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Fourth-order symplectic exponentially-fitted modified Runge-Kutta methods of the Gauss type: a review

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Dedicated to Manuel Calvo for his 65th birthday

Abstract

The construction of symmetric and symplectic exponentially-fitted Runge-Kutta methods for the numerical integration of Hamiltonian systems with oscillatory solutions is reconsidered. In previous papers fourth-order and sixth-order symplectic exponentially-fitted integrators of Gauss type, either with fixed or variable nodes, have been derived. In this paper new fourth-order integrators are constructed by making use of the six-step procedure of Ixaru and Vanden Berghe (*Exponential fitting*, Kluwer Academic Publishers, 2004). Numerical experiments for some oscillatory problems are presented and compared to the results obtained by previous methods.

MSC: 65L05,65L06

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1 Introduction

The construction of Runge-Kutta (RK) methods for the numerical solution of ODEs, which have periodic or oscillating solutions has been considered extensively in the literature [1]-[12]. In this approach the available information on the solutions is used in order to derive more accurate and/or efficient algorithms than the general purpose algorithms for such type of problems. In [13] a particular six-step flow chart is proposed by which specific exponentially-fitted algorithms can be constructed. Up to now this procedure has not yet been applied in all its aspects for the construction of symplectic RK methods of Gauss type.

In principle the derivation of exponentially-fitted (EF) RK methods consists in selecting the coefficients of the method such that it integrates exactly all functions of a particular given linear space, i.e. the set of functions

$$\{1, t, \ldots, t^K, \exp(\pm\lambda t), t\exp(\pm\lambda t), \ldots, t^P \exp(\pm\lambda t)\}\ , \tag{1}$$

where $\lambda \in \mathbb{C}$ is a prescribed frequency. In particular when $\lambda = i\omega, \omega \in \mathbb{R}$ the couple $\exp(\pm\lambda t)$ is replaced by $\sin(\omega t), \cos(\omega t)$. In all previous papers other set of functions have been introduced.

On the other hand, oscillatory problems arise in different fields of applied sciences such as celestial mechanics, astrophysics, chemistry, molecular dynamics and in many cases the modelling gives rise to Hamiltonian systems. It has been widely recognized by several authors [8, 12],[14]-[16] that symplectic integrators have some advantages for the preservation of qualitative properties of the flow over the standard integrators when they are applied to Hamiltonian systems. In this sense it may be appropriate to consider symplectic EFRK methods that preserve the structure of the original flow. In [12] the well-known theory of symplectic RK methods is extended to modified (i.e. by introducing additional parameters) EFRK methods, where the set of functions $\{\exp(\pm\lambda t)\}$ has been introduced, giving sufficient conditions on the coefficients of the method so that symplecticness for general Hamiltonian systems is preserved. Van de Vyver [12] was able to derive a two-stage fourth-order symplectic modified EFRK method of Gauss type with constant knot-points. Calvo *et al.* [2]-[4] have studied two-stage as well as three-stage methods. In their applications for fourth-order methods they consider pure EFRK methods. Their set of functions is the trigonometric polynomial one consisting essentially of the functions $\exp(\pm\lambda t)$ combined with $\exp(\pm 2\lambda t)$.They constructed fourth-order (two-stage case) methods of Gauss type with frequency dependent knot points. On the other hand Vanden Berghe *et al.* have constructed a two-stage EFRK method of fourth-order integrating the set of functions (1) with $(K = 2, P = 0)$ and $(K = 0, P = 1)$, but unfortunately these methods are not symplectic. In addition it has been pointed out in [14] that symmetric methods show a better long time behaviour than non-symmetric ones when applied to reversible differential systems.

In this paper we investigate the construction of two-stage (fourth-order) symmetric and symplectic modified EFRK methods which integrate exactly first-order differential systems whose solutions can be expressed as linear combinations of functions present in the set (1), but also give a review of previous work [2, 12]. Our purpose consists in deriving accurate and efficient modified EF geometric integrators based on the combination of the EF approach, followed from the sixth step flow chart [13], and symmetry and symplecticness conditions. The paper is organized as follows. In Section 2 we present the notations and definitions used in the rest of the paper. In Section 3 we present the previously derived methods of order four. In Section 4 we derive a class of new two-stage symplectic modified EFRK integrators with frequency dependent nodes and based upon some properties of symplectic and symmetric methods also described in [4]. In Section 5 we present some numerical experiments for fourth-order methods with oscillatory Hamiltonian systems and we compare them with the results obtained by other symplectic (EF)RK Gauss integrators given in [2, 12, 14].

2 Notations and definitions

We consider initial value problems for first-order differential systems

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^m \ . \tag{2}$$

In case of Hamiltonian systems $m = 2d$ and there exits a scalar Hamiltonian function $H = H(t, y)$, so that $f(y) = -J\nabla_y H(t, y)$, where 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 where $\nabla_y H(t, y)$ is the column vector of the derivatives of $H(t, y)$ with respect to the components of $y = (y_1, y_2, \ldots, y_{2d})^T$. The Hamiltonian system can then be written as

$$y'(t) = -J\nabla_y H(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^{2d} \ . \tag{3}$$

For each fixed t_0 the flow map of (2) 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, in the case of Hamiltonian systems, ϕ_h is a symplectic map for all h in its domain of definition, i.e. the Jacobian matrix of $\phi_h(y_0)$ satisfies

$$\phi'_h(y_0) J \phi'_h(y_0)^T = J \ .$$

A desirable property of a numerical method ψ_h for the numerical integration of a Hamiltonian system is to preserve qualitative properties of the original flow ϕ_h such as the symplecticness, in addition to provide an accurate approximation of the exact ϕ_h.

Definition 2.1
A numerical method defined by the flow map ψ_h is called symplectic if for all Hamiltonian systems (3) it satisfies the condition

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

One of the well-known examples of symplectic numerical methods is the s-stage RK Gauss methods which possess order $2s$. In this paper we shall deal with so-called (modified) implicit RK-methods, introduced for the first time to obtain explicit EFRK methods [9] and re-used by Van de Vyver [12] for the construction of two-stage symplectic RK methods.

Definition 2.2
A s-stage modified RK method for solving the initial value problems (1) is a one step method defined by

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

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

where the real parameters c_i and b_i are respectively the nodes and the weights of the method. The parameters γ_i make the method modified with repect to the classical RK method, where $\gamma_i = 1, i = 1, \ldots, s$. The s-stage modified RK-method (5)-(6) can also be represented by means of its Butcher's tableau

$$\begin{array}{c|c|ccc} c_1 & \gamma_1 & a_{11} & \ldots & a_{1s} \\ c_2 & \gamma_2 & a_{21} & \ldots & a_{2s} \\ \vdots & \ldots & \vdots & \ddots & \vdots \\ c_s & \gamma_s & a_{s1} & \ldots & a_{ss} \\ \hline & & b_1 & \ldots & b_s \end{array} \tag{7}$$

or equivalently by the quartet (c, γ, A, b).
The conditions for a modified RK method to be symplectic have been obtained by Van de Vyver [12] and they are given in the following theorem.

Definition 2.3
A modified RK-method (5)-(6) for solving the Hamiltonian system (3) is symplectic if the following conditions are satisfied

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

In [2] it is shown that a modified RK-method not only preserves the linear invariants but also quadratic invariants if its coefficients satisfy conditions (8).

3 A review of previously constructed two-stage methods

In all applications we shall write down the results in terms of exponential or hyperbolic functions in order to make it easy for the reader to compare the formulae with previously published material.

3.1 *The method of Van de Vyver [12]*

Van de Vyver considers the modified RK method (7) with $s = 2$ and associates with the internal stages the following linear operators:

$$\mathcal{L}_i[h, \mathbf{a}]y(t) = y(t + c_i h) - \gamma_i y(t) - h \sum_{j=1}^{2} a_{ij} y'(t + c_j h), \quad i = 1, 2 \ , \tag{9}$$

and with the final stage the linear operator

$$\mathcal{L}[h, \mathbf{b}]y(t) = y(t + h) - y(t) - h \sum_{i=1}^{2} b_i y'(t + c_i h) \tag{10}$$

Requiring that the operators vanish for the functions $\exp(\pm\lambda t)$ with fixed nodes $c_i, i = 1, 2$ gives respectively rise to the following equations for the internal ($i = 1, 2$) and final stages

$$\begin{aligned} &\cosh(c_i z) - \gamma_i - z(a_{i1} \sinh(c_1 z) + a_{i2} \sinh(c_2 z)) = 0 \\ &\sinh(c_i z) - z(a_{i1} \cosh(c_1 z) + a_{i2} \cosh(c_2 z)) = 0 \end{aligned} \tag{11}$$

with $z = \lambda h$ and

$$\begin{aligned} &\cosh(z) - 1 - z(b_1 \sinh(c_1 z) + b_2 \sinh(c_2 z)) = 0 \\ &\sinh(z) - z(b_1 \cosh(c_1 z) + b_2 \cosh(c_2 z)) = 0 \end{aligned} \tag{12}$$

The equations (11) and (12) together with the symplecticity conditions

$$\begin{aligned} &b_1 \frac{a_{11}}{\gamma_1} + b_1 \frac{a_{11}}{\gamma_1} - b_1 b_1 = 0, \quad b_1 \frac{a_{12}}{\gamma_1} + b_2 \frac{a_{21}}{\gamma_2} - b_2 b_1 = 0, \\ &b_2 \frac{a_{22}}{\gamma_2} + b_2 \frac{a_{22}}{\gamma_2} - b_2 b_2 = 0, \end{aligned}$$

form a consistent non-linear system for the unknowns a_{ij}, b_i and γ_i. In order to obtain a fourth-order method the Gauss nodes are chosen, i.e. $c_{1,2} = \frac{1}{2} \pm \frac{\sqrt{3}}{6}$. The following solution was obtained:

$$\begin{aligned} a_{11} &= \frac{(\exp(z) - 1)(1 + E^2)}{z(\exp(z) + 1)(1 + E)^2}, & a_{12} &= \frac{2(\exp(z) - E^2)}{z(\exp(z) + 1)(1 + E)^2}, \\ a_{21} &= \frac{2(-1 + \exp(z)E^2)}{z(\exp(z) + 1)(1 + E)^2}, & a_{22} &= a_{11}, \\ \gamma_1 &= \frac{2\exp(z/2)(1 + E + E^2 + E^3)}{\sqrt{E}(1 + E)^2(\exp(z) + 1)}, & \gamma_2 &= \gamma_1, \\ b_1 &= \frac{\exp(z) - 1}{z\exp(c_1 z)(1 + E)}, \quad b_2 = b_1, \end{aligned} \tag{13}$$

with $E = \exp(z\sqrt{3}/3)$.

The series expansions for these coefficients for small values of z are given by:

$$
\begin{aligned}
b_1 &= \frac{1}{2} + \frac{1}{8640}z^4 - \frac{1}{272160}z^6 + \frac{13}{104509440}z^8 - \frac{163}{38799129600}z^{10} + \dots \\
\gamma_1 &= 1 - \frac{1}{288}z^4 + \frac{1}{2160}z^6 - \frac{881}{17418240}z^8 + \frac{617}{117573120}z^{10} + \dots \\
a_{11} &= \frac{1}{4} - \frac{7}{8640}z^4 + \frac{31}{272160}z^6 - \frac{167}{13063680}z^8 + \frac{1861}{1385683200}z^{10} + \dots \\
a_{12} &= -\frac{\sqrt{3}}{6} + \frac{1}{4} + \frac{\sqrt{3}}{216}z^2 - (\frac{\sqrt{3}}{6480} + \frac{7}{8640})z^4 + (\frac{17\sqrt{3}}{3265920} + \frac{31}{272160})z^6 - \\
&\quad (\frac{31\sqrt{3}}{176359680} + \frac{167}{13063680})z^8 + (\frac{691\sqrt{3}}{116397388800} + \frac{1861}{1385683200})z^{10} + \dots \\
a_{21} &= \frac{\sqrt{3}}{6} + \frac{1}{4} - \frac{\sqrt{3}}{216}z^2 + (\frac{\sqrt{3}}{6480} - \frac{7}{8640})z^4 + (-\frac{17\sqrt{3}}{3265920} + \frac{31}{272160})z^6 \\
&\quad +(\frac{31\sqrt{3}}{176359680} - \frac{167}{13063680})z^8 + (-\frac{691\sqrt{3}}{116397388800} + \frac{1861}{1385683200})z^{10} + \dots
\end{aligned}
$$

Let us remark that these series are slowly converging and up to terms z^{22} have to be taken into account to reach an acceptable accuracy. It is also clear that in the limit $z \to 0$ the well-known classical fourth-order Gauss method is reproduced (see also (21)).

3.2 The method of Calvo et al. *[2]*

The method of Calvo *et al.* starts by considering two-stage methods with variable symmetric nodes $c_{1,2} = \frac{1}{2} \pm \theta(h, \lambda)$ such that all linear functionals(9) and (10) are exact for the set $\{1, \exp(\pm\lambda t)\}$. The requirement $\mathcal{L}_i[h, \mathbf{a}]1 = 0, i = 1, 2$ implies that $\gamma_i = 1, i = 1, 2$, meaning that classical RK are considered. The conditions $\mathcal{L}[h, \mathbf{b}] \exp(\pm\lambda t) = 0$ and $\mathcal{L}_i[h, \mathbf{a}] \exp(\pm\lambda t) = 0, i = 1, 2$ results in a unique solution for the b_i's and a_{ij}'s, i.e.

$$
\begin{aligned}
& b_1 = b_2 = \frac{\sinh(z/2)}{z\cosh(z\theta)} \\
& a_{11} = -\frac{\cosh(2z\theta) - \cosh(z(\theta + 1/2))}{z\sinh(2z\theta)}, \quad a_{12} = -\frac{-1 + \cosh(z(\theta - 1/2))}{z\sinh(2z\theta)} \\
& a_{21} = \frac{-1 + \cos(z(\theta + 1/2))}{z\sinh(2z\theta)}, \quad a_{22} = \frac{\cosh(2z\theta) - \cosh(z(\theta - 1/2))}{z\sinh(2z\theta)}
\end{aligned}
\tag{14}
$$

The symplecticness conditions (8) become here

$$
\begin{aligned}
m_{11} &= b_1(2a_{11} - b_1) = 0 \\
m_{22} &= b_1(2a_{22} - b_1) = 0 \\
m_{12} &= m_{21} = b_1(b_1 - a_{12} - a_{21}) = 0
\end{aligned}
\tag{15}
$$

The last condition of (15) is automatically satisfied in view of (14). The conditions m_{11} and m_{22} hold iff

$$
\theta = \frac{1}{z} \operatorname{arccosh}\left(\frac{\cosh(z/2) + \sqrt{8 + \cosh^2(z/2)}}{4} \right) . \tag{16}
$$

Further (14) and (16) imply that $\mathcal{L}[h, \mathbf{b}] \exp(\pm 2\lambda t) = 0$ automatically and therefore the final state is exact for the basis $\{1, \exp(\pm\lambda t), \exp(\pm 2\lambda t)\}$ or when $\lambda = i\omega$ for the trigonometric polynomial basis $\{1, \sin(\omega t), \cos(\omega t), \sin(2\omega t), \cos(2\omega t)\}$.
Also here it is worthwhile to give the series expansions:

$$\begin{aligned}
b_1 &= \tfrac{1}{2} - \tfrac{1}{2160} z^4 + \tfrac{1}{108864} z^6 + \tfrac{1}{2799360} z^8 - \tfrac{23}{1939956480} z^{10} + \ldots \\
a_{11} &= \tfrac{1}{4} - \tfrac{7}{8640} z^4 + \tfrac{31}{272160} z^6 - \tfrac{167}{13063680} z^8 + \tfrac{1861}{1385683200} z^{10} + \ldots \\
a_{12} &= (-\tfrac{\sqrt{3}}{6} + \tfrac{1}{4}) + \tfrac{\sqrt{3}}{432} z^2 + (-\tfrac{1}{4320} + \tfrac{13\sqrt{3}}{311040}) z^4 + (-\tfrac{37\sqrt{3}}{17418240} + \tfrac{1}{217728}) z^6 + \\
&\quad (-\tfrac{1121\sqrt{3}}{45148078080} + \tfrac{1}{5598720}) z^8 + (\tfrac{355363\sqrt{3}}{178786389196800} - \tfrac{23}{3879912960}) z^{10} + \ldots \\
a_{21} &= (\tfrac{\sqrt{3}}{6} + \tfrac{1}{4}) - \tfrac{\sqrt{3}}{432} z^2 - (\tfrac{1}{4320} + \tfrac{13\sqrt{3}}{311040}) z^4 + (\tfrac{37\sqrt{3}}{17418240} + \tfrac{1}{217728}) z^6 + \\
&\quad (\tfrac{1121\sqrt{3}}{45148078080} + \tfrac{1}{5598720}) z^8 - (\tfrac{355363\sqrt{3}}{178786389196800} + \tfrac{23}{3879912960}) z^{10} + \ldots \\
a_{22} &= \tfrac{1}{4} - \tfrac{1}{4320} z^4 + \tfrac{1}{217728} z^6 + \tfrac{1}{5598720} z^8 - \tfrac{23}{3879912960} z^{10} + \ldots \\
\theta &= \tfrac{\sqrt{3}}{6} + \tfrac{\sqrt{3}}{432} z^2 - \tfrac{\sqrt{3}}{311040} z^4 - \tfrac{17\sqrt{3}}{17418240} z^6 - \tfrac{61\sqrt{3}}{15049359360} z^8 + \tfrac{15073\sqrt{3}}{16253308108800} z^{10} + \ldots
\end{aligned}$$

Let us remark here that these series are also slowly converging and up to terms z^{22} have to be taken into account to reach an acceptable accuracy.

4 New two-stage methods

It has been remarked by Hairer *et al.* [14] that symmetric numerical methods show a better long time behaviour than nonsymmetric ones when applied to reversible differential equations, as it is the case of conservative mechanical systems. In [3] it is observed that for modified RK methods whose coefficients are even functions of h the symmetry conditions are given by

$$c(h) + Sc(h) = e, \quad b(h) = Sb(h), \quad \gamma(h) = S\gamma(h), \quad SA(h) + A(h)S = \gamma(h) b^T(h) \ , \tag{17}$$

where

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

Since for symmetric EFRK methods the coefficients contain only even powers of h, the symmetry conditions can be written in a more convenient form by putting [3]

$$c(h) = \frac{1}{2} e + \theta(h), \quad A(h) = \frac{1}{2} \gamma(h) b^T(h) + \Lambda(h) \ , \tag{18}$$

where

$$d(h) = (\theta_1, \ldots, \theta_s)^T \in \mathbb{R}^s \quad \text{and } \Lambda = (\lambda_{ij}) \in \mathbb{R}^{s \times s} \ .$$

Therefore, for a symmetric EFRK method whose coefficients a_{ij} are defined by

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

the symplecticness conditions (8) reduce to

$$\mu_{ij} \equiv \frac{b_i}{\gamma_i}\lambda_{ij} + \frac{b_j}{\gamma_j}\lambda_{ji} = 0, \quad 1 \leq i, j, \leq s \; . \tag{19}$$

The idea of constructing symplectic EFRK taking into account the six-step procedure [13] is new. We briefly shall survey this procedure and suggest some adaptation in order to make the comparison with previous work more easy.

In step (i) we define the appropriate form of an operator related to the discussed problem. Each of the s internal stages (6) and the final stage (5) can be regarded as being a generalized linear multistep method on a nonequidistant grid; we can associated with each of them a linear operator (see (9) and (10)). We further construct the so-called moments which are for Gauss methods the expressions for $L_{i,j}(h, \mathbf{a}) = \mathcal{L}_i[h, \mathbf{a}]t^j, j = 0, \ldots, s-1$ and $L_i(h, \mathbf{b}) = \mathcal{L}[h, \mathbf{b}]t^j, j = 0, \ldots, 2s-1$ at $t = 0$, respectively, with $s = 2$.

In step (ii) the linear systems

$$L_{ij}(h, \mathbf{a}) = 0, \quad i = 1, \ldots, s, \quad j = 0, 1, \ldots, s-1 \; ,$$

$$L_i(h, \mathbf{b}) = 0, \quad i = 0, 1, \ldots, 2s-1 \; .$$

are solved to reproduce the classical Gauss RK collocation methods, showing the maximum number of functions which can be annihilated by each of the operators.

The steps (iii) and (iv) can be combined in the present context. First of all we have to define all reference sets of s and $2s$ functions which are appropriate for the internal and final stages respectively. These sets are in general hybrid sets of the following form

$$\begin{array}{l} 1, t, t^2, \ldots, t^K \text{ or } t^{K'} \\ \exp(\pm\lambda t), t\exp(\pm\lambda t), \ldots, t^P \exp(\pm\lambda t) \text{ or } t^{P'} \exp(\pm\lambda t) \end{array}$$

where for the internal stages $K + 2P = s - 3$ and for the final stage $K' + 2P' = 2s - 3$. The set in which there is no classical component is identified by $K = -1$ and $K' = -1$, while the set in which there is no exponential fitting component is identified by $P = -1$ or $P' = -1$. It is important to note that such reference sets should contain all successive functions inbetween. Lacunary sets are in principle not allowed.

Once the sets chosen the operators (9)-(10) are applied to the members of the sets, in this particular case by taking into account the symmetry and the symplecticness conditions described above. The obtained independent expressions are put to zero and in step (v) the available linear systems are solved. The numerical values for $\lambda_{ij}(h)$, $b_i(h)$, $\gamma_i(h)$ and $\theta_i(h)$

are expressed for real values of λ (the pure exponential case) or for pure imaginary $\lambda = i\,\omega$ (oscillatory case). In order to make the comparison with previous work transparable we have opted to denote the results for real λ-values.
After the coefficients in the Butcher tableau have been filled in, the principal term of the local truncation error can be written down (step (vi)). Essentially, we know [11] that the algebraic order of the EFRK methods remains the same as the one of the classical Gauss method when this six-step procedure is followed, in other words the algebraic order is $\mathcal{O}(h^{2s})$, while the stage order is $\mathcal{O}(h^{s})$. Explicit expressions for this local truncation error will not be discussed here.
Here we shall analyze in particular the construction of symmetric and symplectic EFRK Gauss methods with $s = 2$ stages whose coefficients are even functions of h. These EFRK methods have stage order 2 and algebraic order 4. From the symmetry conditions (17), taking into account (18) it follows that the nodes $c_j = c_j(h^2)$ and weights $b_j = b_j(h^2)$ satisfy

$$c_1 = \frac{1}{2} - \theta, \quad c_2 = \frac{1}{2} + \theta, \quad b_1 = b_2\ ,$$

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

$$a_{11} + a_{22} = \gamma_1 b_1, \quad a_{21} + a_{12} = \gamma_2 b_1\ .$$

The symplecticness conditions (8) or (19) are equivalent to

$$a_{11} = \gamma_1 b_1/2, \quad \frac{a_{12}}{\gamma_1} + \frac{a_{21}}{\gamma_2} = b_1, \quad a_{22} = \gamma_2 b_2/2\ ,$$

which results in

$$\gamma_1 = \gamma_2, \quad \lambda_{21} = -\lambda_{12}\ .$$

Taking into account the above relations the Butcher tableau can be expressed in terms of the unknowns $\theta, \gamma_1, \lambda_{12}$ and b_1 :

$$\begin{array}{c|c|cc} \frac{1}{2}-\theta & \gamma_1 & \dfrac{\gamma_1 b_1}{2} & \dfrac{\gamma_1 b_1}{2} + \lambda_{12} \\ \frac{1}{2}+\theta & \gamma_1 & \dfrac{\gamma_1 b_1}{2} - \lambda_{12} & \dfrac{\gamma_1 b_1}{2} \\ \hline & & b_1 & b_1 \end{array} \qquad (20)$$

For the internal stages, the relation $K + 2P = -1$ results in the respective (K, P)-values:

- $(K = 1, P = -1)$ (the classical polynomial case with hybrid set $\{1, t\}$), and
- $(K = -1, P = 0)$ (the full exponential case with hybrid set $\{\exp(\lambda t), \exp(-\lambda t)\}$).

For the outer stage, we have $K' + 2P' = 1$, resulting in the respective (K', P')-values:

- $(K' = 3, P' = -1)$ (the classical polynomial case with hybrid set $\{1, t, t^2, t^3\}$),

- $(K' = 1, P' = 0)$ (mixed case with hybrid set $\{1, t, \exp(\pm\lambda t)\}$) and
- $(K' = -1, P' = 1)$(the full exponential case with hybrid set $\{\exp(\pm\lambda t), t\exp(\pm\lambda t)\}$).

The hybrid sets $(K = 1, P = -1)$ and $(K' = 3, P' = -1)$ are related to the polynomial case, giving rise to the well-known RK order conditions and to the fourth order Gauss method [17]

$$\begin{array}{c|c|cc} \frac{1}{2}-\frac{\sqrt{3}}{6} & 1 & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{1}{2}+\frac{\sqrt{3}}{6} & 1 & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & & \frac{1}{2} & \frac{1}{2} \end{array} \tag{21}$$

Let us remark that considering the $(K = 1, P = -1)$ set for the internal stages gives rise to $\gamma_1 = 1$, a value which is not compatible with the additional symmetry, symplecticity and order conditions imposed. Therefore in what follows we combine the $(K = -1, P = 0)$ case with either $(K' = 1, P' = 0)$ or $(K' = -1, P' = 1)$.

Case $(K' = 1, P' = 0)$

The operators (9) and (10) are applied to the functions present in the occurring hybrid sets, taking into account the structure of the Butcher tableau (20). Following equations arise with $z = \lambda h$:

$$2b_1 = 1 \tag{22}$$

$$2b_1 \cosh(z/2)\cosh(\theta z) = \frac{\sinh(z)}{z} \tag{23}$$

$$\lambda_{12}\cosh(\theta z) = -\frac{\sinh(\theta z)}{z} \tag{24}$$

$$\lambda_{12}\sinh(\theta z) - \frac{\cosh(\theta z)}{z} = -\frac{\gamma_1}{z}\cosh(z/2) \tag{25}$$

resulting in the results

$$b_1 = 1/2, \qquad \theta = \frac{1}{z}\text{arccosh}\left(\frac{2\sinh(z/2)}{z}\right), \qquad \lambda_{12} = -\frac{\sinh(\theta z)}{z\cosh(\theta z)}$$

$$\gamma_1 = \frac{z}{\cosh(z/2)}\left(\frac{\sinh(\theta z)^2}{z\cosh(\theta z)} + \frac{\cosh(\theta z)}{z}\right).$$

The series expansions for these coefficients for small values of z are given by

$$\theta = \sqrt{3}\left(\tfrac{1}{6} + \tfrac{1}{2160}z^2 - \tfrac{1}{403200}z^4 + \tfrac{1}{145152000}z^6 + \tfrac{533}{9656672256000}z^8 - \tfrac{2599}{2789705318400000}z^{10} + \ldots\right),$$

$$\lambda_{12} = \sqrt{3}\left(-\tfrac{1}{6} + \tfrac{1}{240}z^2 - \tfrac{137}{1209600}z^4 + \tfrac{143}{48384000}z^6 - \tfrac{81029}{1072963584000}z^8 + \tfrac{16036667}{8369115955200000}z^{10} + \ldots\right),$$

$$\gamma_1 = 1 - \tfrac{1}{360}z^4 + \tfrac{11}{30240}z^6 - \tfrac{71}{1814400}z^8 + \tfrac{241}{59875200}z^{10} + \ldots,$$

showing that for $z \to 0$ the classical values are retrieved.

Case $(K' = -1, P' = 1)$

In this approach equations (23)-(25) remain unchanged and they deliver expressions for b_1, γ_1 and λ_{12} in terms of θ. Only (22) is replaced by

$$b_1(\cosh(\theta z)\,(2\cosh(z/2) + z\sinh(z/2)) + 2\theta z\cosh(z/2)\sinh(\theta z)) = \cosh(z) \qquad (26)$$

By combining (23) and (26) one obtains an equation in θ and z, i.e.:

$$\theta\sinh(z)\sinh(\theta z) = \cosh(\theta z)\left(\cosh(z) - \frac{\sinh(z)}{z} - \sinh^2(z/2)\right)$$

It is not anymore possible to write down an analytical solution for θ, but iteratively a series expansion can be derived. We give here those series expansions as obtained for the four unknowns

$$\theta = \sqrt{3}\left(\tfrac{1}{6} + \tfrac{1}{1080}z^2 + \tfrac{13}{2721600}z^4 - \tfrac{1}{7776000}z^6 - \tfrac{1481}{1810626048000}z^8 + \tfrac{573509}{63552974284800000}z^{10} + \ldots\right)\,,$$

$$b_1 = \tfrac{1}{2} - \tfrac{1}{8640}z^4 + \tfrac{1}{1088640}z^6 + \tfrac{1}{44789760}z^8 - \tfrac{149}{775982592000}z^{10} + \ldots$$

$$\lambda_{12} = \sqrt{3}\left(-\tfrac{1}{6} + \tfrac{1}{270}z^2 - \tfrac{223}{2721600}z^4 + \tfrac{17}{9072000}z^6 - \tfrac{259513}{5431878144000}z^8 + \tfrac{9791387}{7944121785600000}z^{10} + \ldots\right)\,,$$

$$\gamma_1 = 1 - \tfrac{1}{480}z^4 + \tfrac{17}{60480}z^6 - \tfrac{2629}{87091200}z^8 + \tfrac{133603}{43110144000}z^{10} + \ldots\,.$$

5 Numerical experiments

In this section we report on some numerical experiments where we test the effectiveness of the new and the previous [2, 12] (modified) Runge-Kutta methods when they are applied to the numerical solution of several differential systems. All the considered codes have the same qualitative properties for the Hamiltonian systems. In the figures we show the decimal logarithm of the maximum global error versus the number of steps required by each code in logarithmic scale. All computations were carried out in double precision and series expansions are used for the coefficients when $|z| < 0.1$.

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

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

with the initial conditions $q_1(0) = 1 - e, q_2(0) = 0, p_1(0) = 0, p_2(0) = ((1+e)/(1-e))^{\frac{1}{2}}$, where $e, (0 \le e < 1)$ represents the eccentricity of the elliptic orbit. The exact solution of this IVP is a 2π-periodic elliptic orbit in the (q_1, q_2)-plane with semimajor axis 1, corresponding the starting point to the pericenter of this orbit. In the numerical experiments presented here we have chosen the same values as in [4], i.e. $e = 0.001, \lambda = i\omega$ with $\omega = (q_1^2 + q_2^2)^{-\frac{3}{2}}$ and the integration is carried out on the interval $[0, 1000]$ with the steps $h = 1/2^m, m = 1, \ldots, 4$. The numerical behaviour of the global error in the solution is presented in figure 1. The results obtained by the four discussed methods (Calvo *et al.* (Calvo), Van de Vyver (Vyver), the new methods with $P = 0$ and $P = 1$) and the classical Gauss method (class.) are represented. The results for the four EFRK methods are approximately falling together. They are however more accurate than the results of the classical Gauss method of the same order.

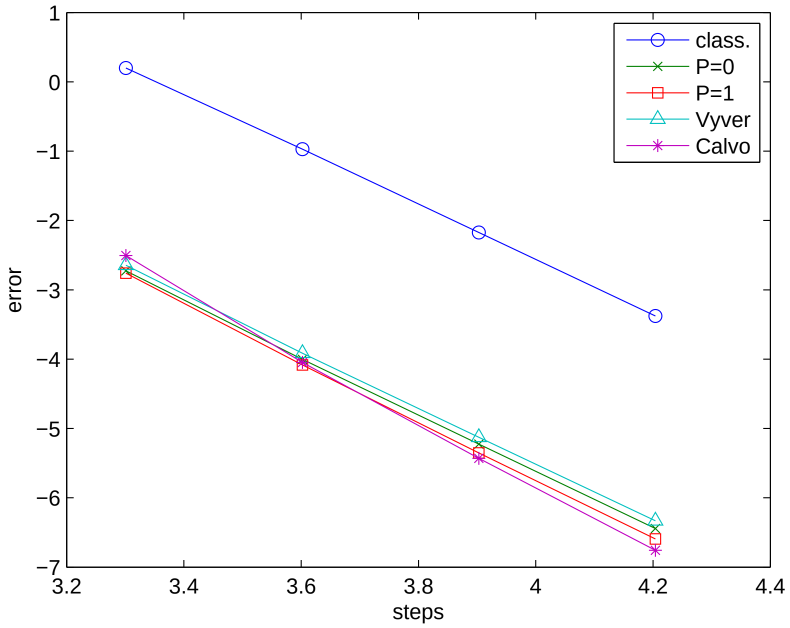


Figure 1.— Maximum global error in the solution of Problem 1.

Problem 2 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 $q_1(0) = 1, q_2(0) = 0, p_1(0) = 0, p_2(0) = 1 + \epsilon$, where ϵ is a small positive parameter. The exact solution of this IVP is given by

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

As in [4] the numerical results are computed with the integration steps $h = 1/2^m, m = 1, \ldots, 4$. We take the parameter $\epsilon = 10^{-3}, \lambda = i\omega$ with $\omega = 1$ and the problem is integrated up to $t_{end} = 1000.$. The global error in the solution is presented in figure 2. The methods of Van de Vyver with the constant nodes gives the most accurate values. Our two new

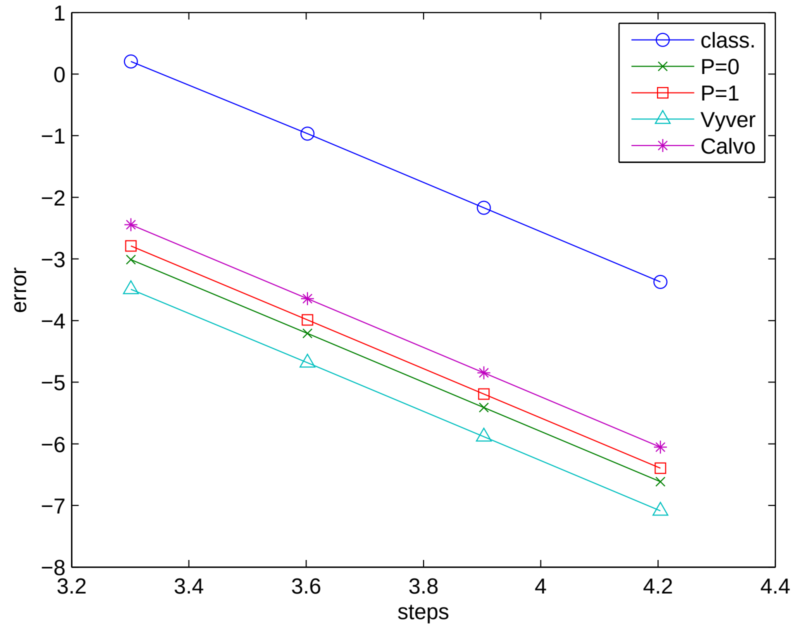


Figure 2.— Maximum global error in the solution of Problem 2.

symmetric methods are more accurate that the one of Calvo *et al.* All EFRK methods are more accurate than the classical Gauss method.

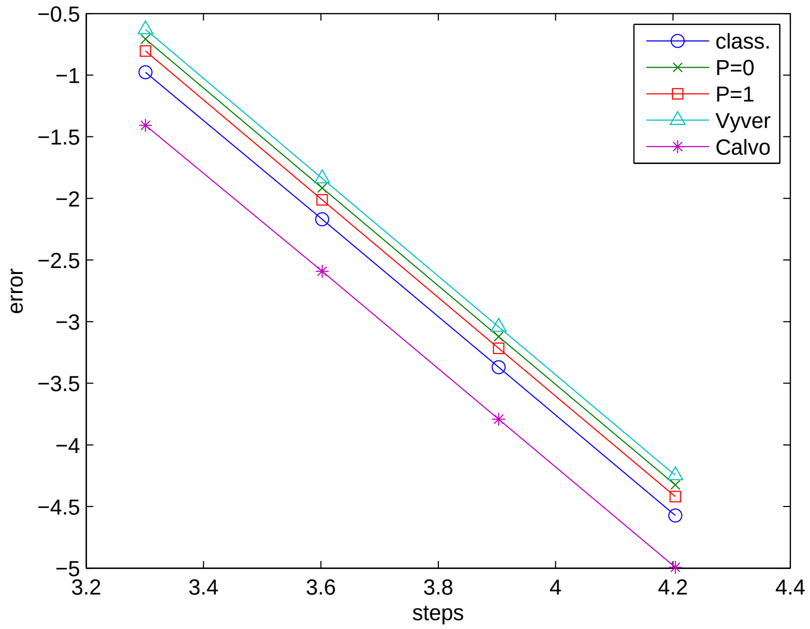
Problem 3 Euler's equations that describe the motion of a rigid body under no forces

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

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

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

it is periodic with period $T = 7.45056320933095$, and sn, cn, dn stand for the elliptic Jacobi functions. Figure 3 shows the numerical results obtained for the global error computed with the interation steps $h = 1/2^m, m = 1, \ldots, 4$, on the interval $[0, 1000]$, and respective λ-values $\lambda = i2\pi/T$ (left) and $\lambda = i/2$ (right). In this problem the choice of the frequency is not so obvious and therefore the differentiation between the classical and the EF methods is not so pronounced. For $\lambda = i2\pi/T$ only the results of Calvo *et al.* are more accurate that the classical Gauss results. For $\lambda = i/2$ all EFRK results are falling together and are slightly more accurate than the classical results.



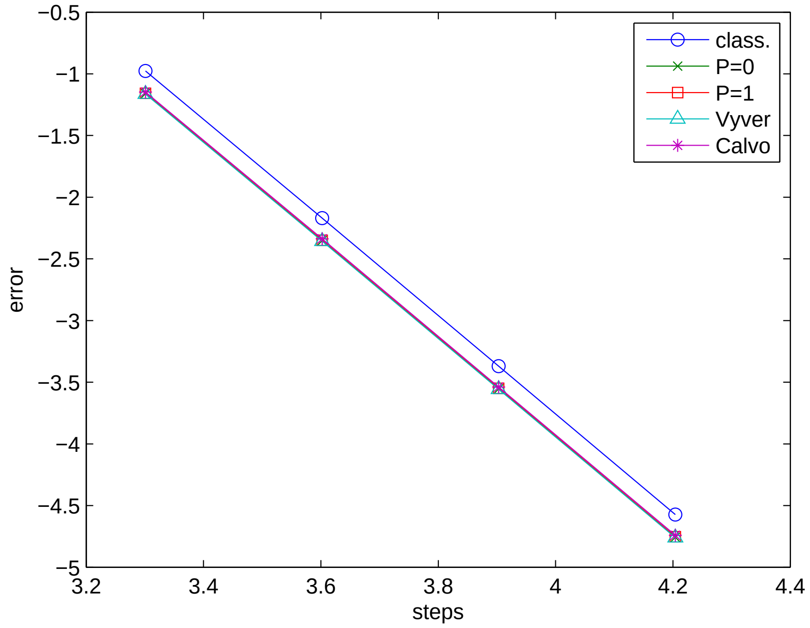


Figure 3.— Maximum global error in the solution of Problem 3. In the upper figure the results obtained with $\lambda = i2\pi/T$ are displayed. In the bottom figure the results obtained with $\lambda = i/2$ are shown.

6 Conclusions

In this paper another approach for constructing symmetric symplectic modified EFRK methods based upon the sixth-step procedure of [13] is presented. Two-stage fourth-order integrators of Gauss type which are symmetric and symplectic and which preserve linear and quadratic invariants have been derived. When the frequency used in the exponential fitting process is put to zero all considered integrators reduce to the classical Gauss integrator of the same order. Some numerical experiments show the utility of these new integrators for some oscillatory problems. The results obtained here are quite similar to the ones obtained in [2] and [12], but they differ in some of the details. The introduced method can be extended to EFRK with larger algebraic order.

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