y(t_0 + h) = \psi_h(y_0) = y(t_0) + hB^T \otimes \gamma' (\text{et}_0 + ch) - r(h),
\]

(60)

\[
y(\text{et}_0 + ch) = \gamma' \otimes y(\text{et}_0) + hA \otimes \gamma' (\text{et}_0 + ch) - R(h),
\]

(61)

where

\[
r(h) = \sum_{k \geq 1} \frac{h^k}{(k-1)!} B_k y^{(k)}(t_0),
\]

(62)

\[
R(h) = (\gamma - e) \otimes y(t_0) + \sum_{k \geq 1} \frac{h^k}{(k-1)!} C_k \otimes y^{(k)}(t_0).
\]

(63)

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

\[
T(h) = Y - y(\text{et}_0 + ch) = hA \otimes (f(\text{et}_0 + ch, Y) - f(\text{et}_0 + ch, y(\text{et}_0 + ch))) + R(h),
\]

(64)

\[
\tau(h) = \psi_h(y_0) - \phi_h(y_0) = hB \otimes (f(\text{et}_0 + ch, Y) - f(\text{et}_0 + ch, y(\text{et}_0 + ch))) + r(h),
\]

(65)

where \( T(h) = (\tau_1(h), \ldots, \tau_s(h))^T \) and \( \tau_i(h) = Y_i - y(t_0 + c_i h), \quad i = 1, \ldots, s \).

In a previous paper [10] we have proved that if the following conditions are satisfied

\[
y - e = O(h^{q+1}), \quad B_k = O(h^{q+1-k}), \quad C_k = O(h^{q+1-k}), \quad k = 1, \ldots, q,
\]

(66)

then the method possesses stage order at least \( q \) (\( T(h) = O(h^{q+1}) \) and \( \tau(h) = O(h^{q+1}) \)).

In view of (53)–(54), the methods SEFRK1(F), SEFRK2(V) and SEFRK3(F) satisfy conditions (66) with \( q = 4 \) and the following result can be written.

**Property 4.2.** The methods SEFRK1(F), SEFRK2(V) and SEFRK3(F) possess stage order \( q = 4 \).

Next we analyze the possibility of superconvergence (i.e., the algebraic order is greater than the stage order \( q \)) for the methods SEFRK1(F), SEFRK2(V) and SEFRK3(F). Assuming that conditions (66) are satisfied and \( \tau_i(h) = O(h^{q+1}), \quad i = 1, \ldots, s \), from (65) and the smoothness of \( f \) the local truncation error for the final stage can be written as

\[
\tau(h) = h \sum_{i=1}^{s} b_i f(t_0 + c_i h) \tau_i(h) + r(h) + O(h^{2q+3}).
\]

(67)

where \( f(t_0 + c_i h) = D_{c_i} f(t_0 + c_i h, y(t_0 + c_i h)) \).

From (64) and the smoothness of \( f \)

\[
\tau_i(h) = h \sum_{j=1}^{s} a_{ij} f(t_0 + c_j h) \tau_j(h) + R_i(h) + O(h^{2q+3}), \quad i = 1, \ldots, s,
\]

and Eq. (67) can be written as

\[
\tau(h) = h^2 \sum_{i,j=1}^{s} b_{ij} a_{ij} f(t_0 + c_i h) f(t_0 + c_j h) \tau_j(h) + h \sum_{i=1}^{s} b_i f(t_0 + c_i h) R_i(h) + r(h) + O(h^{2q+3}).
\]

(68)
Iterating again the process with $\tau_j(h)$ and taking into account that $J_f(t_0 + c_j h) = J_f(t_0) + O(h)$, Eq. (68) can be written as

$$
\tau(h) = h^2 (J_f(t_0))^3 (b^T A^2 \otimes T(h)) + h^2 (J_f(t_0))^2 D_2(h) + h (J_f(t_0) + O(h)) D_1(h) + r(h) + O(h^{q+4}),
$$

and

$$
D_1(h) = b^T \otimes R(h) = b^T (y - e) \otimes y(t_0) + \sum_{k \geq 1} \frac{h^k}{(k-1)!} b^T C_k \otimes y^{(k)}(t_0),
$$

$$
D_2(h) = b^T A \otimes R(h) = b^T A(y - e) \otimes y(t_0) + \sum_{k \geq 1} \frac{h^k}{(k-1)!} b^T A C_k \otimes y^{(k)}(t_0).
$$

From these expansions it follows that

$$
D_1(h) = O(h^{r+1}) \quad \text{iff} \quad b^T (y - e) = O(h^{r+1}), \quad b^T C_k = O(h^{r+1-k}), \quad k = 1, \ldots, r,
$$

$$
D_2(h) = O(h^{q+1}) \quad \text{iff} \quad b^T A(y - e) = O(h^{q+1}), \quad b^T A C_k = O(h^{q+1-k}), \quad k = 1, \ldots, q,
$$

$$
r(h) = O(h^{q+1}) \quad \text{iff} \quad B_k = O(h^{q+1-k}), \quad k = 1, \ldots, r.
$$

Thus, the local truncation error at the final stage behaves as $\tau(h) = O(h^{p+1})$, where

$$
p = \min[q + 3, r + 2, r + 1, \sigma].
$$

In view of (53)–(56), the methods SEFRK1(F), SEFRK2(V) and SEFRK3(F) satisfy (70) with $q = 4$, $r = 6$, $r = 7$ and $\sigma = 8$, and therefore the three methods possess at least order $p = 7$. But the three methods are symmetric by construction, and therefore they have algebraic order 8.

In conclusion we may write the following result:

**Theorem 4.3.** The new symplectic and symmetric methods SEFRK1(F), SEFRK2(V) and SEFRK3(F) have stage order 4 and algebraic order 8 as the standard four-stage RK Gauss method.

### 5. Numerical experiments

In this section we present some numerical experiments to test the effectiveness of the new SEFRK integrators derived in Section 3 when they are applied to the numerical solution of several oscillatory Hamiltonian systems. The new methods have been compared with the standard four-stage eighth-order Gauss method given in [2] denoted as Gauss4, and with the four-stage, eighth-order variable-nodes integrator STFRK4 derived in [27]. It is the symplectic, symmetric and trigonometrically fitted to $1, \cos(\omega t), \sin(\omega t), \ldots, \cos(4\omega t), \sin(4\omega t))$. 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 and 3 we show the decimal logarithm of the maximum global error (log_{10}(err)) versus the number of steps required by each code in logarithmic scale (log_{10}(nsteps)). In Figs. 2 and 4 we plot the decimal logarithm of the maximum error in the invariant Hamiltonian versus the number of steps required by each code in logarithmic scale (log_{10}(nsteps)).

In the implementation of the EF Gauss type methods, due to the implicitness of the stage equations (3), we have used a modified Newton method to solve this nonlinear system. The numerical experiments have been carried out on a PC Intel Pentium computer. The algorithm has been implemented in Python by using the mpmath library with a precision of thirty two significant digits.

**Problem 1.** A perturbed Kepler’s problem defined by the Hamiltonian function

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

with the initial conditions

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

where $\epsilon$ is a small positive parameter. The exact solution of this IVP is given by

$$
q_1(t) = \cos(t + \epsilon t), \quad q_2(t) = \sin(t + \epsilon t), \quad p_1(t) = q_1(t), \quad i = 1, 2.
$$

The numerical results presented in Fig. 1 and Fig. 2 have been computed with the integration steps $h = 1/2^m, m = 0, 1, \ldots, 5$. We take the parameter values $\epsilon = 10^{-3}, \lambda = i\omega$ with $\omega = 1$ and the problem is integrated up to $t_{\text{end}} = 1000$.

**Problem 2.** A two-dimensional nonlinear oscillatory Hamiltonian system

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

with the initial conditions

$$
q_1(0) = \frac{1}{2}, \quad q_2(0) = \frac{1}{2}, \quad p_1(0) = -\frac{1}{\sqrt{2}} - \frac{\omega}{2}, \quad p_2(0) = \frac{1}{\sqrt{2}} - \frac{\omega}{2}.
$$
where \( \alpha = \omega^2 + k^2 + 1 \), \( \beta = \omega^2 - k^2 - 1 \) and the parameters \( \omega > 0 \), \( 0 \leq k < 1 \). 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, given by

\[
q(t) = \frac{1}{\sqrt{2}} \left( \frac{\cos\left(\frac{\pi}{4} + \omega t\right) - \text{sn}(t; k)}{\cos\left(\frac{\pi}{4} + \omega t\right) + \text{sn}(t; k)} \right), \quad p(t) = q'(t),
\]

is a linear combination of periodic functions defined by 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. 3 and Fig. 4 have been computed with the integration steps \( h = 1/(30 \times 2^m) \), \( m = 0, 1, \ldots, 5 \), and \( \lambda = i\omega \).
From the results of the numerical experiments it follows that for the oscillatory Hamiltonian systems under consideration the accuracy of the exponentially and trigonometrically fitted methods is in general superior to the standard ones of the same order and with the same qualitative properties for Hamiltonian systems. In general, the new exponentially fitted methods SEFRK1(F), SEFRK2(V) and SEFRK3(F) are slightly superior to the trigonometrically fitted integrator STFRK4. In particular, the method SEFRK2(V) (variable nodes) results to be the most accurate in Problem 2 whereas in Problem 1 we observe little differences with the methods SEFRK1(F) and SEFRK3(F) (fixed nodes). 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 2), the EF methods whose internal stages are exact for the basis \(\langle 1, \exp(\lambda t), \exp(-\lambda t) \rangle\) and the final stage is exact for the basis \(\langle 1, t, t^2, \exp(\lambda t), \exp(-\lambda t) \rangle\) turn out to be more accurate than those EF methods which are exact for other basis. In general, the Hamiltonian is well preserved by all Gauss type methods. It is remarkable that in Problem 2, the classical nonfitted Gauss method has
the worst behavior for the global error, but it is by far the method that preserves better the Hamiltonian. The new methods appear to be well balanced when considering global and Hamiltonian errors.

6. Conclusions

In this paper an analysis on the construction of symmetric and symplectic EFRK methods of high order is presented. This analysis 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, and it reveals that for symmetric EFRK methods there is a significant reduction of the fitting conditions. Three new four-stage eighth-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 \( \lambda = 0 \) \((\zeta = 0)\), the new integrators reduce to the standard four-stage eighth-order Gauss integrator. It is shown that such fitted methods are a reliable alternative to the standard four-stage eighth-order Gauss integrator and the trigonometrically fitted four-stage eighth-order STFRK4 code derived in [27] 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 Hamiltonian systems show that the new methods improve the results obtained with other (standard or trigonometrically fitted) symplectic integrators.

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References