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Frequency determination and step-length control for exponentially-fitted Runge–Kutta methods ☆

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Abstract

An exponentially fitted Runge–Kutta (EFRK) fifth-order method with six stages is constructed, which exactly integrates first-order differential initial-value problems whose solutions are linear combinations of functions of the form $\{\exp(\omega x), \exp(-\omega x)\}$, ($\omega \in \mathbb{R}$ or $i\mathbb{R}$). By combining this EFRK method with an equivalent classical embedded (4,5) Runge–Kutta method, a technique is developed for the estimation of the occurring ω-values. Error and step-length control is carried out by using the Richardson extrapolation procedure. Some numerical experiments show the efficiency of the introduced methods.

Keywords: Explicit Runge–Kutta methods; Initial-value problems; Oscillating solutions; Exponential fitting

1. Introduction

In the last decade, a lot of research has been performed in the area of the numerical solution of initial-value problems related to systems of first-order ordinary differential equations, i.e.,

$$y' = f(x, y), \quad y(x_0) = y_0. \tag{1.1}$$

Particular tuned methods have been proposed when the solution of the above problem exhibits a pronounced oscillatory character. Behaviour of pendulum-like systems, vibrations, resonances or wave propagation are all phenomena of this type in classical mechanics, while the same is true for the typical behaviour of quantum particles. Up to now, one has considered problems where the frequency was known in advance to develop linear multistep methods, whereby exact integration of a given set of linearly independent functions is achieved. A first good theoretical foundation of

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this technique was given by Gautschi [3] and by Lyche [6]. Since then, a lot of exponentially fitted linear multistep methods have been constructed; most of them were developed for second-order differential equations where the first derivative is absent, and applied to solve equations of the Schrödinger type. Also for first-order equations special tuned algorithms have been constructed. For an exhaustive list of references, we refer to [4,5] and references cited therein. In the class of Runge–Kutta (–Nyström) methods, a few methods with a reduced or null phase error have been considered [8,14–16]. Recently, two authors [9,7] have constructed Runge–Kutta (–Nyström) methods for which they claim that trigonometric functions with known periodicity are integrated exactly. Paternoster [7] used the linear stage representation of a Runge–Kutta method given in Albrecht's approach and derived some examples of implicit Runge–Kutta (–Nyström) methods of low algebraic order (for the definition of this property see [7]). On the other hand, Simos [9] constructed an explicit Runge–Kutta method of algebraic order 4, which integrates certain first-order initial-value problems with periodic or exponential solutions. Simos [10,11] applied some modified Runge–Kutta methods to solve Schrödinger equations. In [12] an alternative derivation of a more general explicit Runge–Kutta method of algebraic order 4, which integrates exactly first-order systems with solutions which can be expressed as linear combinations of $\exp(\omega x)$ and $\exp(-\omega x)$ ($\omega \in \mathbb{R}$ or $i\mathbb{R}$) is constructed and applied to several test systems. In [14] a heuristic way of determining ω is introduced and discussed. In the present paper, a more reliable technique is developed for the determination of the ω-values, which is based on a combined use of embedded classical explicit Runge–Kutta and exponentially fitted (explicit) Runge–Kutta (EFRK) methods.

2. The methods

For the description of EFRK methods, we use the notation introduced in [12,13]. As an example, we give below the form of an embedded EFRK method with six stages.

$$
\begin{aligned}
y_{n+1} &= y_n + h\sum_{i=1}^{5} b_i f(x_n + c_i h, Y_i),\\
\hat{y}_{n+1} &= y_n + h\sum_{i=1}^{6} \hat{b}_i f(x_n + c_i h, Y_i),\\
Y_1 &= y_n,\\
Y_i &= \gamma_i y_n + h\sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, Y_j),
\end{aligned}
\tag{2.2}
$$

with $i = 2,\ldots,6$, or in tableau form

$$
\begin{array}{c|c|ccccc}
c_1 & 1 & & & & & \\
c_2 & \gamma_2 & a_{21} & & & & \\
c_3 & \gamma_3 & a_{31} & a_{32} & & & \\
c_4 & \gamma_4 & a_{41} & a_{42} & a_{43} & & \\
c_5 & \gamma_5 & a_{51} & a_{52} & a_{53} & a_{54} & \\
c_6 & \gamma_6 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} \\
\hline
 & & b_1 & b_2 & b_3 & b_4 & \\
 & & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \hat{b}_4 & \hat{b}_5
\end{array}
$$

A classical embedded Runge–Kutta method has all $\gamma_i=1$ $(i=1,\ldots,6)$ and all A, b and $\hat{b}$ values are just numbers. For EFRK methods these quantities can be ω-dependent functions. For the determination of the ω values we shall make use of an embedded classical RK-method in combination with an explicit EFRK-method; in particular, we consider the well-known (4,5) England's method [2], i.e.,

$$
\begin{array}{c|c|ccccc}
0 & 1 & & & & & \\
\frac{1}{2} & 1 & \frac{1}{2} & & & & \\
\frac{1}{2} & 1 & \frac{1}{4} & \frac{1}{4} & & & \\
1 & 1 & 0 & -1 & 2 & & \\
\frac{2}{3} & 1 & \frac{7}{27} & \frac{10}{27} & 0 & \frac{1}{27} & \\
\frac{1}{5} & 1 & \frac{28}{625} & -\frac{1}{5} & \frac{546}{625} & \frac{54}{625} & -\frac{378}{625} \\
\hline
 & & \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6} & 0 \\
 & & \frac{1}{24} & 0 & 0 & \frac{5}{48} & \frac{27}{56} & \frac{125}{336}
\end{array}
$$

The numerical solution derived from the fourth-order component in the embedded method is used as the initial value for the next step and it will be denoted as $y_{n+1}^{\text{class.}}$. A feature of this method is that the two last elements of b^{T} are zero, implying that if the error estimate is not required then only four stages need to be computed. The local truncation error of the fourth-order component of the embedded method has the following form:

$$\mathrm{LTE}^{\text{class.}} = h^5\psi_1(x,y,f) + \mathcal{O}(h^6), \tag{2.3}$$

and can be estimated by

$$h\sum_{i=1}^{6}(\hat{b}^{\mathrm{T}} - b^{\mathrm{T}})k_i \tag{2.4}$$

with

$$k_i = f\left(x_n + c_i h, y_n + \sum_{j=1}^{i-1} a_{i,j}k_j\right).$$

As an EFRK method we have constructed the exponential-fitted analog of the fourth-order component of England's method. Due to Theorem 1 of [12] an explicit Runge–Kutta method can only exactly integrate a set of two linearly independent functions; for EFRK methods one can choose the set $\{\exp(\omega x), \exp(-\omega x)\}$, or equivalently $\{\sin(\lambda x), \cos(\lambda x)\}$ $\omega = \mathrm{i}\lambda$, instead of the classical set $\{1, x\}$. This means that every stage equation and the final step b-dependent equation in (2.2) has to integrate exactly this set of functions. We also want to preserve the components of c at their classical values in the fourth-order Runge–Kutta scheme, i.e., $c_1 = 0$, $c_2 = c_3 = \frac{1}{2}$ and $c_4 = 1$. The above conditions give rise to the following ten equations (with $v = \omega h$, $\omega \in \mathbb{R}$)

$$\exp(\pm v) - 1 \mp v\sum_{j=1}^{4} b_j \exp(\pm c_j v) = 0,$$

$$\exp(\pm c_i v) - \gamma_i \mp v\sum_{j=1}^{4} a_{ij}\exp(\pm c_j v) = 0 \tag{2.5}$$

with $i = 1, \ldots, 4$. It is clear that a lot of freedom in the determination of the A, b and γ components is still left, but we choose accepting just the classical values for some of them, viz. (this choice is not given a special advantage; other choices are possible):

$$a_{41} = 0, \quad a_{43} = 2, \quad b_2 = 0, \quad \gamma_3 = 1, \quad \gamma_4 = 1. \tag{2.6}$$

By solving the set of Eqs. (2.5), the following ω-dependent coefficients result (here we present the trigonometric solution, i.e., $\omega = \mathrm{i}\lambda, v = h\lambda$):

$$a_{21} = \frac{\sin(v/2)}{v}, \qquad \gamma_2 = \cos(v/2),$$

$$a_{31} = a_{32} = \frac{\sin(v/2)}{v(\cos(v/2)+1)}, \qquad a_{42} = \frac{2\sin(v/2) - 2v}{v},$$

$$b_1 = b_4 = -\frac{v - 2\sin(v/2)}{2v(\cos(v/2)-1)}, \qquad b_3 = \frac{v\cos(v/2) - 2\sin(v/2)}{v(\cos(v/2)-1)}. \tag{2.7}$$

For v-values smaller than 1 series expansions are used for the values of the b-components, the non-zero elements of A and the γ_i-values, different from 1.

The local truncation error of this EFRK-method has the following form:

$$\mathrm{LTE}^{\mathrm{EFRK}} = h^5(\psi_1(x, y, f) + \psi_2(x, y, f, \lambda)) + \mathcal{O}(h^6), \tag{2.8}$$

where the function $\psi_1(x, y, f)$ is defined in (2.3) and where

$$\psi_2(x, y, f, \lambda) = \lambda^2\psi_3(x, y, f) + \mathcal{O}(\lambda^4). \tag{2.9}$$

Typical expressions for the function $\psi_1(x, y, f)$ and $\psi_3(x, y, f)$ for different EFRK-methods with 2, 3 and 4 stages can be found in [13]. The numerical value obtained by the EFRK method (2.6–2.7) will be denoted as y_{n+1}^{EFRK}. A estimate for $h^5\psi_2(x, y, f, \lambda)$ is obtained from

$$y_{n+1}^{\mathrm{EFRK}} - y_{n+1}^{\mathrm{class.}}. \tag{2.10}$$

3. λ-determination and steplength control

On each integration step the following operations are performed:

1. The system is integrated by the classical (4,5) England's method.
2. The $\mathrm{LTE}^{\mathrm{class.}}$ is determined by (2.4).
3. The system is integrated by the constructed EFRK-method, where for each equation in the system an arbitrary λ-value is used. This is denoted by λ_0.
4. The value of $h^5\psi_2(x, y, f, \lambda_0)$ is calculated by Eq. (2.10).
5. For each equation in the system, Eq. (2.9) furnishes $h^5\psi_3(x, y, f)$ as
$$h^5\psi_3(x, y, f) = \frac{h^5\psi_2(x, y, f, \lambda_0)}{\lambda_0^2}.$$
6. Again for each equation an optimal λ value is obtained by making the leading order term in $\mathrm{LTE}^{\mathrm{EFRK}}$ as small as possible in terms of $\alpha = -\psi_1(x, y, f)/\psi_3(x, y, f)$, i.e.,

- if $\alpha > 0$ then $\lambda = \sqrt{\alpha}$,
- if $\alpha < 0$ then $\lambda = i\sqrt{|\alpha|}$. In this case, the exponential functions instead of the trigonometric ones are integrated.

7. The system is re-integrated with the EFRK-method where for each equation the calculated λ-value is used for the determination of the A- and b-coefficients under (2.7). By the described λ determination, the order of the EFRK-method is expected to increase by one unit. This can easily be tested in the following way by considering the equation $y' = -4y$ with $y(0) = 1$, having an exact solution $y(x) = \exp(-4x)$. It is solved twice over the interval $[0, 1]$ by the EFRK-method the first time with a fixed steplength $h = 0.01$ and a second time with $h = 0.02$. In each knot point, the global truncation error $|y_n - y(x_n)|$ is calculated and divided by h^4 and by h^5 in order to determine the x-dependent error form factor of the method, which should be independent of the chosen fixed steplength. The results are plotted in Figs. 1 and 2.
   One should usually expect that in so much the order is assigned correctly the form factor should be one and the same, irrespected of the value of h. In Fig. 1, it is assumed that the order is four and we see that the expectation is violated. More than that the form factor corresponding to the haved step-size is clearly half of the other. However, if the order is assumed as five the form factor is one and the same for the two stepsizes (see Fig. 2). This indicates that five is the correct value of the order.
8. In order to find an estimate for the leading-order term of the LTE corresponding to the calculation with the EFRK-method with adjusted λ-values we used a Richardson extrapolation technique. We apply the EFRK-method to obtain the solution y_{n+1} at x_{n+1}. Under the usual localizing assumption that $y_n = y(x_n)$ it is clear that the $\mathrm{LTE}^{\mathrm{EFRK}}$ can be written in the form

$$\mathrm{LTE}^{\mathrm{EFRK}} = y(x_{n+1}) - y_{n+1} = C(y, f, \lambda)h^6 + \mathcal{O}(h^7),$$

   where $C(y, f, \lambda)$ is some complicated function of y, its derivatives, $f(x, y)$ and its partial derivatives with respect to x and y, all evaluated at the point (x_n, y_n) and of λ.
   A second value of the numerical solution at x_{n+1}, hopefully better, is calculated by applying the same EFRK-method twice with steplength $h/2$ and also starting in x_n; let this be denoted by z_{n+1}. The same set of λ-values can be used for both calculations. Under the usual localizing assumption the local truncation error is now given by

$$\mathrm{LTE}^{\mathrm{EFRK}} = y(x_{n+1}) - z_{n+1} = 2C(y, f, \lambda)(h/2)^6 + \mathcal{O}(h^7),$$

   which, at its turn, produces an estimate of the error in the second calculation, viz.:

$$\mathrm{error} = 2C(y, f, \lambda)(h/2)^6 \approx (z_{n+1} - y_{n+1})/31.$$

   If the user asks for a given tolerance tol, he can control the steplength and the error in the following way:
   if $|\mathrm{error}| \leqslant \mathrm{tol}$ then accept the step and progress with the z_{n+1} value,
   if $|\mathrm{error}| > \mathrm{tol}$ then reject the step and repeat the whole procedure with a new step-length.
   In both cases, the value of the new step is given by

$$h_{\mathrm{new}} = h_{\mathrm{old}} \min(\mathrm{facmax}, \max(\mathrm{facmin}, \mathrm{fac}(\mathrm{tol}/\mathrm{error})^{1/(1+p)})),$$

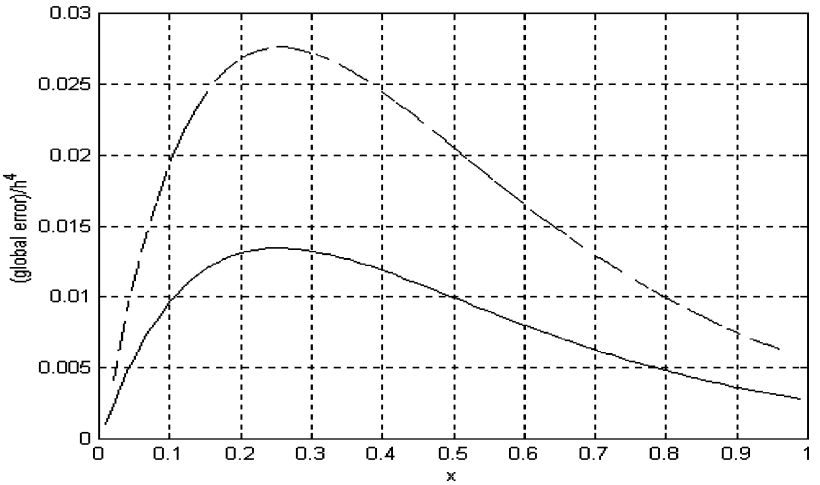

Fig. 1. Plot of the error form factor when the order of the EFRK-method is assumed to be four. The solid line are the results obtained with $h = 0.02$, the dashed line the ones obtained with $h = 0.01$.

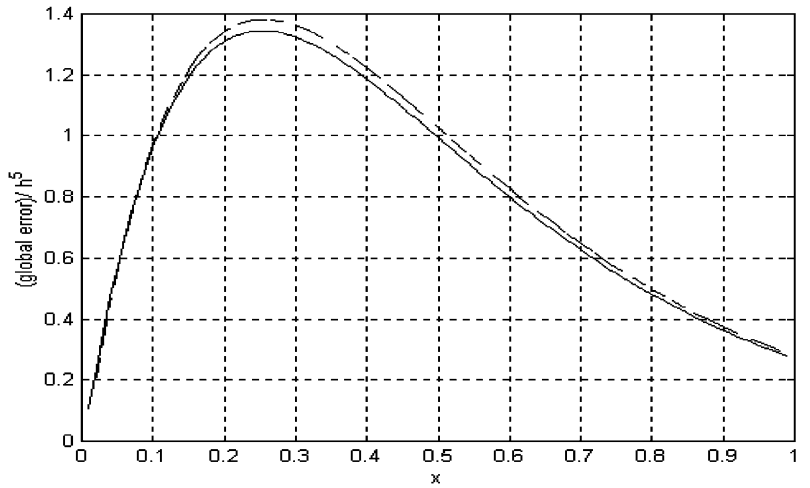

Fig. 2. Plot of the error form factor when the order of the EFRK-method is assumed to be five. The solid line are the results obtained with $h = 0.02$, the dashed line the ones obtained with $h = 0.01$.

with facmax and facmin representing the maximum and minimun acceptable increasing or decreasing factors repectively. The symbol fac stands for a safety factor in order to have an acceptable error in the following step. In the code, we have developed we have taken the following values for these factors:

$$\text{facmax} = 2, \quad \text{facmin} = 0.5, \quad \text{fac} = 0.9.$$

4. Numerical experiments

In this section we solve some initial value problems (single first-order equations as well as systems of first-order equations) having as solution a combination of sine, cosine or exponential functions. In the case of high-order systems, the equations are presented as equivalent first-order systems. These systems have been solved with the described EFRK method and the considered classical embedded RK method; in the EFRK case, we applied the above-described Richardson extrapolation technique. For the classical method, the error was calculated by formula (2.4). Tolerance values, tol of $1E-5$, $1E-7$ and $1E-9$ have been considered. For each equation an arbitrary chosen λ_0-value has been used. For each example, we have calculated the Euclidean norm of the error vector with components defined as the difference between the numerical and the exact values of the solution vector at the endpoint of the integration interval. These data are collected in Table 1 together with the number of accepted and rejected steps and the number of evaluations of the right-hand side (numf) of the systems. The following cases have been considered.

Example 1.

$$y' = x + y, \quad y(0) = 2. \tag{4.11}$$

Its exact solution is $y(x) = 3\exp(3x) - x - 1$. Eq. (4.11) has been solved in the interval $0 \leqslant x \leqslant 4$ with $\lambda_0 = 0.5$.

Example 2.

$$y' = -4y, \quad y(0) = 1, \tag{4.12}$$

with exact solution $y(x)=\exp(-4x)$. Eq. (4.12) has been solved in the interval $0 \leqslant x \leqslant 2$ with $\lambda_0=0.5$.

Example 3.

$$y' = 15\cos(15x), \quad y(0) = 0, \tag{4.13}$$

with exact solution $y(x) = \sin(15x)$. Eq. (4.13) has been solved in the interval $0 \leqslant x \leqslant 3\pi/2$ with $\lambda_0 = 0.2$.

Example 4.

$$y' = y\cos(x), \quad y(0) = 1, \tag{4.14}$$

with exact solution $y(x) = \exp(\sin(x))$, Eq. (4.14) has been solved in the interval $0 \leqslant x \leqslant 10$ with $\lambda_0 = 0.5$.

Example 5.

$$\begin{aligned} y_1' &= -y_1 + y_2, \quad y_1(0) = 3, \\ y_2' &= y_1 - y_2, \quad y_2(0) = 1 \end{aligned} \tag{4.15}$$

with exact solution $y_1(x) = 2 + \exp(-2x)$ and $y_2(x) = 2 - \exp(-2x)$. System (4.15) has been solved in the interval $0 \leqslant x \leqslant 2$ with $\lambda_0 = 0.5$ for each component of the solution as a seed value.

Table 1
Comparison of the Euclidian norms of the end-point global errors obtained by using the fourth-order EFRK and the classical embedded RK-method with step-length control

		log(tol)	Accepted steps	Rejected steps	Numf	Error
Example 1	EFRK	−5	12	0	221	9.33E − 4
		−7	23	0	430	2.40E − 5
		−9	48	0	905	5.70E − 7
	Class	−5	32	0	190	2.05E − 3
		−7	81	1	490	5.32E − 5
		−9	205	2	1240	1.31E − 6
Example 2	EFRK	−5	9	0	164	4.82E − 6
		−7	17	1	335	5.89E − 8
		−9	34	2	677	4.04E − 9
	Class	−5	20	1	124	3.50E − 6
		−7	46	2	286	1.23E − 7
		−9	111	4	688	3.66E − 9
Example 3	EFRK	−5	45	21	1247	5.96E − 5
		−7	91	23	2159	2.42E − 7
		−9	189	33	4211	7.10E − 9
	Class	−5	149	33	1090	1.86E − 5
		−7	362	32	2362	4.29E − 7
		−9	901	49	5698	1.06E − 8
Example 4	EFRK	−5	18	5	430	6.88E − 6
		−7	35	8	810	4.51E − 8
		−9	71	9	1513	3.13E − 9
	Class	−5	36	6	250	2.88E − 5
		−7	82	8	538	6.64E − 7
		−9	196	11	1240	8.15E − 9
Example 5	EFRK	−5	7	0	126	5.84E − 6
		−7	12	0	221	1.61E − 7
		−9	24	1	468	4.81E − 9
	Class	−5	14	0	82	1.09E − 5
		−7	33	2	208	3.27E − 7
		−9	81	3	502	8.60E − 9
Example 6	EFRK	−5	61	0	1152	4.50
		−7	135	2	2596	8.47E − 2
		−9	294	3	5636	1.71E − 3
	Class	−5	225	2	1360	5.98
		−7	572	3	3448	1.43E − 1
		−9	1442	4	8674	3.55E − 3

Example 6.

$$y_1' = 4y_1 - 2y_2, \quad y_1(0) = 2,$$
$$y_2' = -2y_1 + 4y_2, \quad y_2(0) = 0 \tag{4.16}$$

with exact solution $y_1(x) = \exp(2x) + \exp(6x)$ and $y_2(x) = \exp(2x) - \exp(6x)$. System (4.16) has been solved in the interval $0 \leqslant x \leqslant 2$ with $\lambda_0 = 1$ for each component of the solution as a seed value.

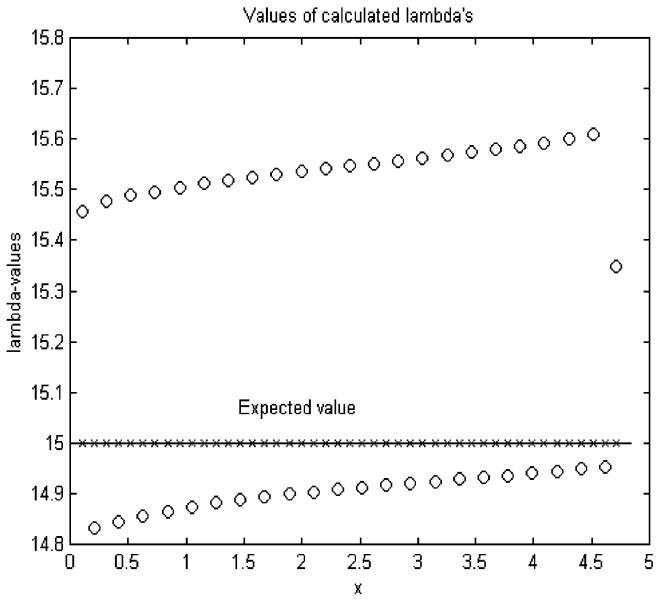

Fig. 3. Plot of the calculated λ-values for Example 3 with $\mathrm{tol} = 1\mathrm{E}-5$. The theoretically expected value 15 is also given.

It is clear from Table 1 that for all examples the number of steps is lower in the EFRK than in the classical method. The higher the asked tolerance the better the EFRK method scores over the classical method in the number of right-hand-side evaluations. For Examples 1–5, the Euclidian norm which in essence represents the absolute error, is compatible with the given tolerance. The absolute error obtained in Example 6 is rather large and deviates drastically from the asked tolerance but one must realize that the two components of the solution have large values in the end point too. Yet the relative error for that example is of acceptable size indeed. In Fig. 3, we plot the calculated values for λ in each knot point for Example 3 for $\mathrm{tol} = 1\mathrm{E}-5$. In this case, the exact value of λ is just 15 in all points. As far, the calculated values they only deviate within 4% from that value. As a matter of fact in all cases where calculated and theoretical values could be compared, analogous results are obtained.

In Fig. 4, we give the results obtained for Example 4. The solid line gives the exact solution, while the circles and the crosses represent in order the results at the mesh points corresponding to the EFRK and the classical method. The figure clearly demonstrates that the number of steps to obtain the solution is much smaller with the EFRK than with the classical method.

5. Conclusions

We have applied a previously described technique to construct an explicit exponentially-fitted Runge–Kutta method, depending on a parameter ω or $\lambda, (\lambda = \mathrm{i}\omega)$. In the limit of $\omega \to 0$ this method tends to the fourth-order method present in the (4,5) England's embedded method.

By combining this EFRK and that embedded method a technique is developed to determine an optimal value for ω or λ, by which the order of the EFRK-method is increased by one unit. Error

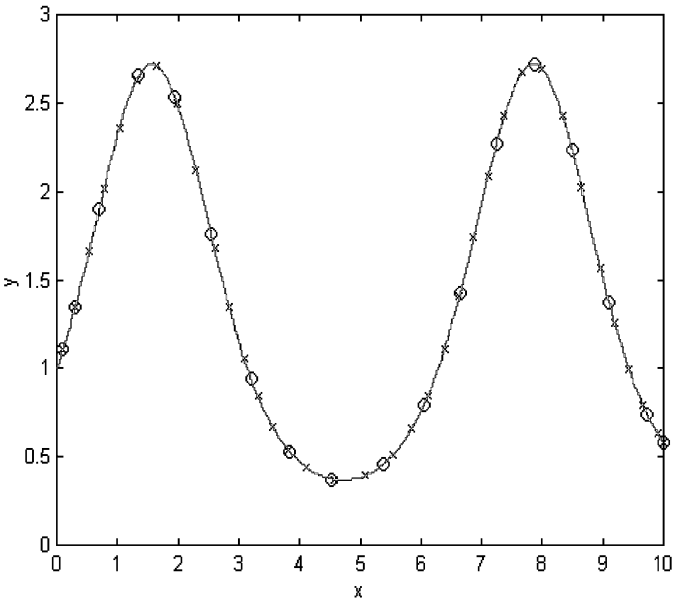

Fig. 4. Plot of the exact solution (solid line) and the numerical results obtained for Example 4 with tol = 1E − 5 with the EFRK (circles) and with the classical Runge–Kutta method (crosses).

and steplength for the EFRK-method is controlled by techniques based on Richardson extrapolation ideas. The introduced method is tested on several initial-value problems. In all cases, the number of steps used to obtain a given tolerance is smaller for the EFRK-method than for the embedded England's method. For high tolerances, the number of right-hand-side evaluations is much smaller for the EFRK-method than for the classical one.

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