JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

Journal of Computational and Applied Mathematics 149 (2002) 407–414

www.elsevier.com/locate/cam

An embedded pair of exponentially fitted explicit Runge–Kutta methods

J.M. Franco

Departamento de Matemática Aplicada, C.P.S. de Ingeniería, Universidad de Zaragoza, María de Luna 3, 50015 Zaragoza, Spain

Received 21 November 2001; received in revised form 21 February 2002

Abstract

An embedded pair of exponentially fitted explicit Runge–Kutta (RK) methods for the numerical integration of IVPs with oscillatory solutions is derived. This pair is based on the exponentially fitted explicit RK method constructed in Vanden Berghe et al., and we confirm that the methods which constitute the pair have algebraic order 4 and 3. Some numerical experiments show the efficiency of our pair when it is compared with the variable step code proposed by Vanden Berghe et al. (J. Comput. Appl. Math. 125 (2000) 107). © 2002 Elsevier Science B.V. All rights reserved.

MSC: 65L05; 65L06

Keywords: Exponential fitting; RK methods; Oscillatory initial value problems

1. Introduction

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

$$y' = f(t, y), \qquad y(t_0) = y_0, \tag{1}$$

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 dynamics, and so forth; and they can be solved by using general purpose methods or 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 [1,2,4–7]

E-mail address: jmfranco@posta.unizar.es (J.M. Franco).

PII: S0377-0427(02)00485-5

in order to solve these classes of problems. A pioneer paper is due to [2], in which adapted RK algorithms with 3 and 4 stages for the integration of ODEs with oscillatory solutions are presented. More recently, Paternoster [4] considers the construction of RK and RK–Nyström methods which integrate trigonometric polynomials exactly. This author derives a family of two-stage RK methods with trigonometric order 1 which present algebraic order up to 3, but the main handicap of these methods is that they are fully implicit. Next, Simos and coworkers [1,5] 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. [6,7] introduced another exponentially fitted explicit RK method which integrates 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 exponentially fitted explicit RK method [7] with error and step length control based on Richardson extrapolation.

Here, we derive a five-stage embedded pair of exponentially fitted Runge–Kutta (EFRK) methods which is based on the four-stage explicit EFRK method presented in [6,7]. We confirm that the methods which constitute the pair have algebraic order 4 and 3, and that this pair corresponds in a unique way to an algebraic pair: the Zonneveld 4(3) pair [3]. The numerical experiments presented in Section 3 show the efficiency of our pair when it is compared with the variable step code proposed in [7].

2. Derivation of the exponentially fitted pair

Vanden Berghe et al. [6,7] constructed an explicit four-stage EFRK method based on the classical fourth-order RK method. This method is derived in such a way that it integrates 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 [4]). In order to carry out this goal, Vanden Berghe et al. [6] have modified the classical explicit RK methods in the following way:

$$g_1 = y_n,$$

$$g_i = \gamma_i(z) y_n + h \sum_{j=1}^{i-1} a_{ij}(z) f(t_j + c_j h, g_j), \quad i = 2, \ldots, s \tag{2}$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i(z) f(t_j + c_j h, g_j), \quad z = \lambda h. \tag{3}$$

These authors introduce the factors γ_i 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 method (2)–(3). So, with the above conditions and the additional requirement that Eq. (3) is exact whenever $f(t, y)$ is 1 or t, Vanden Berghe et al. [6,7] have obtained their four-stage explicit EFRK method.

2.1. The embedded pair

Now our interest is focused on the construction of an embedded pair of explicit EFRK methods based on the above mentioned EFRK method [6,7]. In order to avoid numerical difficulties when the parameter z is small, we impose that for $z \to 0$ the pair of EFRK methods reduces to a classical RK4(3) pair. This imposition implies that at least five stages are required and therefore we consider the following table:

$$
\begin{array}{c|c|ccccc}
0 & 1 & 0 & & & & \\
\frac{1}{2} & \cosh(z/2) & \dfrac{\sinh(z/2)}{z} & 0 & & & \\
\frac{1}{2} & \dfrac{1}{\cosh(z/2)} & 0 & \dfrac{\tanh(z/2)}{z} & 0 & & \\
1 & 1 & 0 & 0 & \dfrac{16\sinh(z/2)}{z} & 0 & \\
\frac{3}{4} & 1 & a_{51}(z) & a_{52}(z) & a_{53}(z) & a_{54}(z) & 0 \\
\hline
 & & b_1(z) & b_2(z) & b_3(z) & b_4(z) & 0 \\
\hline
 & & \bar{b}_1(z) & \bar{b}_2(z) & \bar{b}_3(z) & \bar{b}_4(z) & \bar{b}_5(z)
\end{array}
$$

with

$$
b_1(z) = b_4(z) = \frac{2\sinh(z/2) - z}{2z(\cosh(z/2) - 1)}, \qquad b_2(z) = b_3(z) = \frac{z\cosh(z/2) - 2\sinh(z/2)}{2z(\cosh(z/2) - 1)}.
$$

The fifth stage and the weights $\bar{b}_i(z)$ are introduced in order to obtain another explicit EFRK method so that $\|y_{n+1} - \bar{y}_{n+1}\|$ becomes a local error estimation at each step with a computational cost smaller than the technique based on Richardson extrapolation.

Imposing that the new method integrates exactly the family of functions $\{\exp(\lambda t), \exp(-\lambda t)\}$ and that Eq. (3) is exact whenever $f(t, y)$ is 1, their coefficients satisfy the following five equations:

$$
\begin{aligned}
&(\bar{b}_2 + \bar{b}_3)\sinh(z/2) + \bar{b}_4\sinh(z) + \bar{b}_5\sinh(3z/4) = (\cosh(z) - 1)/z,\\
&\bar{b}_1 + (\bar{b}_2 + \bar{b}_3)\cosh(z/2) + \bar{b}_4\cosh(z) + \bar{b}_5\cosh(3z/4) = \sinh(z)/z,\\
&\bar{b}_1 + \bar{b}_2 + \bar{b}_3 + \bar{b}_4 + \bar{b}_5 = 1,\\
&(a_{52} + a_{53})\sinh(z/2) + a_{54}\sinh(z) = (\cosh(3z/4) - 1)/z,\\
&a_{51} + (a_{52} + a_{53})\cosh(z/2) + a_{54}\cosh(z) = \sinh(3z/4)/z.
\end{aligned} \tag{4}
$$

Eqs. (4) leave four degrees of freedom in the determination of the weights $\bar{b}_i$ and the coefficients a_{5i}. Inspired by the classical Zonneveld 4(3) pair (cf. [3]), we choose the parameter values

$$
\bar{b}_2 = \bar{b}_3, \quad \bar{b}_5 = -\tfrac{16}{3}, \quad a_{51} = \tfrac{5}{32}, \quad a_{52} = \tfrac{7}{32}
$$

and the remaining coefficients are given by

$$\bar{b}_1(z) = \frac{3 - 3\cosh(z) - 32z\sinh(z/4) + 19z\sinh(z/2)}{6z\sinh(z/2) - 3z\sinh(z)},$$

$$\bar{b}_3(z) = \frac{-16z\cosh(z/4) + 19z\cosh(z/2) - 6\sinh(z/2)}{12z\sinh^2(z/4)},$$

$$\bar{b}_4(z) = \frac{3 - 3\cosh(z) + 16z\sinh(z/4) + 19z\sinh(z/2) - 16z\sinh(3z/4)}{6z\sinh(z/2) - 3z\sinh(z)},$$

$$a_{53}(z) = -\frac{32\cosh(z/4) - 32\cosh(z) + 7z\sinh(z/2) + 5z\sinh(z)}{32z\sinh(z/2)},$$

$$a_{54}(z) = \frac{5z - 32\coth(z/2) + [16/\sinh(z/4)]}{32z}.$$

For $z \to 0$ the EFRK pair obtained reduces to the well-known classical Zonneveld 4(3) pair. In addition, the trigonometric form for this EFRK pair emerges having in mind the relations: $\cosh(iv) = \cos(v)$ and $\sinh(iv) = i\sin(v)$.

2.2. Algebraic order of the EFRK pair

As it can be observed, the coefficients of the EFRK pair derived above do not satisfy the row-sum conditions usually imposed in the derivation of RK methods. Therefore, the algebraic order conditions tabulated in [3] are not valid for these methods. Now, the question is to investigate if the methods which constitute the EFRK pair are also of third and fourth order as in the classical Zonneveld 4(3) pair. In order to answer this question we have followed the way given in [3, pp. 143–148] for obtaining the terms of the local truncation error for these methods in the case of nonautonomous first-order differential systems. Having in mind that the parameters of the method are steplength dependent and, with $e = (1,1,1,1,1)^{\mathrm{T}}$, they satisfy

$$\gamma(0) = e, \qquad \gamma'(0) = 0, \qquad \gamma'''(0) = 0, \ldots,$$

$$A(0)e = c, \qquad A'(0) = 0, \qquad A'''(0) = 0, \ldots,$$

the conditions up to fourth-order are the following ones:

Order 2 *requires*:

$$b^{\mathrm{T}}(z)e = 1 + \mathcal{O}(z^4), \qquad b^{\mathrm{T}}(z)c = \tfrac{1}{2} + \mathcal{O}(z^3), \tag{5}$$

Order 3 *requires in addition*:

$$b^{\mathrm{T}}(z)\gamma''(0) = \mathcal{O}(z^2),$$

$$b^{\mathrm{T}}(z)c^2 = \tfrac{1}{3} + \mathcal{O}(z^2), \qquad b^{\mathrm{T}}(z)A(0)c = \tfrac{1}{6} + \mathcal{O}(z^2), \tag{6}$$

Order 4 *requires in addition*:

$$b^{\mathrm{T}}(z)(c\cdot\gamma''(0)) = \mathcal{O}(z), \qquad b^{\mathrm{T}}(z)A''(0)e = \mathcal{O}(z),$$

$$b^{\mathrm{T}}(z)c^3 = \tfrac{1}{4} + \mathcal{O}(z), \qquad b^{\mathrm{T}}(z)(c\cdot A(0)c) = \tfrac{1}{8} + \mathcal{O}(z),$$

$$b^{\mathrm{T}}(z)A(0)c^2 = \tfrac{1}{12} + \mathcal{O}(z), \qquad b^{\mathrm{T}}(z)A^2(0)c = \tfrac{1}{24} + \mathcal{O}(z). \tag{7}$$

If we check the conditions (5)–(7), we obtain

$$b^{\mathrm{T}}(z)e = 1, \quad b^{\mathrm{T}}(z)c = \tfrac{1}{2}, \quad b^{\mathrm{T}}(z)\gamma''(0) = 0, \quad b^{\mathrm{T}}(z)(c\cdot\gamma''(0)) = 0,$$

$$b^{\mathrm{T}}(z)c^2 = \frac{1}{3} - \frac{1}{1440}z^2 + \frac{1}{161280}z^4 - \frac{1}{19353600}z^6 + \frac{1}{2452488192}z^8 + \cdots,$$

$$b^{\mathrm{T}}(z)A(0)c = \frac{1}{6} - \frac{1}{2880}z^2 + \frac{1}{322560}z^4 - \frac{1}{38707200}z^6 + \frac{1}{4904976384}z^8 + \cdots,$$

$$b^{\mathrm{T}}(z)A''(0)e = -\frac{1}{5760}z^2 + \frac{1}{645120}z^4 - \frac{1}{77414400}z^6 + \frac{1}{9809952768}z^8 + \cdots,$$

$$b^{\mathrm{T}}(z)c^3 = \frac{1}{4} - \frac{1}{960}z^2 + \frac{1}{107520}z^4 - \frac{1}{12902400}z^6 + \frac{1}{1634992128}z^8 + \cdots,$$

$$b^{\mathrm{T}}(z)(c\cdot A(0)c) = \frac{1}{8} - \frac{1}{1920}z^2 + \frac{1}{215040}z^4 - \frac{1}{25804800}z^6 + \frac{1}{3269984256}z^8 + \cdots,$$

$$b^{\mathrm{T}}(z)A(0)c^2 = \frac{1}{12} - \frac{1}{5760}z^2 + \frac{1}{645120}z^4 - \frac{1}{77414400}z^6 + \frac{1}{9809952768}z^8 + \cdots,$$

$$b^{\mathrm{T}}(z)A^2(0)c = \frac{1}{24} - \frac{1}{2880}z^2 + \frac{1}{322560}z^4 - \frac{1}{38707200}z^6 + \frac{1}{4904976384}z^8 + \cdots,$$

and therefore we can affirm that the EFRK method with the weights b_i is of fourth order. Analogously, for the weights $\bar{b}_i$ we obtain

$$\bar{b}^{\mathrm{T}}(z)e = 1, \quad \bar{b}^{\mathrm{T}}(z)\gamma''(0) = 0,$$

$$\bar{b}^{\mathrm{T}}(z)c = \frac{1}{2} - \frac{1}{24}z^2 + \frac{5}{4608}z^4 - \frac{61}{2211840}z^6 + \frac{277}{396361728}z^8 + \cdots,$$

$$\bar{b}^{\mathrm{T}}(z)c^2 = \frac{1}{3} - \frac{137}{2880}z^2 + \frac{739}{645120}z^4 - \frac{34819}{1238630400}z^6 + \frac{551849}{784796221440}z^8 + \cdots,$$

$$\bar{b}^{\mathrm{T}}(z)A(0)c = \frac{1}{6} - \frac{137}{5760}z^2 + \frac{739}{1290240}z^4 - \frac{34819}{2477260800}z^6 + \frac{551849}{1569592442880}z^8 + \cdots,$$

and conditions (7) are not fulfilled. So, the EFRK method with the weights $\bar{b}_i$ has algebraic order three.

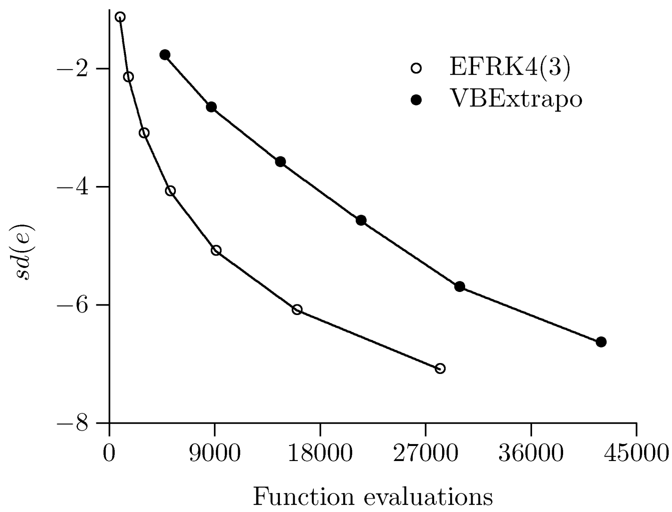

Fig. 1. Linear problem with variable coefficients: $\omega = 10$, $t_{\rm end} = 10$.

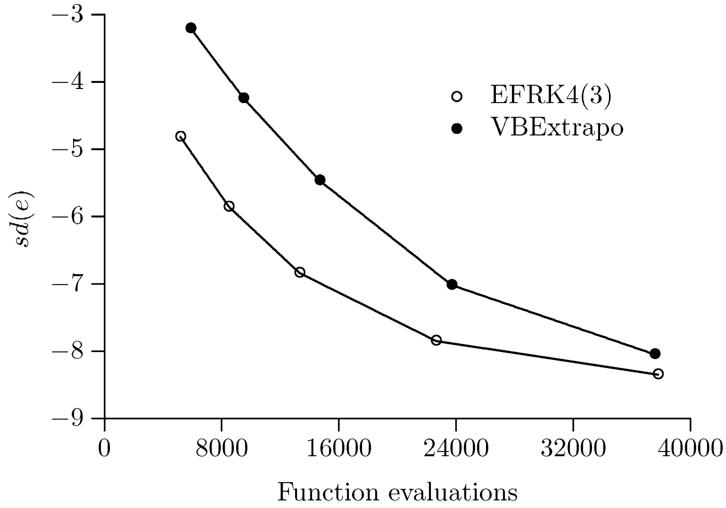

Fig. 2. Undamped Duffing's equation: $t_{\rm end} = 100$.

3. Numerical experiments

In order to evaluate the effectiveness of the EFRK pair we use several model problems which have periodic solutions. The criterion used in the numerical comparisons is the usual lest based on computing the maximum global error over the whole integration interval. In Figs. 1–3 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. The codes used in the comparisons have been denoted by:

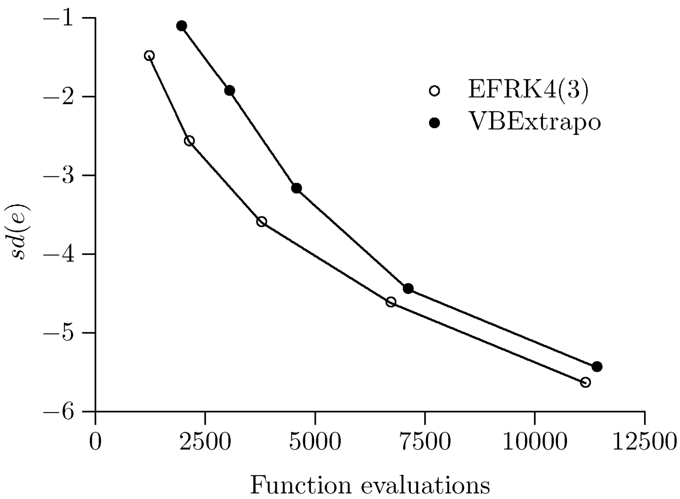

Fig. 3. Nonlinear system: $t_{\text{end}} = 10$.

- EFRK4(3): The trigonometric version of our embedded pair implemented in a variable step code following the way given in [3, pp. 167–169].
- VBExtrapo: The variable step code proposed in [7].

Problem 1. We consider the linear problem with variable coefficients

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

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

whose analytic solution is given by

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

This solution represents a periodic motion that involves a constant frequency and a variable frequency. In our test we choose the parameter values $\omega = 10$, $t_{\text{end}} = 10$ and the numerical results stated in Fig. 1 have been computed with error tolerances $\text{Tol} = 10^{-i}$, $i \geqslant 2$ and $\lambda = i10$.

Problem 2. We consider the periodically forced nonlinear problem (undamped Duffing's equation)

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

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

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 $t_{\text{end}} = 100$ and the numerical results stated in Fig. 2 have been computed with error tolerances $\text{Tol} = 10^{-i}$, $i \geqslant 3$ and $\lambda = i$.

Problem 3. We consider the nonlinear system

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

$$y_2'' = -4t^2 y_2 + \frac{2y_1}{\sqrt{y_1^2 + y_2^2}}, \quad y_2(0) = 0, \quad y_2'(0) = 0,$$

whose analytic solution is given by

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

This solution represents a periodic motion with variable frequency. In our test we choose the parameter value $t_{\text{end}} = 10$ and the numerical results stated in Fig. 3 have been computed with error tolerances $\text{Tol} = 10^{-i}$, $i \geqslant 2$ and $\lambda = it_n$ $(n \geqslant 1)$ at each step.

In view of the numerical results obtained in Problems 1–3, we may conclude that the code EFRK4(3) is clearly more efficient than the code VBExtrapo (see Figs. 1–3). This conclusion is not surprising because the technique based on embedded pairs for to estimate the local error requires a smaller computational cost than the technique based on Richardson extrapolation.

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

Acknowledgements

This research has been partially supported by Projects PB97-1018 of the DGES and P226-68 of the University of Zaragoza. We are grateful to J.J. Martínez for helping us in preparing the manuscript.

References

[1] G. Avdelas, T.E. Simos, J. Vigo-Aguiar, An embedded exponentially-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation and related periodic initial-value problems, Comput. Phys. Commun. 131 (2000) 52–67.
[2] D.G. Bettis, Runge–Kutta algorithms for oscillatory problems, J. Appl. Math. Phys. (ZAMP) 30 (1979) 699–704.
[3] E. Hairer, S.P. Nørsett, S.P. Wanner, Solving Ordinary Differential Equations I, Nonstiff Problems, Springer, Berlin, 1993.
[4] B. Paternoster, Runge–Kutta(–Nyström) methods for ODEs with periodic solutions based on trigonometric polynomials, Appl. Numer. Math. 28 (1998) 401–412.
[5] T.E. Simos, An exponentially-fitted Runge–Kutta method for the numerical integration of initial-value problems with periodic or oscillating solutions, Comput. Phys. Commun. 115 (1998) 1–8.
[6] G. Vanden Berghe, H. De Meyer, M. Van Daele, T. Van Hecke, Exponentially-fitted explicit Runge–Kutta methods, Comput. Phys. Commun. 123 (1999) 7–15.
[7] G. Vanden Berghe, H. De Meyer, M. Van Daele, T. Van Hecke, Exponentially fitted Runge–Kutta methods, J. Comput. Appl. Math. 125 (2000) 107–115.