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Exponentially fitted explicit Runge-Kutta-Nyström methods

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Abstract

Exponentially fitted Runge–Kutta–Nyström (EFRKN) methods for the numerical integration of second-order IVPs with oscillatory solutions are derived. These methods integrate exactly differential systems whose solutions can be expressed as linear combinations of the set of functions $\{\exp(\lambda t), \exp(-\lambda t)\}, \lambda \in \mathbb{C}$, or equivalently $\{\sin(\omega t), \cos(\omega t)\}$ when $\lambda = i\omega, \omega \in \mathbb{R}$. Explicit EFRKN methods with two and three stages and algebraic orders 3 and 4 are constructed. In addition, a 4(3) embedded pair of explicit EFRKN methods based on the FSAL technique is obtained, which permits to introduce an error and step length control with a small cost added. Some numerical experiments show the efficiency of our explicit EFRKN methods when they are compared with other exponential fitting type codes proposed in the scientific literature. (\hat{c}) 2003 Elsevier B.V. All rights reserved.

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1. Introduction

In the last decade a great interest in the research of new methods for the numerical integration of initial value problems

$$y'' = f(t, y), \quad t \in [t_0, T],$$

$$y(t_0) = y_0, \quad y'(t_0) = y'_0,$$
(1)

whose solution exhibits a pronounced oscillatory character has arisen. Such problems often arise in different fields of applied sciences such as celestial mechanics, astrophysics, electronics, molecular

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dynamics, and so forth; and they can be solved by using general purpose methods or by using codes specially adapted to the structure or to the solution of the problem. In the case of specially adapted methods, particular Runge-Kutta (RK) algorithms have been proposed by several authors [1-3,5, 7-12] in order to solve these classes of problems. A pioneer paper is due to Bettis [2], in which adapted RK algorithms with 3 and 4 stages for the integration of ODEs with oscillatory solutions are presented. More recently, in [3,7,8] the construction of RK and RK–Nyström methods which integrate trigonometric polynomials exactly or which have zero phase error (phase-fitted methods) is considered. These authors derive families of two-stage RK methods and families of two and three-stage RKN methods with trigonometric order 1 and algebraic order up to 6, but the main handicap of these methods is that they are fully implicit. Next, Simos and coworkers [1,9] constructed explicit RK methods which integrate certain first-order initial value problems with periodic or exponential solutions. On the other hand, Vanden Berghe et al. [11,12] introduced other exponentially fitted RK (EFRK) methods which integrate exactly first-order systems whose solutions can be expressed as linear combinations of functions of the form $\{e^{\lambda t}, e^{-\lambda t}\}$ or $\{\cos(\omega t), \sin(\omega t)\}$. In addition, these authors have implemented a variable step code by using their four-stage explicit EFRK method [12] with error and step length control based on Richardson extrapolation. This variable step code has been improved in [5] by constructing an embedded pair EFRK4(3) which corresponds in a unique way with the algebraic pair Zonneveld 4(3) given in [6].

Here, we analyze the construction of exponentially fitted Runge–Kutta–Nyström (EFRKN) methods based on an extension of the ideas proposed in [11,12] which have been recently used by Simos [10]. Our goal is to obtain practical and efficient explicit EFRKN methods as well as local error estimations that allow the implementation of these methods in a variable step code with a small computational cost added. The paper is organized as follows: In Section 2 we introduce a class of explicit EFRKN methods together with the appropriate conditions so that the functions $\{e^{\lambda t}, e^{-\lambda t}\}$ or $\{\cos(\omega t), \sin(\omega t)\}$ can be integrated exactly by these methods. We also make a study of the local truncation error, obtaining the order conditions (up to fifth order) for this class of methods. In Section 3 we derive explicit EFRKN methods with two and three stages and algebraic orders 3 and 4 as well as a 4(3) embedded pair based on the FSAL technique. Finally, in Section 4 some numerical experiments are presented to show the efficiency of our explicit EFRKN methods when they are compared with other exponential fitting codes proposed in the scientific literature.

2. Explicit EFRKN methods

In [11,12], Vanden Berghe and coworkers have introduced a class of explicit EFRK methods that integrate exactly differential systems whose solutions can be expressed as linear combinations of the set of functions $\{\exp(\lambda t), \exp(-\lambda t)\}$ or equivalently $\{\sin(\omega t), \cos(\omega t)\}$ when $\lambda = i\omega$, $\omega \in \mathbb{R}$. This means that the stage equations and the final step equation have to integrate exactly these sets of functions (see [7]).

Here we intend to extend the ideas proposed in [11,12] to the case of RK–Nyström methods. In order to carry out this goal we introduce a modification in the *s*-stage classical explicit RKN methods ($s \ge 2$), which have been recently used by Simos [10]:

$$g_1 = y_n + c_1 h \gamma_1(z) y'_n, (2)$$

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$$g_i = y_n + c_i h \gamma_i(z) y'_n + h^2 \sum_{j=1}^{i-1} a_{ij}(z) f(t_n + c_j h, g_j), \quad i = 2, \dots, s,$$
(3)

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{i=1}^{s} \bar{b}_i(z) f(t_n + c_i h, g_i),$$
(4)

$$y'_{n+1} = y'_n + h \sum_{i=1}^{3} b_i(z) f(t_n + c_i h, g_i), \quad z = \lambda h,$$
(5)

and may be expressed in Butcher tableau form as

$$\frac{c | \gamma(z) | A(z)}{| \overline{b}^{T}(z)|} = \frac{c_{1} | \gamma_{1}(z) | 0}{c_{2} | \gamma_{2}(z) | a_{21}(z) | 0}$$

$$\frac{c | \gamma(z) | A(z)}{| \overline{b}^{T}(z)|} = \frac{c_{3} | \gamma_{3}(z) | a_{31}(z) | a_{32}(z) | 0}{c_{3} | \gamma_{3}(z) | a_{31}(z) | a_{32}(z) | 0}$$

$$\frac{c_{3} | \gamma_{3}(z) | a_{31}(z) | a_{32}(z) | 0}{c_{3} | c_{31}(z) | a_{32}(z) | 0}$$

$$\frac{c_{3} | \gamma_{3}(z) | a_{31}(z) | a_{32}(z) | 0}{c_{3} | c_{31}(z) | a_{32}(z) | 0}$$

$$\frac{c_{3} | \gamma_{3}(z) | a_{31}(z) | a_{32}(z) | 0}{c_{3} | c_{31}(z) | a_{32}(z) | 0}$$

$$\frac{c_{3} | \gamma_{3}(z) | a_{31}(z) | a_{32}(z) | 0}{c_{3} | c_{31}(z) | a_{32}(z) | 0}$$

$$\frac{c_{3} | \gamma_{3}(z) | a_{31}(z) | a_{32}(z) | 0}{c_{3} | c_{31}(z) | a_{32}(z) | 0}$$

Algorithm (2)–(5) coincides with an *s*-stage classical RK–Nyström method when the coefficients $\gamma_i(z) = 1$, i = 1, ..., s, and the remaining coefficients are constant. So, the factors $\gamma_i(z)$ are introduced in the stage definition so that the family of functions $\{\exp(\lambda t), \exp(-\lambda t)\}$, or equivalently $\{\sin(\omega t), \cos(\omega t)\}$, can be integrated exactly by the method. Then, if we impose that method (2)–(5) is exact for differential systems whose solutions are $y(t)=e^{\pm\lambda t}$, and we bear in mind the meaning of the stages g_i , it is natural to consider that $g_i = y(t_n + c_i h) = e^{\pm\lambda(t_n+c_i h)}$ and $f(t_n + c_i h, g_i) = y''(t_n + c_i h) = \lambda^2 e^{\pm\lambda(t_n+c_i h)}$. This leads to the following equations for the coefficients of the method

$$e^{\pm c_1 z} = 1 \pm c_1 z \gamma_1(z), \tag{6}$$

$$e^{\pm c_i z} = 1 \pm c_i z \gamma_i(z) + z^2 \sum_{j=1}^{i-1} a_{ij}(z) e^{\pm c_j z}, \quad i = 2, \dots, s,$$
(7)

$$e^{\pm z} = 1 \pm z + z^2 \sum_{i=1}^{s} \bar{b}_i(z) e^{\pm c_i z},$$
(8)

$$e^{\pm z} = 1 \pm z \sum_{i=1}^{s} b_i(z) e^{\pm c_i z}, \quad z = \lambda h.$$
 (9)

Having in mind the relations $\cosh(z) = (e^z + e^{-z})/2$ and $\sinh(z) = (e^z - e^{-z})/2$, Eq. (6) implies that $c_1 = 0$ and $\gamma_1(z) = 1$, and Eqs. (7)–(9) can be expressed in the form

$$\sum_{j=1}^{i-1} a_{ij}(z) \cosh(c_j z) = \frac{\cosh(c_i z) - 1}{z^2},$$

$$\sum_{j=1}^{i-1} a_{ij}(z) \sinh(c_j z) = \frac{\sinh(c_i z) - c_i z \gamma_i(z)}{z^2}, \quad i = 2, \dots, s,$$
(10)

$$\sum_{i=1}^{s} \bar{b}_i(z) \cosh(c_i z) = \frac{\cosh(z) - 1}{z^2}, \quad \sum_{i=1}^{s} \bar{b}_i(z) \sinh(c_i z) = \frac{\sinh(z) - z}{z^2}, \tag{11}$$

$$\sum_{i=1}^{s} b_i(z) \sinh(c_i z) = \frac{\cosh(z) - 1}{z}, \quad \sum_{i=1}^{s} b_i(z) \cosh(c_i z) = \frac{\sinh(z)}{z}.$$
 (12)

The conditions defined by Eqs. (10)–(12) characterize when an explicit RKN method (2)–(5) with $c_1 = 0$ and $\gamma_1(z) = 1$ is exponentially fitted, and therefore they will be denominated as exponential fitting conditions (EF conditions). An explicit RKN method (2)–(5) with $c_1 = 0$ and $\gamma_1(z) = 1$, which satisfies the EF conditions (10)–(12), will be denominated an explicit EFRKN method.

On the other hand, the structure of method (2)–(5) indicates that it produces the solution of y''=0 exactly at the outer point t_{n+1} of the one-step interval, irrespective of what are the coefficients (i.e. the method reduces to $y_{n+1} = y_n + hy'_n$, $y'_{n+1} = y'_n$). So, the advance formulas (4) and (5) of an explicit EFRKN method are exact for the functions: 1, t, $e^{\pm \lambda t}$.

In the trigonometric case ($\lambda = i\omega$, $\omega \in \mathbb{R}$), z = iv with $v = \omega h$, and the EF conditions emerge having in mind the relations $\cosh(iv) = \cos(v)$ and $\sinh(iv) = i\sin(v)$. In this case, the advance formulas of the EFRKN method are exact for the functions: 1, t, $\cos(\omega t)$, $\sin(\omega t)$.

2.1. Algebraic order of the EFRKN methods

Now, we made a study of the local truncation error for the EFRKN methods in order to obtain the order conditions for this class of methods.

In the case of a classical RKN method, the local truncation error in the approximation of the solution and its derivative may be expressed as

$$e_{n+1} = y(t_{n+1}) - y_{n+1} = \sum_{j=0}^{p-1} h^{j+1} \left(\sum_{\rho(n_t)=j} \tau^{(j+1)}(n_t) F^{(j)}(n_t)(y_n) \right) + \mathcal{O}(h^{p+1})$$
$$e_{n+1}' = y'(t_{n+1}) - y_{n+1}' = \sum_{j=0}^{p} h^j \left(\sum_{\rho(n_t)=j} \tau^{'(j)}(n_t) F^{(j)}(n_t)(y_n) \right) + \mathcal{O}(h^{p+1}),$$

where n_t represents a Nyström tree of order $\rho(n_t)$, $F^{(j)}(n_t)$ denotes the elementary differential associated to n_t and the terms $\tau^{(j+1)}(n_t)$ and $\tau'^{(j)}(n_t)$ depend on the coefficients of the RKN method. So, an RKN method is of order p if

$$e_{n+1} = \mathcal{O}(h^{p+1}), \quad e'_{n+1} = \mathcal{O}(h^{p+1}),$$

or equivalently

$$\tau^{(j+1)}(n_t) = 0, \quad \forall n_t \in N \text{-trees, with } \rho(n_t) \leq p-1,$$

$$\tau^{'(j)}(n_t) = 0, \quad \forall n_t \in N \text{-trees, with } \rho(n_t) \leq p.$$

The terms $\tau^{(j+1)}(n_t)$ and $\tau'^{(j)}(n_t)$ and therefore the order conditions (up to order ≤ 5) are tabulated in [6]. In addition, if the row-sum conditions (usually imposed in the derivation of RKN methods)

are satisfied, then the number of order conditions is simplified. The quantities

$$\|\tau^{(p+1)}\| = \|(\tau^{(p+1)}(n_{t1}), \dots, \tau^{(p+1)}(n_{ti}))\|, \quad \|\tau^{'(p+1)}\| = \|(\tau^{'(p+1)}(n_{t1}), \dots, \tau^{'(p+1)}(n_{tk}))\|,$$

are denominated the principal terms of the local truncation error (see [4]).

In the case of EFRKN methods, the coefficients are step length dependent and therefore the algebraic order conditions tabulated in [6] are not valid for these methods. In addition, as it can be observed in [5,11,12], the exponentially fitted methods do not satisfy the row-sum conditions but their coefficients are even functions of h. So, in order to obtain the order conditions for EFRKN methods, we consider the following assumptions

$$\gamma(0) = e, \quad A(0)e = \frac{c^2}{2},$$
(13)

$$\bar{b}(z) = \bar{b}^{(0)} + \bar{b}^{(2)}h^2 + \bar{b}^{(4)}h^4 + \cdots, \quad b(z) = b^{(0)} + b^{(2)}h^2 + b^{(4)}h^4 + \cdots,$$
(14)

$$\gamma(z) = e + \gamma^{(2)}h^2 + \gamma^{(4)}h^4 + \cdots, \quad A(z) = A^{(0)} + A^{(2)}h^2 + A^{(4)}h^4 + \cdots,$$
(15)

where $e = (1, ..., 1)^{T}$ and $c^{2} = c \cdot c = (c_{1}^{2}, ..., c_{s}^{2})^{T}$.

Using the assumptions mentioned above and following the way given in Hairer [6, pp. 143–148] for obtaining the terms of the local truncation error, the order conditions for the EFRKN methods (up to fifth order) are the following ones:

Order 1 requires:

$$b^{(0)\mathrm{T}}e = 1. \tag{16}$$

Order 2 requires in addition:

$$b^{(0)T}c = \frac{1}{2}, \quad \bar{b}^{(0)T}e = \frac{1}{2}.$$
 (17)

Order 3 requires in addition:

$$b^{(2)T}e = 0, \quad b^{(0)T}c^2 = \frac{1}{3},$$

 $\bar{b}^{(0)T}c = \frac{1}{6}.$ (18)

Order 4 requires in addition:

$$b^{(0)T}(c \cdot \gamma^{(2)}) = 0, \quad b^{(2)T}c = 0,$$

$$b^{(0)T}c^{3} = \frac{1}{4}, \quad b^{(0)T}A^{(0)}c = \frac{1}{24},$$

$$\bar{b}^{(2)T}e = 0, \quad \bar{b}^{(0)T}c^{2} = \frac{1}{12}.$$
(19)

Order 5 requires in addition:

$$b^{(4)T}e = 0 = b^{(2)T}c^2 = b^{(0)T}A^{(2)}e, \quad b^{(0)T}c^4 = \frac{1}{5},$$

$$b^{(0)T}(c \cdot A^{(0)}c) = \frac{1}{30}, \quad b^{(0)T}A^{(0)}c^2 = \frac{1}{60},$$

$$\bar{b}^{(0)T}(c \cdot \gamma^{(2)}) = 0, \quad \bar{b}^{(2)T}c = 0, \quad \bar{b}^{(0)T}c^3 = \frac{1}{20}, \quad \bar{b}^{(0)T}A^{(0)}c = \frac{1}{120}.$$
(20)

With the help of these order conditions we have obtained (in the next section) practical and efficient explicit EFRKN methods as well as an 4(3) embedded pair of explicit EFRKN methods. To end this section, we present some properties related with the algebraic order reached by the explicit EFRKN methods.

Property 2.1. An explicit EFRKN method with $s \ge 2$ satisfies the assumptions

$$\gamma(0) = e, \quad A(0)e = \frac{c^2}{2}.$$

Proof. Using the second condition given in (10),

$$\gamma_i(z) = \frac{\sinh(c_i z)}{c_i z} - \frac{z}{c_i} \sum_{j=1}^{i-1} a_{ij}(z) \sinh(c_j z) = 1 + \mathcal{O}(z^2), \quad i = 2, \dots, s$$

and therefore $\gamma_i(0) = 1$, $i = 2, \dots, s$.

Using now the first condition given in (10)

$$\sum_{j=1}^{i-1} a_{ij}(z) \cosh(c_j z) = \frac{c_i^2}{2} + \mathcal{O}(z^2), \quad i = 2, \dots, s,$$

and therefore

$$\sum_{j=1}^{i-1} a_{ij}^{(0)} = \frac{c_i^2}{2}, \quad i = 2, \dots, s. \qquad \Box$$

Theorem 2.2. An explicit EFRKN method with $s \ge 2$ and whose coefficients satisfy assumptions (14)–(15) has algebraic order ≥ 2 .

Proof. Using conditions (11) and the expansions of the hyperbolic functions we have

$$\sum_{i=1}^{s} \bar{b}_i(z) = \frac{1}{2} + \mathcal{O}(z^2), \quad \sum_{i=1}^{s} \bar{b}_i(z)c_i = \frac{1}{6} + \mathcal{O}(z^2),$$

and therefore

$$\sum_{i=1}^{s} \bar{b}_{i}^{(0)} = \frac{1}{2}, \quad \sum_{i=1}^{s} \bar{b}_{i}^{(0)} c_{i} = \frac{1}{6}.$$

Analogously, conditions (12) yield

$$\sum_{i=1}^{s} b_i(z) = 1 + \mathcal{O}(z^2), \quad \sum_{i=1}^{s} b_i(z)c_i = \frac{1}{2} + \mathcal{O}(z^2),$$

and therefore

$$\sum_{i=1}^{s} b_i^{(0)} = 1, \quad \sum_{i=1}^{s} b_i^{(0)} c_i = \frac{1}{2}.$$

So, the order conditions (16) and (17) are satisfied and the explicit EFRKN method has algebraic order at least 2. \Box

3. Construction of explicit EFRKN methods

In this section we analyze the construction of explicit EFRKN methods (up to order 4) with the help of the order conditions obtained in the previous section. In addition, we derive an 4(3) embedded pair and we analyze the principal terms of the local truncation error.

3.1. EFRKN methods with s = 2

We consider the explicit EFRKN methods defined by the table of coefficients

If we impose the EF conditions (10)–(12), the coefficients are given by

$$\gamma_{2}(z) = \frac{\sinh(c_{2}z)}{c_{2}z}, \quad a_{21}(z) = \frac{\cosh(c_{2}z) - 1}{z^{2}},$$

$$\bar{b}_{2}(z) = \frac{\sinh(z) - z}{z^{2}\sinh(c_{2}z)}, \quad \bar{b}_{1}(z) = \frac{\cosh(z) - 1}{z^{2}} - \bar{b}_{2}(z)\cosh(c_{2}z),$$

$$b_{2}(z) = \frac{\cosh(z) - 1}{z\sinh(c_{2}z)}, \quad b_{1}(z) = \frac{\sinh(z)}{z} - b_{2}(z)\cosh(c_{2}z),$$

(21)

with c_2 a free parameter. By Theorem 2.2, coefficients (21) define a method with algebraic order ≥ 2 , and we use the free parameter in order to reach third order. Conditions (18) imply that $c_2=2/3$. So, we have obtained a third-order explicit method whose principal terms of the local truncation error are

$$\|\tau^{(4)}\|_2 = \sqrt{0.000386 + 0.000193\lambda^4}, \quad \|\tau^{'(4)}\|_2 = \sqrt{0.00176 + 0.000364\lambda^4},$$

which will be denominated as EFRKN3. For small values of z it is preferable to use series expansions for the coefficient values of the method:

$$\begin{aligned} \gamma_2(z) &= 1 + \frac{2}{27} z^2 + \frac{2}{1215} z^4 + \frac{4}{229635} z^6 + \cdots, \\ a_{21}(z) &= \frac{2}{9} + \frac{2}{243} z^2 + \frac{4}{32805} z^4 + \frac{2}{2066715} z^6 + \cdots, \\ \bar{b}_2(z) &= \frac{1}{4} - \frac{13}{2160} z^2 + \frac{271}{816480} z^4 - \frac{1877}{125971200} z^6 + \cdots, \\ \bar{b}_1(z) &= \frac{1}{4} - \frac{17}{2160} z^2 + \frac{55}{163296} z^4 - \frac{13231}{881798400} z^6 + \cdots, \\ b_2(z) &= \frac{3}{4} + \frac{1}{144} z^2 + \frac{13}{38880} z^4 - \frac{709}{58786560} z^6 + \cdots, \\ b_1(z) &= \frac{1}{4} - \frac{1}{144} z^2 + \frac{11}{38880} z^4 - \frac{731}{58786560} z^6 + \cdots. \end{aligned}$$

In addition, these expressions show that assumptions (14)–(15) are satisfied by the method.

3.2. EFRKN methods with s = 3

In this case, the explicit EFRKN methods are defined by the table of coefficients

Imposing that the advance formulas (4) and (5) are exact whenever f(t, y) = 1, or equivalently

$$b_1(z) + b_2(z) + b_3(z) = 1, \quad \bar{b}_1(z) + \bar{b}_2(z) + \bar{b}_3(z) = 1/2,$$
(22)

and the EF conditions (10)–(12), the coefficients $b_i(z)$, $\bar{b}_i(z)$, $\gamma_i(z)$, $a_{21}(z)$ and $a_{32}(z)$ are determined in terms of the arbitrary coefficients c_2 , c_3 and $a_{31}(z)$. In addition, the derived method satisfies the third-order conditions and some of the conditions given in (19). So, we use the free parameters c_2 , c_3 and $a_{31}(z)$ in order to reach fourth order. Conditions (19) yield the nonlinear system

$$3 - 4(c_2 + c_3) + 6c_2c_3 = 0,$$

$$a_{31}(0)(-12c_2 + 18c_2^2) + 2c_2^2c_3 + 6c_2c_3^2 - 12c_2^2c_3^2 - 2c_3^3 + 3c_2c_3^3 = 0,$$
(23)

which have infinitely many solutions.

If we chose $a_{31}(z) = 0$, then the nodes are given by $c_2 = 1/2$, $c_3 = 1$, and the remaining coefficients of the method are

$$\begin{aligned} \gamma_{2}(z) &= \frac{2\sinh(z/2)}{z}, \quad a_{21}(z) = \frac{\cosh(z/2) - 1}{z^{2}}, \\ \gamma_{3}(z) &= \frac{2\tanh(z/2)}{z}, \quad a_{32}(z) = \frac{2\sinh^{2}(z/2)}{z^{2}\cosh(z/2)}, \\ b_{1}(z) &= b_{3}(z) = \frac{2\sinh(z/2) - z}{4z\cosh^{2}(z/4)}, \quad b_{2}(z) = \frac{2 - 2\cosh(z) + z\sinh(z)}{z(\sinh(z) - 2\sinh(z/2))}, \\ \bar{b}_{1}(z) &= \frac{2(z\cosh(z) - \sinh(z)) + (4 - z^{2})\sinh(z/2) - 2z\cosh(z/2)}{2z^{2}(\sinh(z) - 2\sinh(z/2))}, \\ \bar{b}_{2}(z) &= \frac{2 - 2\cosh(z) + z\sinh(z)}{2z(\sinh(z) - 2\sinh(z/2))}, \\ \bar{b}_{3}(z) &= \frac{2z\cosh(z/2) - (4 + z^{2})\sinh(z/2) + 2(\sinh(z) - z)}{2z^{2}(\sinh(z) - 2\sinh(z/2))}. \end{aligned}$$
(24)

So, we have obtained a fourth-order explicit method whose principal terms of the local truncation error are

$$\|\tau^{(5)}\|_2 = \sqrt{0.0000887 + 0.000014\lambda^4}, \quad \|\tau^{'(5)}\|_2 = \sqrt{0.0000837 + 0.000017\lambda^4},$$

which will be denominated as EFRKN4. For small values of z, the series expansions for the coefficients are given by

$$\begin{split} \gamma_2(z) &= 1 + \frac{1}{24} z^2 + \frac{1}{1920} z^4 + \frac{1}{322560} z^6 + \frac{1}{92897280} z^8 + \frac{1}{4087480200} z^{10} + \cdots, \\ \gamma_3(z) &= 1 - \frac{1}{12} z^2 + \frac{1}{120} z^4 - \frac{17}{20160} z^6 + \frac{31}{362880} z^8 - \frac{691}{79833600} z^{10} + \cdots, \\ a_{21}(z) &= \frac{1}{8} + \frac{1}{384} z^2 + \frac{1}{46080} z^4 + \frac{1}{10321920} z^6 + \frac{1}{3715891200} z^8 \\ &+ \frac{1}{1961990553600} z^{10} + \cdots, \\ a_{32}(z) &= \frac{1}{2} - \frac{1}{48} z^2 + \frac{31}{11520} z^4 - \frac{173}{645120} z^6 + \frac{25261}{928972800} z^8 - \frac{675691}{245248819200} z^{10} + \cdots, \\ \bar{b}_1(z) &= \frac{1}{6} - \frac{1}{480} z^2 + \frac{199}{483840} z^4 - \frac{17}{19353600} z^6 + \frac{29}{1362493440} z^8 \\ &- \frac{71173}{133905855283200} z^{10} + \cdots, \\ \bar{b}_2(z) &= \frac{1}{3} + \frac{1}{720} z^2 - \frac{1}{80640} z^4 + \frac{1}{9676800} z^6 - \frac{1}{1226244096} z^8 \\ &+ \frac{691}{11588212736000} z^{10} + \cdots, \\ \end{split}$$

and they satisfy assumptions (14)–(15).

Conditions (22) imply that the advance formulas (4) and (5) of the method EFRKN4 are exact for the functions: $1, t, t^2, e^{\pm \lambda t}$.

3.3. EFRKN methods with s = 4 (FSAL)

Now we analyze the case of EFRKN methods with 4 stages by using the FSAL technique [4] (the last evaluation at any step is the same as the first evaluation at the next step). In this case, the methods require 3 evaluations per step except at the first step in which 4 evaluations are required,

and they are defined by the table of coefficients

Imposing that the weights of the advance formulas (4) and (5) satisfy

$$b_1(z) + b_2(z) + b_3(z) + b_4(z) = 1, \quad \bar{b}_1(z) + \bar{b}_2(z) + \bar{b}_3(z) = 1/2,$$

$$b_2(z)c_2 + b_3(z)c_3 + b_4(z) = 1/2,$$
 (25)

in addition to the EF conditions (10)–(12), the coefficients $b_i(z)$, $\bar{b}_i(z)$, $\gamma_i(z)$, $a_{21}(z)$ and $a_{32}(z)$ are determined in terms of the arbitrary parameters c_2 , c_3 and $a_{31}(z)$. With these conditions, the resulting method has order 3 and it satisfies some of the conditions given in (19). So, we use the free parameters c_2 , c_3 and $a_{31}(z)$ in order to reach fourth order. In this case, conditions (19) yield that

$$a_{31}(0) = \frac{c_3(c_2^2(1-12c_3)+6c_2^3c_3-c_3^2+3c_2c_3(1+c_3))}{6c_2(c_2-1)(2c_2-1)}.$$
(26)

The choice $a_{31}(z)=a_{31}(0)$ defines a two-parameter family of fourth-order explicit EFRKN methods. Now, we select the nodes so that the principal terms of the local truncation error should be as small as possible. We have found that the choice $c_2 = 1/4$, $c_3 = 7/10$ give

$$\|\tau^{(5)}\|_2 = \sqrt{2.14 \times 10^{-7} + 5.36 \times 10^{-8} \lambda^4}, \quad \|\tau^{'(5)}\|_2 = \sqrt{3.08 \times 10^{-6} + 1.43 \times 10^{-6} \lambda^4}$$

and the remaining coefficients of the method are

$$\begin{split} \gamma_{2}(z) &= \frac{4\sinh(z/4)}{z}, \quad a_{21}(z) = \frac{\cosh(z/4) - 1}{z^{2}}, \\ \gamma_{3}(z) &= \frac{1000\sinh(7z/10) + (1000 + 7z^{2} - 1000\cosh(7z/10))\tanh(z/4)}{700z}, \\ a_{31}(z) &= \frac{7}{1000}, \quad a_{32}(z) = \frac{1000\cosh(7z/10) - 1000 - 7z^{2}}{1000z^{2}\cosh(z/4)}, \\ \bar{b}_{1}(z) &= \frac{\sinh(9z/40)(z^{2}\cosh(9z/40) + 2\cosh(19z/40) - 2\cosh(21z/40) - 2z\sinh(19z/40))}{z^{2}(\sinh(z/4) + \sinh(9z/20) - \sinh(7z/10))}, \\ \bar{b}_{2}(z) &= -\frac{2z - 2z\cosh(7z/10) + 2\sinh(3z/10) + 2\sinh(7z/10) + z^{2}\sinh(7z/10) - 2\sinh(z)}{2z^{2}(\sinh(z/4) + \sinh(9z/20) - \sinh(7z/10))}, \\ \bar{b}_{3}(z) &= \frac{-2z\cosh(z/4) + (2 + z^{2})\sinh(z/4) + 2(z + \sinh(3z/4) - \sinh(z))}{2z^{2}(\sinh(z/4) + \sinh(9z/20) - \sinh(7z/10))}, \\ b_{1}(z) &= \frac{N_{1}}{D}, \quad b_{2}(z) = \frac{N_{2}}{D}, \quad b_{3}(z) = \frac{N_{3}}{D}, \quad b_{4}(z) = \frac{N_{4}}{D}, \end{split}$$

where
$$D = z(6\sinh(z/4) + 5\sinh(3z/10) + 20\sinh(9z/20) - 15\sinh(7z/10) - 14\sinh(3z/4) + 9\sinh(z)),$$

 $N_1 = -9 + 6\cosh\left(\frac{z}{4}\right) + 15\cosh\left(\frac{3z}{10}\right) - 15\cosh\left(\frac{7z}{10}\right) - 6\cosh\left(\frac{3z}{4}\right) + 9\cosh(z)$
 $-5z\sinh\left(\frac{3z}{10}\right) + 10z\sinh\left(\frac{9z}{20}\right) - 4z\sinh\left(\frac{3z}{4}\right),$
 $N_2 = 4\left(z\cosh\left(\frac{z}{2}\right) - 2\sinh\left(\frac{z}{2}\right)\right)\left(-5\sinh\left(\frac{z}{5}\right) + 2\sinh\left(\frac{z}{2}\right)\right),$
 $N_3 = 10\left(z\cosh\left(\frac{z}{2}\right) - 2\sinh\left(\frac{z}{2}\right)\right)\left(-2\sinh\left(\frac{z}{4}\right) + \sinh\left(\frac{z}{2}\right)\right),$
 $N_4 = -9 + 14\cosh\left(\frac{z}{4}\right) + 5\cosh\left(\frac{3z}{10}\right) - 5\cosh\left(\frac{7z}{10}\right) - 14\cosh\left(\frac{3z}{4}\right) + 9\cosh(z)$
 $-4z\sinh\left(\frac{z}{4}\right) + 10z\sinh\left(\frac{9z}{20}\right) - 5z\sinh\left(\frac{7z}{10}\right).$

This method will be denominated EFRKN4F, and for small values of z the series expansions for the coefficient are given by

$$\begin{split} \gamma_2(z) &= 1 + \frac{z^2}{96} + \frac{z^4}{30720} + \frac{z^6}{20643840} + \frac{z^8}{23781703680} + \frac{z^{10}}{41855798476800} + \cdots, \\ \gamma_3(z) &= 1 - \frac{z^2}{300} + \frac{159z^4}{80000} - \frac{13967z^6}{288000000} + \frac{8931917z^8}{72576000000000} \\ &\quad - \frac{69131417z^{10}}{2217600000000000} + \cdots, \\ a_{21}(z) &= \frac{1}{32} + \frac{z^2}{6144} + \frac{z^4}{2949120} + \frac{z^6}{2642411520} + \frac{z^8}{3805072588800} \\ &\quad + \frac{z^{10}}{8036313307545600} + \cdots, \\ a_{32}(z) &= \frac{119}{500} + \frac{77z^2}{30000} + \frac{256067z^4}{5760000000} - \frac{351701z^6}{76800000000} \\ &\quad + \frac{9222666821z^8}{66355200000000000} - \frac{1519748735123z^{10}}{74379443200000000000} + \cdots, \\ \bar{b}_1(z) &= \frac{1}{14} + \frac{z^2}{5040} - \frac{629z^4}{120960000} + \frac{4099z^6}{56448000000} \\ &\quad - \frac{992337887z^8}{107296358400000000} + \frac{209z^6}{2343352467456000000000} + \cdots, \\ \bar{b}_2(z) &= \frac{8}{27} - \frac{z^2}{3240} - \frac{1937z^4}{54432000} + \frac{209z^6}{5443200000} - \frac{26260033z^8}{689762304000000000} \\ &\quad + \frac{200929607z^{10}}{1158800670720000000000} + \cdots, \end{split}$$

$$\begin{split} \bar{b}_3(z) &= \frac{25}{189} + \frac{z^2}{9072} + \frac{1907z^4}{1907217728000} - \frac{4661z^6}{60963840000} \\ &+ \frac{1859736289z^8}{1931334451200000000} - \frac{494432457737z^{10}}{42180344414208000000000} + \cdots, \\ b_1(z) &= \frac{1}{14} + \frac{z^2}{8400} - \frac{503z^4}{117600000} + \frac{45331z^6}{705600000000} - \frac{6814329551z^8}{7823692800000000000} \\ &+ \frac{14555700385913z^{10}}{47178776943594068320256000000000000} + \cdots, \\ b_2(z) &= \frac{32}{81} - \frac{z^2}{4050} + \frac{473z^4}{97200000} - \frac{1612757z^6}{24494400000000} \\ &+ \frac{25977716983z^8}{3017710080000000000} - \frac{4838146239331z^{10}}{42796615680000000000000} + \cdots, \\ b_3(z) &= \frac{250}{567} + \frac{z^2}{4536} + \frac{797z^4}{381024000} - \frac{679589z^6}{13716864000000} \\ &+ \frac{12694368991z^8}{1689917644800000000} - \frac{27398706112457z^{10}}{263627152588800000000000000} + \cdots, \\ b_4(z) &= \frac{5}{54} - \frac{z^2}{10800} - \frac{19z^4}{7087500} + \frac{835117z^6}{1632960000000} \\ &- \frac{1355296393z^8}{182891520000000000000} + \frac{31702189865821z^{10}}{313841848320000000000000000000} + \cdots, \end{split}$$

which satisfy assumptions (14)–(15).

Conditions (25) imply that the advance formula (4) of the method EFRKN4F is exact for the functions: $1, t, t^2, e^{\pm \lambda t}$, whereas the advance formula (5) is exact for the functions: $1, t, t^2, t^3, e^{\pm \lambda t}$.

3.4. The 4(3) embedded pair

Now our interest is focused on the construction of an embedded pair of explicit EFRKN methods based on the above EFRKN4F method. In order to carry out this goal, we consider another explicit EFRKN method of 4 stages and order 3

$$y_{n+1}^{*} = y_n + hy_n' + h^2 \sum_{i=1}^{4} \bar{b}_i^{*}(z) f(t_n + c_i h, g_i),$$

$$y_{n+1}^{'*} = y_n' + h \sum_{i=1}^{4} b_i^{*}(z) f(t_n + c_i h, g_i),$$

with the same stages that the EFRKN4F method. It should be noted that the fourth-order approximations y_n and y'_n are used as the initial values for obtaining the third-order approximations y^*_{n+1} and y'^*_{n+1} , that is to say, the embedded pair is applied in local extrapolation mode or higher-order

mode. In order to obtain the third-order method, we impose that the new weights $\bar{b}_i^*(z)$ and $b_i^*(z)$ satisfy the EF conditions (11) and (12) and the condition

$$b_1^*(z) + b_2^*(z) + b_3^*(z) + b_4^*(z) = 1.$$
(28)

This last condition implies that the advance formula (5) of the method is exact for the functions: 1, $t, t^2, e^{\pm \lambda t}$. With these conditions, the resulting method has order 3, it satisfies the order conditions (16)–(18), and the weights are determined in terms of the arbitrary parameters $b_4^*(z)$, $\bar{b}_3^*(z)$ and $\bar{b}_4^*(z)$. Inspired by the classical RKN4(3) pair obtained in [4], we choose the parameter values

$$b_4^*(z) = -1/3$$
, $b_3^*(z) = 3/20$, $b_4^*(z) = -1/20$

and the remaining weights are given by

$$\bar{b}_1^*(z) = \frac{20z\cosh(z/4) - 20\sinh(z/4) + 3z^2\sinh(9z/20) - 20\sinh(3z/4) - z^2\sinh(3z/4)}{20z^2\sinh(z/4)},$$

$$= \frac{(20 + z^2)\sin(z) - 20z - 3z^2\sinh(7z/10)}{20z^2\sinh(7z/10)}$$

$$b_{2}^{*}(z) = \frac{(20 + 2^{\circ})\sin(2) - 202 - 92^{\circ}\sin(2/10)}{20z^{2}\sinh(z/4)},$$

$$b_{1}^{*}(z) = \frac{N_{1}^{*}}{3z(\sinh(z/4) + \sinh(9z/20) - \sinh(7z/10))},$$

$$b_{2}^{*}(z) = \frac{N_{2}^{*}}{3z(\sinh(z/4) + \sinh(9z/20) - \sinh(7z/10))},$$

$$b_{3}^{*}(z) = \frac{N_{3}^{*}}{3z(\sinh(z/4) + \sinh(9z/20) - \sinh(7z/10))},$$

where

$$N_{1}^{*} = 3\cosh\left(\frac{z}{4}\right) + 3\cosh\left(\frac{3z}{10}\right) - 3\cosh\left(\frac{7z}{10}\right) - 3\cosh\left(\frac{3z}{4}\right) + z\sinh\left(\frac{3z}{10}\right)$$
$$+ 4z\sinh\left(\frac{9z}{20}\right) - z\sinh\left(\frac{3z}{4}\right),$$
$$N_{2}^{*} = -3 - 3\cosh\left(\frac{3z}{10}\right) + 3\cosh\left(\frac{7z}{10}\right) + 3\cosh\left(\frac{7z}{10}\right) + 3\cosh(z) - z\sinh\left(\frac{3z}{10}\right)$$
$$- 4z\sinh\left(\frac{7z}{10}\right) + z\sinh(z),$$
$$N_{3}^{*} = 3 - 3\cosh\left(\frac{z}{4}\right) + 3\cosh\left(\frac{3z}{4}\right) - 3\cosh(z) + 4z\sinh\left(\frac{z}{4}\right) + z\sinh\left(\frac{3z}{4}\right) - z\sinh(z).$$

The new embedded pair will be denominated EFRKN4(3)F, and for small values of z the series expansions for the weights of the third-order formula are given by

$$\bar{b}_{1}^{*}(z) = -\frac{7}{150} - \frac{529z^{2}}{45000} - \frac{4192z^{4}}{14765625} - \frac{441517z^{6}}{18900000000} - \frac{76458659z^{8}}{7484400000000000} - \frac{113878959611z^{10}}{40864824000000000000} + \cdots,$$

$$\begin{split} \bar{b}_2^*(z) &= \frac{67}{150} + \frac{9977z^2}{360000} + \frac{79636507z^4}{60480000000} + \frac{1270638757z^6}{4838400000000} \\ &+ \frac{4090303650217z^8}{153280512000000000000} + \frac{27719213106114401z^{10}}{16738231910400000000000000000} + \cdots, \\ b_1^*(z) &= \frac{13}{21} + \frac{23z^2}{10080} - \frac{10597z^4}{564480000} + \frac{330971z^6}{1354752000000} \\ &- \frac{6575318689z^8}{2145927168000000000} + \frac{238284355301z^{10}}{6248939913216000000000} + \cdots, \\ b_2^*(z) &= -\frac{20}{27} - \frac{253z^2}{6480} - \frac{294689z^4}{1088640000} - \frac{640751z^6}{870912000000} \\ &- \frac{1829801551z^8}{1379524608000000000} - \frac{5947927819z^{10}}{12051526975488000000000} + \cdots, \\ b_3^*(z) &= \frac{275}{189} + \frac{667z^2}{18144} + \frac{882353z^4}{3048192000} + \frac{239671z^6}{487710720000} \\ &+ \frac{16959017983z^8}{3862668902400000000} - \frac{6350406603661z^{10}}{168721377656832000000000} + \cdots, \end{split}$$

which satisfy assumptions (14)–(15).

For $z \rightarrow 0$ the EFRKN4(3)F pair reduces to the classical RKN4(3) pair obtained in [4].

4. Numerical experiments

In order to evaluate the effectiveness of the EFRKN methods derived in the above section, we use several model problems which have periodic or almost periodic solutions. The new EFRKN methods have been implemented in fixed step and variable step codes, and have been compared with other exponential fitting type codes proposed in [5,11,12]. Numerical considerations indicate that Taylor series should be used for the coefficients of the new EFRKN methods when |z| < 0.3, and they contain terms up to z^{10} in order to obtain the coefficients with arithmetic precision of 16 digits. The criterion used in the numerical comparisons is the usual test based on computing the maximum global error over the whole integration interval. In Figs. 1–5 we have depicted the efficiency curves for the tested codes. These figures show the decimal logarithm of the maximum global error (sd(e)) against the computational effort measured by the number of function evaluations required by each code.

4.1. Comparisons with fixed step-size

As test problems we have considered a linear model problem as well as a nonlinear problem, and the codes used in the comparisons have been denoted by

- EFRKN4F: The trigonometric version of the method derived in Section 3.3.
- EFRKN4: The trigonometric version of the method derived in Section 3.2.
- VBERGHE4: The fourth-order and four-stage EFRK method obtained in [11].



Fig. 1. Linear problem with resonance: $t_{end} = 1000$.

Problem 1. We consider the linear problem with resonance

 $y'' + y = 0.001 \cos(t), \quad t \in [0, t_{end}],$ $y(0) = 1, \quad y'(0) = 0,$

whose analytic solution is given by $y(t) = \cos(t) + 0.0005t \sin(t)$.

In our test we choose the parameter value $t_{end} = 1000$, and the numerical results stated in Fig. 1 have been computed with integration steps $h = 1/2^j$, j = 0, 1, ..., 4 and $\lambda = i$.

Problem 2. We consider the nonlinear problem

$$y_1'' + 100y_1 + \frac{2y_1y_2}{y_1^2 + y_2^2} = f_1(t), \quad y_1(0) = 1, \quad y_1'(0) = \varepsilon,$$

$$y_2'' + 25y_2 + \frac{y_1^2 - y_2^2}{y_1^2 + y_2^2} = f_2(t), \quad y_2(0) = -\varepsilon, \quad y_2'(0) = 5,$$

with $\varepsilon = 10^{-3}$ and

$$f_1(t) = \frac{2\cos(10)\sin(5t) + 2\varepsilon(\sin(5t)\sin(t) - \cos(10t)\cos(t)) - \varepsilon^2\sin(2t)}{\cos^2(10t) + \sin^2(5t) + 2\varepsilon(\sin(t)\cos(10t) - \cos(t)\sin(5t)) + \varepsilon^2} + 99\varepsilon\sin(t),$$

$$f_2(t) = \frac{\cos^2(10t) - \sin^2(5t) + 2\varepsilon(\sin(t)\cos(10t) + \cos(t)\sin(5t)) - \varepsilon^2\cos(2t)}{\cos^2(10t) + \sin^2(5t) + 2\varepsilon(\sin(t)\cos(10t) - \cos(t)\sin(5t)) + \varepsilon^2} - 24\varepsilon\cos(t).$$

The analytic solution of this initial-value problem is given by

$$y_1(t) = \cos(10t) + \varepsilon \sin(t), \quad y_2(t) = \sin(5t) - \varepsilon \cos(t),$$

and represents a periodic motion with two dominant frequencies and a small perturbation of low frequency. In our test we choose the parameter value $t_{end} = 100$ and the different components of the



Fig. 2. Nonlinear problem: $t_{end} = 100$.

system have been integrated with different λ -values: $\lambda_1 = i10$ for the first component and $\lambda_2 = i5$ for the second component. The numerical results stated in Fig. 2 have been computed with integration steps $h = 1/2^j$, j = 1, 2, ..., 5.

As it can be observed in Figs. 1 and 2, the new fourth-order EFRKN methods show a more efficient behaviour than the exponentially fitted method VBERGHE4. In addition, among the fourth-order EFRKN methods, the code EFRKN4F which has optimized the principal terms of the local truncation error performs more efficiently than the code EFRKN4.

4.2. Comparisons with variable step-size

In this case we have considered the test problems used in [5] and the codes used in the comparisons have been denoted by

- EFRKN4(3)F: The trigonometric version of the embedded pair derived in Sections 3.3 and 3.4.
- EFRK4(3): The trigonometric version of the embedded pair obtained in [5].
- VBExtrapo: The variable step code proposed by Vanden Berghe et al. [12].

Problem 3. We consider the linear problem with variable coefficients

$$y'' + 4t^2 y = (4t^2 - \omega^2)\sin(\omega t) - 2\sin(t^2), \quad t \in [0, t_{end}],$$

$$y(0) = 1, \quad y'(0) = \omega,$$

whose analytic solution is given by

$$y(t) = \sin(\omega t) + \cos(t^2)$$



Fig. 3. Linear problem with variable coefficients: $\omega = 10$, $t_{end} = 10$.

This solution represents a periodic motion that involves a constant frequency and a variable frequency. In our test we choose the parameter values $\omega = 10$, $t_{end} = 10$, and the numerical results stated in Fig. 3 have been computed with error tolerances Tol = 10^{-j} , $j \ge 2$ and $\lambda = i10$.

Problem 4. We consider the periodically forced nonlinear problem (undamped Duffing's equation)

$$y'' + y + y^3 = (\cos(t) + \varepsilon \sin(10t))^3 - 99\varepsilon \sin(10t), \quad t \in [0, t_{end}]$$

$$y(0) = 1, \quad y'(0) = 10\varepsilon,$$

with $\varepsilon = 10^{-3}$. The analytic solution is given by

 $y(t) = \cos(t) + \varepsilon \sin(10t),$

and represents a periodic motion of low frequency with a small perturbation of high frequency. In our test we choose the parameter value $t_{end} = 100$, and the numerical results stated in Fig. 4 have been computed with error tolerances Tol = 10^{-j} , $j \ge 3$ and $\lambda = i$.

Problem 5. We consider the nonlinear system

$$y_1'' = -4t^2 y_1 - \frac{2y_2}{\sqrt{y_1^2 + y_2^2}}, \quad y_1(0) = 1, \quad y_1'(0) = 0, \quad t \in [0, t_{end}],$$
$$y_2'' = -4t^2 y_2 + \frac{2y_1}{\sqrt{y_1^2 + y_2^2}}, \quad y_2(0) = 0, \quad y_2'(0) = 0,$$

whose analytic solution is given by

$$y_1(t) = \cos(t^2), \quad y_2(t) = \sin(t^2).$$

This solution represents a periodic motion with variable frequency. In our test we choose the parameter value $t_{end} = 10$, and the numerical results stated in Fig. 5 have been computed with error tolerances Tol = 10^{-j} , $j \ge 2$ and $\lambda = it_n$ ($n \ge 1$) at each step.



Fig. 4. Undamped Duffing's equation: $t_{end} = 100$.



Fig. 5. Nonlinear system: $t_{end} = 10$.

As it can be observed in Figs. 3–5, the new embedded pair EFRKN4(3)F shows a more efficient behaviour than the exponentially fitted variable step codes EFRK4(3) and VBExtrapo.

In view of the numerical results obtained in Problems 1–5, we may conclude that the new fourth-order EFRKN methods derived in Section 3 perform more efficiently than other exponential fitting type codes recently proposed in the scientific literature.

All the computations have been carried out in double-precision arithmetic in a PC computer of the University of Zaragoza.

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