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New embedded explicit pairs of exponentially fitted Runge–Kutta methods☆

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ABSTRACT

Two new embedded pairs of exponentially fitted explicit Runge–Kutta methods with four and five stages for the numerical integration of initial value problems with oscillatory or periodic solutions are developed. In these methods, for a given fixed ω the coefficients of the formulae of the pair are selected so that they integrate exactly systems with solutions in the linear space generated by $\{\sinh(\omega t), \cosh(\omega t)\}$, the estimate of the local error behaves as $\mathcal{O}(h^4)$ and the high-order formula has fourth-order accuracy when the stepsize $h \to 0$. These new pairs are compared with another one proposed by Franco [J.M. Franco, An embedded pair of exponentially fitted explicit Runge–Kutta methods, J. Comput. Appl. Math. 149 (2002) 407–414] on several problems to test the efficiency of the new methods.

1. Introduction

In the past years, there has been a growing interest in exponentially fitted (EF) methods for the numerical solution of IVPs which have periodic or oscillating solutions. Since one of the pioneers in this area, Bettis [1], showed the first paper with adapted RK algorithms, several authors like Paternoster [2], Simos [3], Vanden Berghe et al. [4–6], Gautschi [7], Franco [8], Simos et al. [9], have developed methods based on Runge–Kutta formulae. Particularly, Vanden Berghe et al. obtained methods with frequency-dependent coefficients that are able to integrate exactly first-order ordinary differential systems with solutions belonging to a linear space generated by a set of functions of type $\{\sinh(\omega t), \cosh(\omega t)\}$, where ω is a prescribed frequency.

Franco [8] used this idea to develop an embedded pair which is based on the four-stage explicit EFRK method presented by Vanden Berghe et al. [4,5] and he showed that his new embedded pair has algebraic order 4(3) and it was related in a unique way to the Zonneveld 4(3) pair. In addition, he compared the efficiency of this new method against another one introduced by Vanden Berghe et al. [5,6] which used the same EFRK technique but with error and step length control based on Richardson's extrapolation.

After that, our objective is to construct explicit embedded pairs of exponentially fitted methods with algebraic order 4(3) and compare its efficiency relative to Franco's pair [8], which is composed by a four-stage explicit EFRK method of algebraic order four and an additional stage to construct the embedded pair of algebraic order three. Then, we are going to develop two new pairs 4(3) with other techniques: the first one is a new explicit EFRK method of algebraic order four derived from the well-known rule of $\frac{3}{8}$ and the third-order method uses the FSAL technique [10]; in the second one, we obtain an embedded pair 4(3) with five stages with some simplifying assumption [10]. Finally, several numerical experiments are carried out to compare the efficiency of all these types of explicit embedded pairs.

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This research was initiated by both authors one year ago and would have been a part of the Dissertation of the first author if he had not died suddenly; the second author continued the work and now wishes to dedicate the present paper to the memory of his dear friend and companion Antonio.

2. Some preliminary results

Consider autonomous IVPs

$$\begin{aligned} &y'(t) = f(y(t)) \quad \text{with } t \in [0, T], \\ &y(0) = y_0, \ \in \mathbb{R}^m, \end{aligned} \tag{1}$$

with periodic or oscillatory solution. For a given fixed frequency $\omega \in i\mathbb{R}$ the above IVP will be solved by an explicit exponentially fitted Runge–Kutta method (EFRK) of s stages defined by:

$$\begin{aligned} &g_i = f\left(\gamma_i(\nu)y_n + h\sum_{j=1}^{i-1} a_{ij}(\nu)g_j\right), \quad i = 1, \ldots, s, \\ &y_{n+1} \equiv \psi_h(y_n) = y_n + h\sum_{i=1}^{s} b_i(\nu)g_i, \end{aligned} \tag{2}$$

with $\nu = \omega h$, and $\gamma_i(\nu), b_i(\nu), a_{ij}(\nu)$ are real $\mathcal{C}^\infty$ functions in some neighborhood of $\nu = 0$, defining the method. Here, $\psi_h = \psi_{h,f}$ denotes the numerical flow associated to f.

The method (2) is assumed to integrate exactly all IVP (1) with solution $y(t) \in \langle \sinh(\omega t), \cosh(\omega t)\rangle$. Note that for standard RK methods, $\gamma_i = 1$ and a_{ij}, b_i are real constants.

Using a notation similar to the one used by Butcher, an explicit s-stage EFRK method is represented by:

$$\begin{array}{c|c|cccccc} 0 & \gamma_1 & 0 & & & & \\ c_2 & \gamma_2 & a_{21} & 0 & & & \\ c_3 & \gamma_3 & a_{31} & a_{32} & 0 & & \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \\ c_s & \gamma_s & a_{s1} & a_{s2} & \ldots & a_{s\,s-1} & 0 \\ \hline & & b_1 & b_2 & \ldots & b_{s-1} & b_s \end{array} \equiv \begin{array}{c|c|c} c & \gamma & A \\ \hline & & b^T \end{array}$$

where $A \in \mathbb{R}^{s\times s}$ and $\gamma, b, c \in \mathbb{R}^s$.

For $\gamma_i(\nu) \equiv 1$, $i = 1, \ldots, s$ Eqs. (2) are formally the same as those of explicit s-stage RK formula and therefore, even with the variable coefficient $a_{ij}(\nu), b_i(\nu)$, Butcher's theory can be used to derive an order theory with the same elementary differentials used there. However, the inclusion of the additional parameters $\gamma_i(\nu) \neq 1$ implies the existence of new elementary differentials, here termed as *ghost* elementary differentials, in the Taylor series expansion of the numerical solution. As an example, we consider the stages of a generic explicit two-stage RK method for an autonomous differential equation $y' = f(y)$. Then,

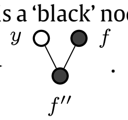
$$\begin{aligned} &g_1 = f(y_n), \\ &g_2 = f(\gamma_2 y_n + ha_{21}g_1) = f(y_n + ha_{21}f_n + \delta_2 y_n), \end{aligned}$$

with $\gamma_2(\nu) = 1 + \delta_2(\nu)$. Now, denoting by $f := f(y_n)$ and $y := y_n$, the series expansion of the second stage up to second order is:

$$g_2 = f + ha_{21}f'f + \frac{1}{2}h^2a_{21}^2f''(f, f) + \delta_2\mathbf{f}'\mathbf{y} + ha_{21}\delta_2\mathbf{f}''(\mathbf{f}, \mathbf{y}) + \frac{1}{2}\delta_2^2\mathbf{f}''(\mathbf{y}, \mathbf{y}) + \cdots. \tag{3}$$

The *ghost* elementary differentials (highlighted in boldface) will be present in the Taylor series expansion of the numerical solution and generate additional order conditions.

To deal with *ghost* elementary differentials, in addition to the set of standard rooted trees $\mathcal{T}$ (denoted with 'black' nodes), we will consider another set of trees $\mathcal{G}$ associated to the *ghost* elementary differentials.

For the graphical representation of the new trees of $\mathcal{G}$, we consider the 'black' vertices for representing an f and 'white' vertices for a y. Note that the root always is a 'black' node, a 'white' node has no sons, and therefore 'white' nodes only appear as leafs of some branch, e.g. $f''(y, f) \longleftrightarrow$ 

.

Definition. The set of rooted trees $\mathcal{G}$ is recursively defined as follows:

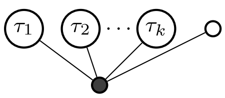
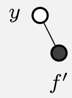
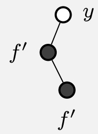
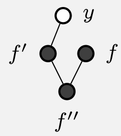
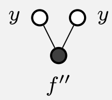
- $\tau_0 = \circ \in \mathcal{G}$ is the tree relative to y.
- if $\tau_1, \ldots, \tau_k \in \mathcal{G} \bigcup \mathcal{T}$, then $\tau = [\tau_1, \ldots, \tau_k, \tau_0] \in \mathcal{G}$. 

Table 1
Some *ghost* elementary differentials.

$F(\tau)(y)$	$\Phi_A(\tau)$	τ	$\rho(\tau)$	$\rho'(\tau)$
$f'y$	$b^T\delta$		2	1
$f'f'y$	$b^TA\delta$		3	2
$f''(f'y, f)$	$b^T(A\delta \cdot Ae)$		4	3
$f''(y, y)$	$b^T\delta^2$		3	1

We note that for this class of EFRK methods, the vector of nodes $c = c(\nu)$ does not satisfy the simplifying assumption $Ae = c, e = (1, \dots, 1)^t$ and therefore the vector function Φ_A must be computed recursively on the order of the rooted trees by using only $A(\nu)$.

The local error at y_0 with stepsize h is given by

$$e_l = \psi_h(y_0) - y(h, y_0),$$

where $y(h, y_0)$ is the exact solution of (1), and it has the power series expansion [11]

$$e_l = \sum_{\tau \in \mathcal{T}} \frac{h^{\rho(\tau)}}{\sigma(\tau)} \alpha(\tau) \left(b^T(\nu)\Phi_A(\tau) - \frac{1}{\Gamma(\tau)} \right) F(\tau)(y_0) + e_{ghost}, \tag{4}$$

where $\mathcal{T}$ is the set of rooted trees with order $\rho(\tau) \geq 1$, $F(\tau)(y_0)$ is the elementary differential of f associated to $\tau \in \mathcal{T}$ at y_0, $\alpha(\tau)$ is the number of monotonic labellings of τ and $\sigma(\tau)$ is the symmetry coefficient.

So, the local error is composed of two terms. The first term is the standard local error and yields the order conditions for order p,

$$\Gamma(\tau) b^T \Phi(\tau) = 1, \quad \forall\, \tau \text{ so that } \rho(\tau) \leq p.$$

The second one, that we have called *ghost local error*, corresponds to all the terms that contain *ghost* elementary differentials.

Before studying the second case, we rewrite the stages of the Runge–Kutta method (2) in autonomous form

$$g_i = f\left(y_n + h \sum_{j=1}^{i-1} a_{ij}(\nu) g_j + \delta_i(\nu) y_n \right), \quad i = 1, \dots, s.$$

Remark. Note that the series expansions of the functions $\delta_i(\nu)$, $b_i(\nu)$ and $a_{ij}(\nu)$ are even, (see also [8]), and therefore

$$\delta^{(2k-1)}(\nu) = A^{(2k-1)}(\nu) = b^{(2k-1)}(\nu) = 0, \quad k = 1, \dots,$$

and in particular $\delta(\nu) = \mathcal{O}(\nu^q)$, $q \geq 2$.

In Table 1 some examples to know how *ghost* elementary differentials are related with their order condition and their corresponding tree are given.

Taking into account the above comments, we obtain for the *ghost error* the following expression

$$e_{ghost} = \sum_{\tau \in \mathcal{G}, \rho(\tau) \geq 2} \frac{h^{\rho'(\tau)}}{\sigma(\tau)} \alpha(\tau) b^T(\nu) \Phi_A(\tau) F(\tau)(y_0),$$

with $\rho'(\tau) = \rho(\tau) - \rho_G(\tau)$, where $\rho_G(\tau) \geq 1$ is the number of leafs of τ relative to y (the number of white nodes in the tree).

Table 2
Order conditions.

$b^T e = 1 + \mathcal{O}(\nu^4)$,	$b^T Ae = \frac{1}{2} + \mathcal{O}(\nu^3)$,	$b^T A^2 e = \frac{1}{6} + \mathcal{O}\left(\nu^2\right)$,
$b^T A^3 e = \frac{1}{24} + \mathcal{O}(\nu)$,	$b^T (Ae)^2 = \frac{1}{3} + \mathcal{O}(\nu^2)$,	$b^T (Ae \cdot A^2 e) = \frac{1}{8} + \mathcal{O}(\nu)$,
$b^T A(Ae)^2 = \frac{1}{12} + \mathcal{O}(\nu)$,	$b^T (Ae)^3 = \frac{1}{4} + \mathcal{O}(\nu)$,	
...		
$b^T \delta = \mathcal{O}(\nu^4)$,	$b^T A\delta = \mathcal{O}(\nu^3)$,	$b^T (\delta \cdot Ae) = \mathcal{O}(\nu^3)$,

Proposition. *With the previous notation and from the fact that $\nu = \omega h$, the method (2) has order p if:*

- $b(\nu)^T \Phi_{A(\nu)}(\tau) - \frac{1}{\Gamma(\tau)} = \mathcal{O}(h^{p'})$ *with* $p' \geq p + 1 - \rho(\tau)\ \forall \tau \in \mathcal{T}$ *with order* $\rho(\tau) \leq p$
- $b(\nu)^T \Phi_{A(\nu)}(\tau) = \mathcal{O}(h^{p'})$ *with* $p' \geq p + 1 - \rho'(\tau)\ \forall \tau \in \mathcal{G}$ *with order* $\rho(\tau) \leq p$.

We have computed the h-power series expansion of the local error, obtaining the set of fourth-order conditions presented in Table 2, where $e = (1, \ldots, 1)^T$.

3. Construction of the embedded pairs

Following the approach of Vanden Berghe et al. in [4,6], to construct s-stage EFRK methods with respect to a given linear space of functions defined by a basis $\mathcal{F}$, we associate to (2) the $s + 1$ linear functionals

$$\mathcal{L}_i[y](t) := y(t + c_i h) - \gamma_i y(t) - h \sum_{j=1}^{i-1} a_{ij} y'(t + c_j h), \quad i = 0, \ldots, s,$$

where $c_0 = 1$ and $a_{0j} = b_j$, $j = 1, \ldots, s$. Then, we choose the available parameters of the method ψ_h so that all linear functionals $\mathcal{L}_i$ vanish for the functions of $\mathcal{F} = \{\sinh(\omega t), \cosh(\omega t)\}$, and we may ensure that the corresponding method (2) will integrate exactly all IVPs (1) with solutions belonging to the linear space generated by $\mathcal{F}$. For the sake of simplicity, we have carried out this process for the well-known rule of 3/8 ($c_1 = 0, c_2 = 1/3, c_3 = 2/3, c_4 = 1$) obtaining the exponentially fitted method with coefficients a_{ij}, γ_i given by:

$$\begin{aligned}
\gamma_2 &= \cosh(\mu), & a_{21} &= \frac{\sinh(\mu)}{3\mu}, \\
a_{31} &= -\frac{1}{3}, & a_{32} &= \frac{\sinh(2\mu) + \mu}{3\mu \cosh(\mu)}, \\
\gamma_3 &= \frac{\cosh(\mu) - \mu \sinh(\mu)}{\cosh(\mu)} & a_{41} &= 1, \\
\gamma_4 &= \frac{\cosh(\mu) + 3\mu \sinh(\mu)\,(2\cosh(\mu) - 1)}{\cosh(2\mu)}, & a_{42} &= -1, \\
a_{43} &= \frac{\cosh(\mu)(4\sinh(\mu) + 3\mu) - \sinh(\mu)}{3\mu \cosh(2\mu)}, & \mu &= \frac{\nu}{3}.
\end{aligned}$$

In order to determine the vector b we impose the conditions of standard algebraic order 2 ($b^T e = 1$ and $b^T c = \frac{1}{2}$) and in addition that the numerical approximation at $t_n + h$ be exact for $\{\sinh(\omega t), \cosh(\omega t)\}$.

$$\begin{aligned}
&b_1 + b_2 + b_3 + b_4 = 1, \\
&\frac{1}{3} b_2 + \frac{2}{3} b_3 + b_4 = \frac{1}{2}, \\
&b_1 \cosh(c_1 \nu) + b_2 \cosh(c_2 \nu) + b_3 \cosh(c_3 \nu) + b_4 \cosh(c_4 \nu) = \frac{\sinh(\nu)}{\nu}, \\
&b_1 \sinh(c_1 \nu) + b_2 \sinh(c_2 \nu) + b_3 \sinh(c_3 \nu) + b_4 \sinh(c_4 \nu) = \frac{(\cosh(\nu) - 1)}{\nu}.
\end{aligned}$$

These equations have the unique solution

$$\begin{aligned}
b_1 = b_4 &= -\frac{\nu\sigma_3 + 2 - 4\tau_3^2 + 2\tau_3}{4\sigma_3(\tau_3 - 1)\nu}, \\
b_2 = b_3 &= \frac{2\sigma_3 \nu \tau_3 - \nu\sigma_3 + 2 - 4\tau_3^2 + 2\tau_3}{4\sigma_3(\tau_3 - 1)\nu},
\end{aligned}$$

where $\sigma_3 = \sinh(\mu)$, $\tau_3 = \cosh(\mu)$. With the above choice, it is not difficult to show that all conditions for the fourth-order solution of the Table 2 are fulfilled.

In order to construct the embedded pair, we add the FSAL stage ($c_5 = 1$) to compute the coefficients of vector $\hat{b}$ of order 3 and therefore the cost of this pairs is four effective stages per integration step.

Imposing the condition $\hat{b}^T e = 1$ and also that the method be exact for $\langle \sinh(\omega t), \cosh(\omega t)\rangle$, we have the equations:

$$\begin{aligned}
&\hat{b}_1 + \hat{b}_2 + \hat{b}_3 + \hat{b}_4 + \hat{b}_5 = 1,\\
&\hat{b}_1 \cosh(c_1\nu) + \hat{b}_2 \cosh(c_2\nu) + \hat{b}_3 \cosh(c_3\nu) + (\hat{b}_4 + \hat{b}_5)\cosh(c_4\nu) = \frac{\sinh(\nu)}{\nu},\\
&\hat{b}_1 \sinh(c_1\nu) + \hat{b}_2 \sinh(c_2\nu) + \hat{b}_3 \sinh(c_3\nu) + (\hat{b}_4 + \hat{b}_5)\sinh(c_4\nu) = \frac{\cosh(\nu) - 1}{\nu}.
\end{aligned}$$

Choosing $\hat{b}_3$ and $\hat{b}_5$ as free parameters, in order to satisfy the third-order conditions, we obtain a relationship between $\hat{b}_3$ and $\hat{b}_5$ with condition $\hat{b}^T A(0)c = 1/6 \Leftrightarrow \hat{b}_3 = \frac{3}{8} - \frac{3}{4}\hat{b}_5$. For a correct tuning of the embedded pair, the third-order approximation, depending on $\hat{b}_5$, should be chosen to enable correct error estimation. The usual criteria (see [12]) to select the available parameters is that the quantities

$$B = \frac{|\hat{T}_5|}{|\hat{T}_4|}, \qquad C = \frac{|\hat{T}_5 - T_5|}{|\hat{T}_4|}, \tag{5}$$

are required not to be large. Here $|T_5|$ (or $|\hat{T}_4|$, $|\hat{T}_5|$) is the ℓ_2-norm of the coefficients of the elementary differentials in the development of the local error of y_{n+1} solution ($\hat{y}_{n+1}$ solution respectively), i.e.

$$|T_{p+1}| = \sqrt{\sum_{\rho(\tau)=p+1} \left(\frac{\alpha(\tau)}{\sigma(\tau)}\left(b^T(\nu)\Phi_A(\tau) - \frac{1}{\Gamma(\tau)}\right)\right)^2}.$$

Also, the absolute stability region for the lower-order formula should be reasonably close to the higher-order formula. Therefore, taking $\hat{b}_5 = \frac{1}{10}$ we obtain the values $B = 0.88$, $C = 1.11$, and the coefficients are given by:

$$\begin{aligned}
\hat{b}_1 &= -\frac{\frac{28}{5}\nu\tau_3 + \frac{12}{5}\nu - 16\sigma_3\tau_3 - 8\sigma_3}{8\nu(2\tau_3^2 - \tau_3 - 1)},\\
\hat{b}_2 &= \frac{\frac{28}{5}\sigma_3\nu\tau_3 - \frac{8}{5}\nu\sigma_3 - 16\tau_3^2 + 8\tau_3 + 8}{8\nu\sigma_3(\tau_3 - 1)},\\
\hat{b}_3 &= \frac{3}{10},\\
\hat{b}_4 &= -\frac{\frac{8}{5}\sigma_3\nu\tau_3^2 + \frac{8}{5}\sigma_3\nu\tau_3 + \frac{4}{5}\nu\sigma_3 - 16\tau_3^3 + 8\tau_3^2 + 8\tau_3}{8\nu(2\tau_3^2 - \tau_3 - 1)\sigma_3},\\
\hat{b}_5 &= \frac{1}{10}.
\end{aligned}$$

Note that for values $|\nu| \ll 1$, for computational purposes it is convenient to use a truncated Taylor's series of the coefficients due mainly to severe cancelation errors and the fast convergence of the series.

Notes. The idea of the FSAL stage cannot be used for the classic Runge–Kutta, due to the fact that it only has three different values of c_i.

The order conditions given in [8], can be deduced from the above set given in Table 2 if we consider only the first terms. So,

- $\mathcal{O}(\nu^4) = b^T\delta = \frac{\nu^2}{2} b^T\delta''(0) + \mathcal{O}(\nu^4) \Leftrightarrow b^T\delta''(0) = \mathcal{O}(\nu^2)$
- $\mathcal{O}(\nu^3) = b^T(\delta \cdot Ae) = \frac{\nu^2}{2} b^T(\delta''(0)\cdot Ae) + \mathcal{O}(\nu^4) \Leftrightarrow b^T(\delta''(0)\cdot Ae) = \mathcal{O}(\nu)$
- $\mathcal{O}(\nu^3) = b^T A\delta = \frac{\nu^2}{2} b^T A\delta''(0) + \mathcal{O}(\nu^4) \Leftrightarrow b^T A\delta''(0) = \mathcal{O}(\nu)$ which is missing in [8].

Next, we will develop a new family of pairs 4(3) with five stages with the simplifying assumptions [13]

$$\begin{aligned}
&b^T A = b^T - (b\cdot c)^T,\\
&Ae = c,\\
&Ac = \frac{1}{2}c^2 - \frac{c_2^2}{2}e_2,\\
&Ac^2 = \frac{1}{3}c^3 - \frac{c_2^3}{3}e_2
\end{aligned} \tag{6}$$

with $e_2 = (0, 1, 0, \ldots, 0)^T$. Manipulating carefully the set of nonlinear equations composed by (6) and the order conditions for algebraic fourth order, we arrive to a family of fourth-order methods depending on two free parameters c_3 and c_4 given

Table 3
Comparison of RK4(3) methods.

Method	$\lvert\cdot\rvert_2$	IAS
New4(3)	1.87×10^{-4}	$[-3.21, 0]$
DP4(3)	5.86×10^{-4}	$[-3.15, 0]$
Nor4(3)	1.21×10^{-2}	$[-2.79, 0]$

by:

$$
\begin{aligned}
b_3 &= \frac{2c_4-1}{12(c_3-c_4)(c_3-1)c_3}, & b_4 &= \frac{2c_3-1}{12(c_4-c_3)(c_4-1)c_4},\\
b_5 &= \frac{6c_4c_3-4c_3-4c_4+3}{12(c_3-1)(c_4-1)}, & b_2 &= 0,\\
b_1 &= 1-b_3-b_4-b_5, & c_2 &= \frac{2c_3}{3},\\
a_{32} &= \frac{c_3^2}{2c_2}, & a_{31} &= c_3-a_{32}\\
a_{42} &= -\frac{3c_4^2(2c_4-3c_3)}{4c_3^2} & a_{43} &= \frac{-c_4^2(c_3-c_4)}{c_3^2},\\
a_{54} &= \frac{(2c_3-1)(c_3-1)(c_4-1)}{c_4(6c_3c_4-4c_3-4c_4+3)(c_3-c_4)}, & a_{52} &= \frac{3(6a_{54}c_4(c_4-c_3)+3c_3-2)}{4c_3^2}\\
a_{53} &= \frac{a_{54}c_4(2c_3-3c_4)+1}{c_3^2} & a_{51} &= 1-a_{52}-a_{53}-a_{54},\\
a_{41} &= c_4-a_{42}-a_{43} & a_{51} &= c_5-a_{52}-a_{53}-a_{54}
\end{aligned}
$$

where $c_4 \neq \frac{3-4c_3}{6c_3-4}$ and the obvious relations $c_i \neq c_j$, $i \neq j$.

For the third-order embedded method, the order equations lead to:

$$\hat{b}_2 = 0, \qquad \hat{b}^T c^i = \frac{1}{i+1}, \quad i = 0, 1, 2,$$

with $\hat{b}_5$ as free parameter.

The values of $(c_3, c_4, \hat{b}_5)$ have been chosen subject to the following constraints: Firstly, to minimize the ℓ_2-norm of the coefficients of the elementary differentials in the leading term of the local error expansion. Secondly, that the high-order formula of the pair possesses a large stability interval. Thirdly, that the estimate of the local error given by the pair provides a reliable stepsize policy. For the first point, we get

$$|T_5|_2^2 = \frac{243-714c_3+595c_3^2+(2c_3-1)c_4\left(2(501-595c_3)+1315(2c_3-1)c_4\right)}{207360},$$

that is zero for $c_3 = 2/5$ and $c_4 = 1$, but the fourth-order solution collapses, because of the vanishing denominator of b_i. In this way, and taking into account the above requirements we have obtained the values of the parameters

$$c_3 = \frac{89}{225}, \qquad c_4 = \frac{289}{300}, \qquad \hat{b}_5 = -\frac{1}{5},$$

giving the values $B \simeq C = 0.52$ in (5). Table 3 shows the Euclidean norm of the coefficients of the principal term of the local error and the interval of absolute stability (IAS) of the new methods together with the ones DP4(3) due to Dormand and Prince [13] and Nor4(3) due to Nørsett [14].

Carrying out a similar process like the above embedded pair, we obtain the exponentially fitted version given by:

$$
\begin{aligned}
a_{21} &= \sinh\left(\frac{178}{675}\nu\right) \Big/ \nu,\\
a_{31} &= 89/900,\\
a_{32} &= \frac{900\sinh\left(\frac{89}{225}\nu\right)-89\nu}{900\nu\cosh\left(\frac{178}{675}\nu\right)},\\
a_{41} &= 67490459/76041600,\\
a_{42} &= -83437479/25347200,\\
a_{43} &= \frac{76041600\sinh\left(\frac{289}{300}\nu\right)-67490459\nu+250312437\nu\cosh\left(\frac{178}{675}\nu\right)}{76041600\nu\cosh\left(\frac{89}{225}\nu\right)},\\
a_{51} &= 1131789887/904356412,
\end{aligned}
$$

$$a_{52} = -254859075/53197436,$$
$$a_{53} = 31234577700/6795972449,$$
$$a_{54} = \left(462126126532\sinh(\nu) - 578344632257\nu + 2213960784525\nu\cosh\left(\frac{178}{675}\nu\right) - 2123951283600\nu\cosh\left(\frac{89}{225}\nu\right)\right)\Big/\left(462126126532\nu\cosh\left(\frac{289}{300}\nu\right)\right),$$
$$\gamma_1 = 1,$$
$$\gamma_2 = \cosh(178\nu/675),$$
$$\gamma_3 = \frac{\cosh\left(\frac{89}{675}\nu\right)\left(\frac{89}{450}\sinh\left(\frac{89}{675}\nu\right)\nu + 1\right)}{\cosh\left(\frac{178}{675}\nu\right)},$$
$$\gamma_4 = \frac{76041600\cosh\left(\frac{511}{900}\nu\right) - 250312437\nu\sinh\left(\frac{89}{675}\nu\right) + 67490459\,\nu\sinh\left(\frac{89}{225}\nu\right)}{76041600\cosh\left(\frac{89}{225}\nu\right)},$$
$$\gamma_5 = \left(462126126532\cosh\left(\frac{11}{300}\nu\right) - 2213960784525\,\nu\,\sinh\left(\frac{1889}{2700}\nu\right) + 2123951283600\,\nu\,\sinh\left(\frac{511}{900}\nu\right) + 578344632257\nu\sinh\left(\frac{289}{300}\nu\right)\right)\Big/\left(462126126532\cosh\left(\frac{289}{300}\nu\right)\right).$$

With the above set of parameters, it is easy to show that the conditions of Table 2 are fulfilled.
Due to the lengthy expressions of the vectors b, $\hat{b}$, we give only their series expansions up to fourth order.

$$b_1 = \frac{3198}{25721} - \frac{3584591}{8333604000}\nu^2 - \frac{5119242101713}{28350920808000000000}\nu^4 + \mathcal{O}(\nu^6)$$
$$b_2 = 0,$$
$$b_3 = \frac{7036875}{12370288} + \frac{1130487}{989623040}\nu^2 - \frac{716370877619}{336669758208000000}\nu^4 + \mathcal{O}(\nu^6)$$
$$b_4 = \frac{1410000}{1624469} - \frac{6228487}{877213260}\nu^2 + \frac{25164120037429}{298427951052000000}\nu^4 + \mathcal{O}(\nu^6),$$
$$b_5 = -\frac{1679}{2992} + \frac{3096341}{484704000}\nu^2 - \frac{13255812002537}{164896300800000000}\nu^4 + \mathcal{O}(\nu^6),$$
$$\hat{b}_1 = \frac{6213}{51442} + \frac{2951}{61730400}\nu^2 - \frac{1267188167083}{63002046240000000}\nu^4 + \mathcal{O}(\nu^6)$$
$$\hat{b}_2 = 0,$$
$$\hat{b}_3 = \frac{26325}{45479} + \frac{34579}{109149600}\nu^2 - \frac{51015557597}{4125854880000000}\nu^4 + \mathcal{O}(\nu^6)$$
$$\hat{b}_4 = \frac{118200}{147679} - \frac{10769}{29535800}\nu^2 + \frac{2937099857609}{90432712440000000}\nu^4 + \mathcal{O}(\nu^6),$$
$$\hat{b}_5 = -\frac{1}{2}.$$

4. Numerical experiments

In order to test the efficiency of the new exponentially fitted pairs obtained in the above section, we have compared the behavior of variable stepsize codes based on the following pairs:

- EF4(3)4S for the exponentially fitted pair based in the 3/8 rule with four effective stages per step using the FSAL technique.
- EF4(3)5S for the exponentially fitted pair with five effective stages per step.
- JMF4(3)5S for the exponentially fitted pair in [8] with five effective stages per step.

We present here the results for the following three problems:

Problem 1. Duffing's equation, (see, e.g. [15])

$$y'' + (\lambda^2 + k^2)y = 2k^2y^3, \quad t \in [0, 40],$$
$$y(0) = 0, \qquad y'(0) = \lambda,$$

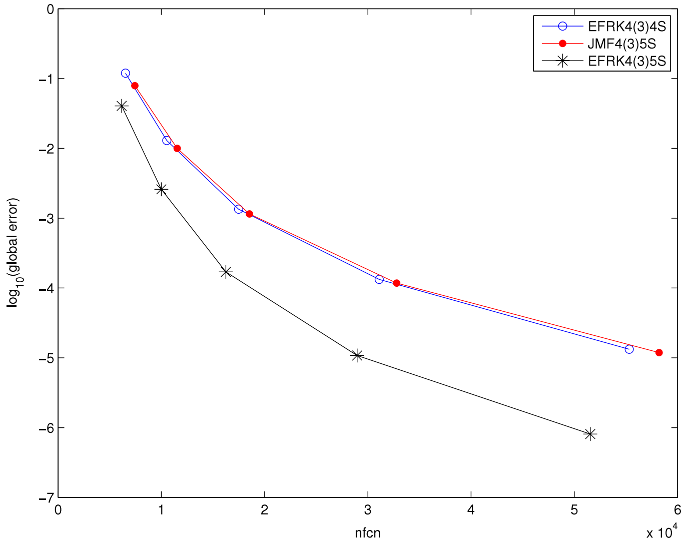


Fig. 1. Efficiency plot for Problem 1.

with $k = 0.035$ and $\lambda = 5$. The analytic solution is given by:

$$y(t) = \mathrm{sn}\left(\lambda t, \left(\frac{k}{\lambda}\right)^2\right)$$

where sn represents the elliptic Jacobi function. We choose $\omega = 5i$ (see Fig. 1).

Problem 2. The rigid solid equations, (see, e.g. [16,17])

$$y' = ((\alpha - \beta)y_2y_3, (1-\alpha)y_3y_1, (\beta - 1)y_1y_2)^T, \quad t \in [0, 40],$$
$$y(0) = (0, 1, 1)^T,$$

with $\alpha = 1 + \frac{1}{\sqrt{1.51}}$, $\beta = 1 - \frac{0.51}{\sqrt{1.51}}$. The exact solution is given by:

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

where sn, cn, dn are Jacobi's elliptical functions. This solution describes the motion of a rigid solid without forces operating on it. It has been taken $\omega = \frac{2\pi}{T} i$ with $T = 7.45056320933095$ (see Fig. 2).

Problem 3. Kepler's perturbed problem (see, e.g. [15])

Kepler's perturbed problem is given by the Hamiltonian function:

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

where ε is a low positive parameter. The initial conditions are

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

and the theoretical solution is

$$q_1(t) = \cos(t + \varepsilon t), \qquad q_2(t) = \sin(t + \varepsilon t).$$

It has been taken $\omega = (q_1^2(0) + q_2^2(0))^{-3/4}$ and $\varepsilon = 10^{-3}$ (see Fig. 3).

In order to make comparisons, we have computed for a given tolerance (usually in the range 10^{-i}, $i = 2, \ldots, 7$) the logarithm of the maximum norm of the global error in the solution over the whole integration interval and the computational cost measured by the number of functions evaluations (nfcn) for the above set of problems.

In the next figures we have plotted the efficiency curves for all the problems considered. As it can be seen in these figures, the codes which use the new EF4(3) pairs appear to be the more efficient than Franco's pair. In particular, the EF4(3)5S is clearly the most efficient. This fact is supported by the optimization carried out with the additional stage for the construction of the embedded pair.

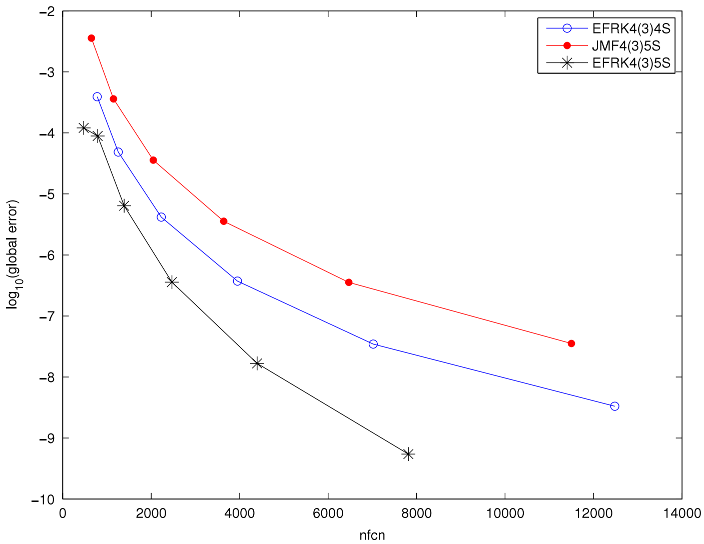


Fig. 2. Efficiency plot for Problem 2.

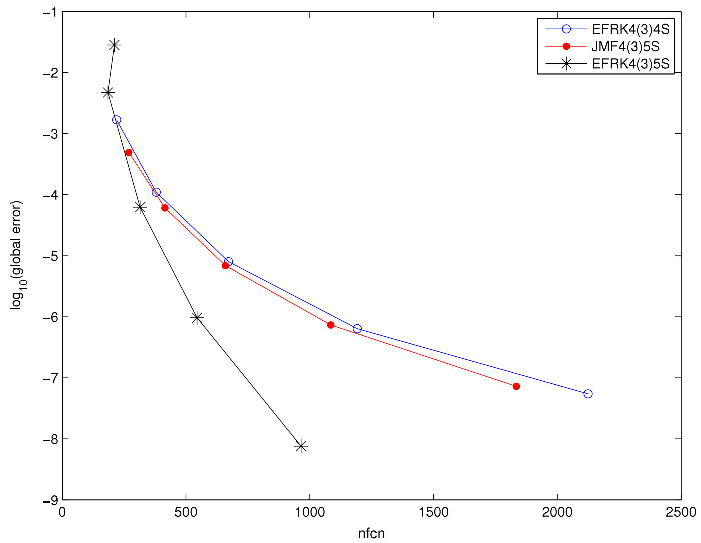


Fig. 3. Efficiency plot for Problem 3.

5. Conclusions

We have constructed two new pairs of orders 4(3), EF4(3)4S and EF4(3)5S, of exponentially fitted explicit methods with four and five effective stages respectively. Taking into account the results of an extensive set of representative numerical experiments, we may conclude that the new embedded pairs are more efficient than the previous ones constructed by Franco for these kinds of problems and are very suited for oscillatory problems whose frequency is known approximately in advance.

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