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ON THE ECONOMIZATION OF EXPLICIT RUNGE-KUTTA METHODS

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A modification to explicit Runge-Kutta (RK) methods is proposed. Schemes are constructed which require less derivative-evaluations to achieve a certain order than the classical RK methods do. As an example, we give a second-order method requiring one evaluation, two third-order methods using one and two evaluations, respectively and finally a fourth-order method which requires two evaluations. Numerical examples illustrate the behaviour of these schemes.

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1. INTRODUCTION

For the numerical integration of the first-order initial value problem

$$\frac{d}{dt} y(t) = f(t, y(t)), \quad y(t_0) = y_0, \quad t \geq t_0 \quad (1.1)$$

explicit Runge-Kutta (RK) methods are frequently used. These methods are defined by

$$\begin{aligned} y_{n+1} &= y_n + h \sum_{i=1}^m b_i k_n^{(i)}, \\ k_n^{(1)} &= f(t_n, y_n), \\ k_n^{(i)} &= f(t_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} k_n^{(j)}), \quad i=2, \dots, m \\ c_i &= \sum_{j=1}^{i-1} a_{ij}, \end{aligned} \quad (1.2)$$

where y_n is an approximation to $y(t_n)$, h is the step size and $t_n = t_0 + nh$, $n=1, 2, \dots$. Explicit Runge-Kutta methods unquestionably have obtained great popularity and this is easily understood if we consider their properties: (i) the straightforward implementation on a computer and (ii) the one-step nature of the scheme is preserved whilst an arbitrarily high order can be achieved. However, included in the disadvantages of explicit RK methods is the necessity of (relatively) many evaluations of the right-hand side function f

of (1.1) in order to achieve a certain order of accuracy. It is well-known (see e.g.[2]) that an RK method of order $p \leq 4$ requires at least p f-evaluations and for $p > 4$ this number increases rapidly. Here, we propose methods in which the number of f-evaluations can be reduced whilst retaining the order of accuracy. This is achieved by using some of the f-evaluations already computed in the previous step(s). More precisely, in (1.2) some of the $k_n^{(i)}$ are replaced by $k_{n-\ell}^{(j)}$ with both i and $j \in \{1, \dots, m\}$, $i \neq j$ and $\ell \geq 1$.

It is not clear in advance how many k -vectors should be used from the previous step(s) and what the best values for i, j and ℓ are. However, it is possible to make some general remarks:

First, concerning the value of j we see that if the values of c_i are increasing (with increasing i) - which is the case in many RK schemes - we should choose j as large as possible; this results in the use of a "recent" f-evaluation which will reduce the local truncation error of the new schemes.

Next, if in stage i , $k_n^{(i)}$ is replaced by $k_{n-\ell}^{(j)}$, the free parameters a_{ij} disappear and can no longer be used to satisfy the consistency conditions. Therefore, a low value of i will leave us with more free parameters than a large value of i .

Furthermore, in this paper we concentrate on $\ell=1$, viz. only k -vectors of the preceding step are employed.

Finally, we have to decide how many k -vectors will be used from the preceding step. First of all, we remark that we will perform at least one f-evaluation in each step, because a saving of all $k_n^{(i)}$'s will result in an integration process which evaluates the derivative only in the initial part of the integration interval and this, of course, cannot be considered as a serious way of integrating (1.1). The question remains: how many f-evaluations are necessary to obtain a particular order of accuracy. As a guidance, let us consider the following Table:

order of accuracy	1	2	3	4	5	6		
# consistency conditions	1	2	4	8	17	37		
# stages	1	2	3	4	5	6	7	8
# free parameters in the classical case	1	3	6	10	15	21	28	36
attainable order in the classical case	1	2	3	4	4	5	6	6
# free parameters if $k_n^{(1)}$ is replaced	-	3	6	10	15	21	28	36
# free parameters if $k_n^{(1)}, k_n^{(2)}$ are replaced	-	-	5	9	14	20	27	35
# free parameters if $k_n^{(1)}, \dots, k_n^{(3)}$ are replaced	-	-	-	7	12	18	25	32
# free parameters if $k_n^{(1)}, \dots, k_n^{(4)}$ are replaced	-	-	-	-	9	15	22	29

As the consistency conditions are nonlinear equations in the parameters of the scheme, it is certainly not possible to deduce from this Table conclusions concerning the optimal order; on the other hand, this Table indicates that we may hope for the existence of an RKE(nf=1,p=2,m=2) method, an RKE(nf=1,p=3,m=3) method, an RKE(nf=2,p=4,m=4) method, an RKE(nf=1,p=4,m=5) method, an RKE(nf=3,p=5,m=6) method, etc. where we introduced the shortened notation RKE(nf,p,m) to denote an m-stage, p-th order *economized* RK method requiring nf f-evaluations per step.

Note that for RKE schemes in which $m-nf > nf$ (i.e. in which the number of "saved" k-values is larger than the number of evaluations actually performed in one step), more than one back-step is involved.

It should be observed that these schemes bear some resemblance to hybrid linear multistep methods (see for example Gragg and Stetter[10], Gear[9], Butcher[3], Kohfeld and Thompson[15], Danchick[5] and Lyche[18]). The RKE methods can be regarded as hybrid methods with more than one "off-step" point and applied in predictor-corrector (PC) mode using different predictors. However, following this PC view-point, the RKE schemes do not end up with an evaluation of the final result, because in all RKE schemes, $k_n^{(1)}$ will be replaced by $k_{n-1}^{(j)}$. On the other hand, most of the methods discussed by the above authors do perform this final evaluation (the so-called $P_1EP_2E\dots P_{m-1}ECE-$ mode; see [17]).

Moreover, it is this lack of f-evaluations at step points (t_n, y_n) , which prevents the RKE scheme to fit into the multistep RK methods as defined by van der Houwen [12] and by Byrne and Lambert[4]. To see this, let us consider the most simple RKE scheme:

$$\begin{aligned} k_n^{(1)} &= k_{n-1}^{(2)}, \\ k_n^{(2)} &= f(t_n + c_2 h, y_n + c_2 h k_n^{(1)}); \\ y_{n+1} &= y_n + h(b_1 k_n^{(1)} + b_2 k_n^{(2)}) \end{aligned}$$

which can be reformulated (using $\bar{y}_{n+c_2} := y_n + c_2 h k_n^{(1)}$) as

$$\begin{aligned} \bar{y}_{n+c_2} &= y_n + c_2 h f(t_{n-1} + c_2 h, \bar{y}_{n-1+c_2}), \\ y_{n+1} &= y_n + b_1 h f(t_{n-1} + c_2 h, \bar{y}_{n-1+c_2}) + b_2 h f(t_n + c_2 h, \bar{y}_{n+c_2}). \end{aligned} \tag{1.3}$$

Obviously, two sequences of approximations are generated; one sequence in the step points and another in the off-step points, and, as a consequence, y_{n+1} cannot be expressed in terms of preceding approximations y_n, y_{n-1}, \dots at the step points.

Using this formulation, there appears also a resemblance to cyclic multi-step methods (or block methods); see, for example, Donelson and Hansen [6]. However, in this type of methods all formulae within one cycle (or block) are applied with the same step size and have (approximately) the same order of accuracy. In (1.3), these features are not necessarily fulfilled.

2. CONSTRUCTION OF RKE SCHEMES

Here we will derive RKE schemes of orders 2, 3 and 4. Special attention is paid to the first integration step in which, of course, no k -values from preceding steps can be used. Occasionally, this first step will require even more f -evaluations than in the original RK scheme. Furthermore, we will show possibilities to exploit the free parameters and, finally, the (linear) stability of the schemes will be discussed. For reasons of notational convenience, the ODE (1.1) will be treated in its autonomous form.

2.1 An RKE(nf=1, p=2, m=2) scheme

Let us start with the most simple RKE scheme

$$\begin{aligned} k_n^{(1)} &= k_{n-1}^{(2)}, \\ k_n^{(2)} &= f(y_n + c_2 h k_n^{(1)}); \\ y_{n+1} &= y_n + h(b_1 k_n^{(1)} + b_2 k_n^{(2)}). \end{aligned} \quad (2.1)$$

In deriving the consistency relations for RKE schemes we substitute, as often as necessary, the expression for $k_{n-1}^{(j)}$ into the "economized" $k_n^{(i)}$ -vectors; or, more precisely, until sufficient high powers of h are involved. For (2.1) we find

$$k_n^{(1)} = k_{n-1}^{(2)} = f(y_{n-1} + c_2 h k_{n-1}^{(1)}) = f(y_{n-1} + c_2 h k_{n-2}^{(2)}) = f(y_{n-1} + c_2 h f_{n-2}) + O(h^2). \quad (2.2)$$

Then, as usual, we make a Taylor expansion (of all $k_n^{(i)}$) about (t_n, y_n) and,

straightforwardly, find the order conditions

$$\begin{aligned} b_1 + b_2 &= 1, \\ b_1(c_2 - 1) + b_2 c_2 &= \frac{1}{2}. \end{aligned} \quad (2.3)$$

This yields the one-parameter family of RKE(1,2,2) schemes giving by (adopting the Butcher-array notation[2])

$$\begin{array}{c|cc} & & \\ \hline c_2 & c_2 & \\ \hline & c_2^{-1/2} & 3/2 - c_2 \end{array} \quad (2.4)$$

where c_2 is a free parameter. For the scheme (2.4), the principal term in the local truncation error (cf. [17]) is given by (using tensor notation, see [11, p.118])

$$\frac{5}{12} h^3 f_j f_j^k + \left(\frac{5}{12} - c_2 + \frac{1}{2} c_2^2 \right) h^3 f_{jk} f_j^k. \quad (2.5)$$

Hence, by choosing $c_2 = (6 - \sqrt{6})/6$, the second term in this expression vanishes.

Now, let us consider the (linear) stability of scheme (2.1) by applying it to the scalar test equation $y' = \lambda y$ (cf. [17]). Introducing $z = \lambda h$ and defining $A(z)$ and $B(z)$ by $y_{n+1} = A(z)y_n$ and $h k_n^{(2)} = B(z)y_n$, we have

$$\begin{aligned} h k_n^{(1)} &= h k_{n-1}^{(2)} = B(z)y_{n-1} = B(z)/A(z) y_n, \\ h k_n^{(2)} &= z(1 + c_2 B(z)/A(z))y_n \stackrel{d}{=} B(z)y_n, \\ y_{n+1} &= (1 + b_1 B(z)/A(z) + b_2 B(z))y_n \stackrel{d}{=} A(z)y_n. \end{aligned} \quad (2.6)$$

From these last equations $A(z)$ and $B(z)$ can be solved and we find the *characteristic equation*

$$A(z)^2 - A(z)[1 + z(b_2 + c_2)] + z(c_2 - b_1) = 0. \quad (2.7)$$

As usual, the *stability region* in the complex z -plane is defined as the region for which the roots $A(z)$ of (2.7) are less than 1 in modulus. On substituting $b_1 = c_2 - 1/2$, $b_2 = 3/2 - c_2$, (2.7) reduces to

$$A(z)^2 - A(z)[1 + 3z/2] + z/2 = 0. \quad (2.7')$$

Consequently, the parameter c_2 cannot be exploited to enlarge the stability region. Notice, that the characteristic equation (2.7') is identical to that of the two-step (second-order) Adams-Bashforth method, the stability region of which can be found in [19,p.135].

Finally, the treatment of the first step has to be specified. We suggest to perform a classical two-stage RK method (hence, $k_0^{(1)}$ is obtained by $f(y_0)$) using the same value of c_2 , i.e. $c_2=(6-\sqrt{6})/6$. Requiring this step to be second-order accurate, we have to satisfy the classical order conditions $b_1+b_2=1$, $b_2c_2=\frac{1}{2}$.

Summarizing, we have the method

$$\begin{array}{c|cc} 0 & & \\ (6-\sqrt{6})/6 & (6-\sqrt{6})/6 & \\ \hline & (4-\sqrt{6})/10 & (6+\sqrt{6})/10 \end{array} \quad \text{for } n=0 \quad (2.8a)$$

and

$$\begin{array}{c|cc} - & & \\ (6-\sqrt{6})/6 & (6-\sqrt{6})/6 & \\ \hline & (3-\sqrt{6})/6 & (3+\sqrt{6})/6 \end{array} \quad \text{for } n \geq 1. \quad (2.8b)$$

2.2 RKE(nf,p=3,m=3) schemes

In this section we will derive 3-stage RKE methods, using 1 and 2 f-evaluations. The "cheapest" scheme which maintains third-order accuracy is given by

$$\begin{aligned} k_n^{(1)} &= k_{n-1}^{(2)}, \\ k_n^{(2)} &= k_{n-1}^{(3)}, \\ k_n^{(3)} &= f(y_n + (c_3 - a_{32})hk_n^{(1)} + a_{32}hk_n^{(2)}); \\ y_{n+1} &= y_n + h(b_1k_n^{(1)} + b_2k_n^{(2)} + b_3k_n^{(3)}). \end{aligned} \quad (2.9)$$

Again, repeatedly substituting the expression for $k_n^{(3)}$ into $k_n^{(2)}$ and $k_n^{(1)}$ ($=k_{n-2}^{(3)}$) and Taylor expansion about (t_n, y_n) , (2.9) is of third-order if

$$\begin{aligned}
b_1 + b_2 + b_3 &= 1, \\
b_1(c_3-2) + b_2(c_3-1) + b_3c_3 &= \frac{1}{2}, \\
c_3^2 + a_{32} + b_1(2-4c_3) + b_2(\frac{1}{2}-3c_3) - 2b_3c_3 &= 1/6, \\
b_1(c_3-2)^2 + b_2(c_3-1)^2 + b_3c_3^2 &= 1/3.
\end{aligned} \tag{2.10}$$

Choosing c_3 as a free parameter we easily find

$$\begin{aligned}
b_1 &= \frac{1}{2}c_3^2 - c_3 + 5/12, \\
b_2 &= -c_3^2 + 3c_3 - 4/3, \\
b_3 &= \frac{1}{2}c_3^2 - 2c_3 + 23/12, \\
a_{32} &= -\frac{1}{2}c_3^2 + 2c_3.
\end{aligned} \tag{2.11}$$

Let us first derive the characteristic equation corresponding to the scheme (2.9). Again using $y_{n+1} := A(z)y_n$ and $hk_n^{(3)} := B(z)y_n$ and solving for $A(z)$ (and $B(z)$), we find

$$A^3(z) - A^2(z)[1+(a_{32}+b_3)z] + A(z)(2a_{32}-c_3-b_2)z + (c_3-a_{32}-b_1)z = 0. \tag{2.12}$$

If the relations given by (2.11) are substituted, (2.12) reduces to

$$A^3(z) - A^2(z)(1 + \frac{23}{12}z) + A(z)\frac{4}{3}z - \frac{5}{12}z = 0, \tag{2.12'}$$

which is identical to the characteristic equation of the three-step (third-order) Adams-Bashforth method. The corresponding stability region can be found in [19, p.136].

Obviously, the free parameter c_3 cannot be used to enlarge the stability region of this RKE method; therefore we consider its influence on the local truncation error. The principal term in this error is of the form

$$h^4 \left(\frac{3}{8} f_j^j f_k^k f_l^l + q_1 f_j^j f_k^k f_l^l + q_2 f_j^j f_k^k f_l^l + q_3 f_j^j f_k^k f_l^l \right), \tag{2.13}$$

where q_1 , q_2 and q_3 are functions of the free parameter c_3 . Now, by choosing $c_3 \approx .63397\dots$, we achieve that the sum of the absolute values $\sum |q_i|$ is minimized (see also [16]). This value of c_3 yields $q_1 \approx .42$, $q_2 \approx 0$, $q_3 \approx 0$.

Finally, we have to specify the scheme for the first two steps. Here, however, we have some additional constraints on these first steps: in the derivation of the order conditions, we used the expression of $k_{n-\ell}^{(3)}$ for $\ell \geq 1$, because $k_2^{(1)}$ is defined by $k_0^{(3)}$ and $k_2^{(2)}$ by $k_1^{(3)}$. Therefore, we must take care that $k_0^{(3)}$ and $k_1^{(3)}$ (which are obtained by a classical RK method) have the same expansion as we have for $k_n^{(3)}$ (which is obtained by an RKE method). This expansion is given by

$$k_n^{(3)} = f + c_3 h f_j f^j + \left(\frac{3}{2}c_3^2 - c_3\right) h^2 f_j f_k^j f^k + \frac{1}{2}c_3^2 h^2 f_{jk} f^j f^k + O(h^3). \quad (2.14)$$

Moreover, we want the first steps to be of third-order accuracy. It turns out that it is not possible to achieve this goal with a classical RK method using only three stages. Therefore, we propose the following four-stage third-order scheme for the first two stages

0					
$\frac{1}{2}$		$\frac{1}{2}$			
1		-1	2		
c_3		$-3c_3^2 + 3c_3$	$3c_3^2 - 2c_3$	0	
		1/6	2/3	1/6	0

(2.15)

Notice that this is in fact Kutta's third-order method, extended with $k_0^{(4)}$ which serves merely to provide the correct expansion (2.14) in the RKE scheme. Summarizing, apply (2.15) in the first and second integration step and save $k_0^{(4)}$ and $k_1^{(4)}$; rename them to $k_0^{(3)}$ and $k_1^{(3)}$, respectively and apply, for $n \geq 2$, the RKE scheme (2.9). In the numerical tests we used $c_3 = 0.634$.

Finally, we briefly mention another third-order RKE scheme, given by

$$\begin{aligned} k_n^{(1)} &= f(y_n), \\ k_n^{(2)} &= k_{n-1}^{(3)}, \\ k_n^{(3)} &= f(y_n + (c_3 - a_{32})h k_n^{(1)} + a_{32}h k_n^{(2)}); \\ y_{n+1} &= y_n + h(b_1 k_n^{(1)} + b_2 k_n^{(2)} + b_3 k_n^{(3)}). \end{aligned} \quad (2.16)$$

Although this scheme is not optimal with respect to the number of f -evaluations, it will turn out that this method possesses a rather large *imaginary stability boundary* β_{imag} , which is defined as the point where the boundary of the

stability region intersects the imaginary axis (cf.[12]). The reason for mentioning this result is the following: since the introduction of vector-computers, there is a renewed interest in explicit methods, for example in the field of hyperbolic differential equations. For this type of problems, a relatively large value of β_{imag} is of great importance (see e.g. [20]). The third-order consistency conditions for (2.16) are solved by

$$\begin{aligned} b_3 &= \frac{5 - 3c_3}{6c_3}, & b_2 &= \frac{2 - 3c_3}{6(1-c_3)}, \\ b_1 &= 1 - b_2 - b_3, & a_{32} &= \frac{1 - b_2(3-6c_3)}{6(c_3-1)(b_2+b_3)}, \end{aligned} \quad (2.17)$$

where c_3 is free. Selecting $c_3=0.52$ yields $\beta_{\text{imag}}=1.63$, which is optimal. Although this value is smaller than the "classical" value $\sqrt{3}$, the *effective* imaginary stability boundary (i.e. β_{imag}/nf) is 40% larger than the classical value. Moreover, it is 15% larger than the effective imaginary stability boundary of the classical fourth-order RK method, which has $\frac{1}{2}\sqrt{2}$. However, in this connection we remark that Kinnmark and Gray [14], recently have indicated how to construct RK methods of orders 3 (for $m=3,5,\dots$) and 4 (for $m=4,6,\dots$) possessing an effective imaginary stability boundary equal to $[(m-1)^2-1]^{\frac{1}{2}}/m$, which approaches $1 - 1/m$, for m large. This last value was proven by Vichnevetsky [21] to be the limit for any consistent RK method.

Finally, to achieve the appropriate expansion for $k_0^{(3)}$ in the first step, the RK scheme (2.15) can be used.

2.3 An RKE(nf=2,p=4,m=4) scheme

Finally, we give a fourth-order RKE scheme, requiring 2 f-evaluations. It is defined by

$$\begin{aligned} k_n^{(1)} &= k_{n-1}^{(3)}, \\ k_n^{(2)} &= k_{n-1}^{(4)}, \\ k_n^{(3)} &= f(y_n + (c_3 - a_{32})hk_n^{(1)} + a_{32}hk_n^{(2)}), \\ k_n^{(4)} &= f(y_n + (c_4 - a_{42} - a_{43})hk_n^{(1)} + a_{42}hk_n^{(2)} + a_{43}hk_n^{(3)}); \\ y_{n+1} &= y_n + h(b_1k_n^{(1)} + b_2k_n^{(2)} + b_3k_n^{(3)} + b_4k_n^{(4)}). \end{aligned} \quad (2.18)$$

Proceeding in the same way as in the preceding Sections, we derive the fourth-order consistency conditions:

$$\begin{aligned}
b_1 + b_2 + b_3 + b_4 &= 1, \\
b_1(c_3-1) + b_2(c_4-1) + b_3c_3 + b_4c_4 &= 1/2, \\
b_1q_3 + b_2q_6 + b_3q_9 + b_4q_{12} &= 1/6, \\
b_1(c_3-1)^2 + b_2(c_4-1)^2 + b_3c_3^2 + b_4c_4^2 &= 1/3, \\
b_1q_4 + b_2q_7 + b_3q_{10} + b_4q_{13} &= 1/24, \\
b_1q_5 + b_2q_8 + b_3q_{11} + b_4q_{14} &= 1/24, \\
b_1(c_3-1)q_3 + b_2(c_4-1)q_6 + b_3c_3q_9 + b_4c_4q_{12} &= 1/8, \\
b_1(c_3-1)^3 + b_2(c_4-1)^3 + b_3c_3^3 + b_4c_4^3 &= 1/4,
\end{aligned} \tag{2.19a}$$

where

$$\begin{aligned}
q_1 &= 2 + (c_3 - a_{32})(c_3 - 3) + a_{32}(c_4 - 3), \\
q_2 &= 2 + (c_4 - a_{42} - a_{43})(c_3 - 3) + a_{42}(c_4 - 3) + a_{43}(c_4 - 2), \\
q_3 &= \frac{1}{2} + (c_3 - a_{32})(c_3 - 2) + a_{32}(c_4 - 2), \\
q_4 &= -1/6 + (c_3 - a_{32})q_1 + a_{32}q_2, \\
q_5 &= -1/6 + \frac{1}{2}(c_3 - a_{32})(c_3 - 2)^2 + \frac{1}{2}a_{32}(c_4 - 2)^2, \\
q_6 &= \frac{1}{2} + (c_4 - a_{42} - a_{43})(c_3 - 2) + a_{42}(c_4 - 2) + a_{43}(c_3 - 1), \\
q_7 &= -1/6 + (c_4 - a_{42} - a_{43})q_1 + a_{42}q_2 + a_{43}q_3, \\
q_8 &= -1/6 + \frac{1}{2}(c_4 - a_{42} - a_{43})(c_3 - 2)^2 + \frac{1}{2}a_{42}(c_4 - 2)^2 + \frac{1}{2}a_{43}(c_3 - 1)^2, \\
q_9 &= (c_3 - a_{32})(c_3 - 1) + a_{32}(c_4 - 1), \\
q_{10} &= (c_3 - a_{32})q_3 + a_{32}q_6, \\
q_{11} &= \frac{1}{2}(c_3 - a_{32})(c_3 - 1)^2 + \frac{1}{2}a_{32}(c_4 - 1)^2, \\
q_{12} &= (c_4 - a_{42} - a_{43})(c_3 - 1) + a_{42}(c_4 - 1) + a_{43}c_3, \\
q_{13} &= (c_4 - a_{42} - a_{43})q_3 + a_{42}q_6 + a_{43}q_9, \\
q_{14} &= \frac{1}{2}(c_4 - a_{42} - a_{43})(c_3 - 1)^2 + \frac{1}{2}a_{42}(c_4 - 1)^2 + \frac{1}{2}a_{43}c_3^2.
\end{aligned} \tag{2.19b}$$

There exists a remarkably simple solution to this nonlinear system, which

reads

$$\begin{array}{c|ccc}
 - & & & \\
 - & - & & \\
 1/2 & -1/3 & 5/6 & \\
 1 & 7/12 & -1 & 17/12 \\
 \hline
 & 0 & 1/6 & 2/3 & 1/6
 \end{array} \tag{2.20}$$

For the characteristic equation we find (using the auxiliary functions $B(z)$ and $C(z)$ defined by $hk_n^{(3)} =: B(z)y_n$ and by $hk_n^{(4)} =: C(z)y_n$)

$$A^3(z) + r_2(z)A^2(z) + r_1(z)A(z) + r_0(z) = 0,$$

with

$$r_2(z) = -[z^2 a_{43}(a_{32} + b_4) + z(b_3 + b_4 + c_3 - a_{32} + a_{42}) + 1], \tag{2.21}$$

$$r_1(z) = z^2 [a_{42}c_3 - a_{32}c_4 + 2a_{32}a_{43} - b_2a_{43} - b_3(a_{32} - a_{42}) + b_4(c_3 - a_{32} - c_4 + a_{42} + a_{43})] + z(c_3 - a_{32} + a_{42} - b_1 - b_2),$$

$$r_0(z) = -z^2 [a_{42}c_3 - a_{32}(c_4 - a_{43}) + b_1(a_{32} - a_{42}) - b_2(c_3 - a_{32} - c_4 + a_{42} + a_{43})],$$

yielding $\beta_{\text{real}} = 0.50$ and $\beta_{\text{imag}} = 0.64$ if (2.20) is substituted, where β_{real} is the *real* stability boundary (cf. Section 2.2).

Again, the first step has to be treated separately. We find that $k_n^{(3)}$ and $k_n^{(4)}$ in (2.18) have the expansions

$$\begin{aligned}
 k_n^{(3)} = & f + c_3 h f_j f_j^j + h^2 (q_9 f_j f_j^j f_k^k + \frac{1}{2} c_3^2 f_{jk} f_j^j f_k^k) + \\
 & + h^3 (q_{10} f_j f_j^j f_k^k f_l^l + q_{11} f_j f_j^j f_k^k f_l^l + c_3 q_9 f_j f_j^j f_k^k f_l^l + \\
 & \frac{1}{6} c_3^3 f_{jkl} f_j^j f_k^k f_l^l) + O(h^4)
 \end{aligned}$$

and

$$\begin{aligned}
 k_n^{(4)} = & f + c_4 h f_j f_j^j + h^2 (q_{12} f_j f_j^j f_k^k + \frac{1}{2} c_4^2 f_{jk} f_j^j f_k^k) + \\
 & + h^3 (q_{13} f_j f_j^j f_k^k f_l^l + q_{14} f_j f_j^j f_k^k f_l^l + c_4 q_{12} f_j f_j^j f_k^k f_l^l + \\
 & \frac{1}{6} c_4^3 f_{jkl} f_j^j f_k^k f_l^l) + O(h^4).
 \end{aligned} \tag{2.22}$$

Using a classical five-stage fourth-order RK method, it appeared to be impossible to construct $k_0^{(i)}$ -vectors having the appropriate expansion.

Therefore, we suggest the following six-stage fourth-order starting scheme

0							
1/2	1/2						
1/2	0	1/2					
1	0	0	1				
1/2	-1/6	5/6	1/6	-1/3			
1	3/4	-5/6	1/2	7/12	0		
	1/6	1/3	1/3	1/6	0	0	

(2.23)

This starting scheme is to be used in combination with (2.20). In the first four stages the classical fourth-order RK scheme is easily recognized and $k_0^{(5)}$ and $k_0^{(6)}$ should be renamed to $k_0^{(3)}$ and $k_0^{(4)}$, respectively before (2.20) is used for $n \geq 1$.

Finally, we did not try to find other solutions to (2.19) which may have better stability characteristics.

3. ZERO-STABILITY

As can be seen from the stability polynomials (cf. (2.7'), (2.12') and (2.21)), the RKE schemes possess a multistep character. Therefore, we have to consider the concept of zero-stability. Following Lambert [17, p.33 and p.163], the RKE scheme is said to be zero-stable if no root of its characteristic equation evaluated at $z=0$, lies outside the unit disc, and those on the unit circle being simple.

It is readily verified that all RKE schemes proposed are zero-stable indeed. As is the case in Adams-type methods, they have one (principle) root equal to one and all other (parasitic) roots vanish.

4. NUMERICAL ILLUSTRATION

As it is to be expected that we sacrificed accuracy by the economization techniques, it is interesting to see to what extent the reduction in computational effort per step can compensate for this decrease in accuracy. Therefore, we applied the RKE schemes derived in Section 2 to several test problems. Each RKE scheme will be compared with a classical RK scheme of the same order; for this purpose we choose the (second-order) improved Euler method, Kutta's third-order method and the classical fourth-order RK method [17]. As the number of f -evaluations is not the same for all these methods, the step size in each application is adjusted as to result in a fixed computational effort (measured in f -evaluations only). This effort is denoted by Σf in the Tables of results.

4.1 Orbit equation

First, we integrate the two-body gravitational problem (class D in the testset of Hull et. al.[13])

$$\begin{aligned}
 y_1' &= y_3, & y_1(0) &= 1 - \epsilon, \\
 y_2' &= y_4, & y_2(0) &= 0, \\
 y_3' &= -y_1/r^3, & y_3(0) &= 0, \\
 y_4' &= -y_2/r^3, & y_4(0) &= [(1+\epsilon)(1-\epsilon)]^{\frac{1}{2}},
 \end{aligned} \tag{4.1}$$

where $r = (y_1^2 + y_2^2)^{\frac{1}{2}}$ and the excentricity $\epsilon = 0.5$. The exact solution is given by

$$\begin{aligned}
 y_1(t) &= \cos(u) - \epsilon, & y_2(t) &= (1-\epsilon^2)^{\frac{1}{2}} \sin(u), \\
 y_3(t) &= -\sin(u)/(1-\epsilon\cos(u)), & y_4(t) &= (1-\epsilon^2)^{\frac{1}{2}} \cos(u)/(1-\epsilon\cos(u)),
 \end{aligned} \tag{4.2}$$

where

$$u - \epsilon \sin(u) - t = 0.$$

More than three orbital periods are covered by the integration range $[0, 20]$. In Table 1, we tabulate the results obtained by the various methods for several values of Σf . The errors given, are the maximal global errors in the endpoint, measured over all components. As can be seen from this Table, the

Table 1. Global errors in the maximum norm for problem (4.1)

Σf	RKE(1,2,2)	Impr. Euler method	RKE(1,3,3)	Kutta's third-order method	RKE(2,4,4)	RK4 method
1200	.53 ₁₀ ⁻¹	.37	.33 ₁₀ ⁻¹	.99 ₁₀ ⁻¹	.38 ₁₀ ⁻³	.25 ₁₀ ⁻²
2400	.11 ₁₀ ⁻¹	.74 ₁₀ ⁻¹	.42 ₁₀ ⁻²	.13 ₁₀ ⁻¹	.86 ₁₀ ⁻⁵	.10 ₁₀ ⁻³
4800	.24 ₁₀ ⁻²	.17 ₁₀ ⁻¹	.53 ₁₀ ⁻³	.16 ₁₀ ⁻²	.92 ₁₀ ⁻⁶	.48 ₁₀ ⁻⁵
9600	.55 ₁₀ ⁻³	.40 ₁₀ ⁻²	.67 ₁₀ ⁻⁴	.20 ₁₀ ⁻³	.82 ₁₀ ⁻⁷	.25 ₁₀ ⁻⁶

RKE schemes yield, for the same computational effort, errors which are smaller than those obtained by the classical RK schemes. In the average, the gain factors are 7, 3 and 6 for methods of order 2, 3 and 4, respectively.

4.2 Euler's equation

Next, we solve Euler's equation of motion for a rigid body without external forces (see [1], and [13], problem B5)

$$\begin{aligned} y_1' &= y_2 y_3, & y_1(0) &= 0, \\ y_2' &= -y_1 y_3, & y_2(0) &= 1, \\ y_3' &= -k^2 y_1 y_2, & y_3(0) &= 1, \quad k^2=0.51 \end{aligned} \quad (4.3)$$

on $t \in [0, 20]$; its exact solution is given by the Jacobian elliptic functions

$$y_1(t) = \operatorname{sn}(t; k), \quad y_2(t) = \operatorname{cn}(t; k), \quad y_3(t) = \operatorname{dn}(t; k). \quad (4.4)$$

Following the same testing procedure as described in the previous Section, we obtain the results as given in Table 2.

Table 2. Global errors in the maximum norm for problem (4.3)

Σf	RKE(1,2,2)	Impr. Euler method	RKE(1,3,3)	Kutta's third-order method	RKE(2,4,4)	RK4 method
1200	$.92_{10^{-3}}$	$.18_{10^{-2}}$	$.29_{10^{-4}}$	$.85_{10^{-4}}$	$.39_{10^{-6}}$	$.23_{10^{-5}}$
2400	$.23_{10^{-3}}$	$.45_{10^{-3}}$	$.37_{10^{-5}}$	$.11_{10^{-4}}$	$.22_{10^{-7}}$	$.15_{10^{-6}}$
4800	$.57_{10^{-4}}$	$.11_{10^{-3}}$	$.46_{10^{-6}}$	$.14_{10^{-5}}$	$.13_{10^{-8}}$	$.90_{10^{-8}}$

Again, the RKE methods are more efficient. Now, gainfactors 2,3 and 6.5 are obtained for the methods of the respective orders 2,3 and 4.

4.3 Restricted three-body problem

Our last test example describes the restricted problem of three bodies (earth-moon-spaceship [7,8]) and reads

$$\begin{aligned} y_1' &= y_3, & y_1(0) &= 1.2, \\ y_2' &= y_4, & y_2(0) &= 0, \\ y_3' &= y_1 + 2y_4 - \mu'(y_1 + \mu)/r_1^3 - \mu(y_1 - \mu')/r_2^3, & y_3(0) &= 0, \\ y_4' &= y_2 - 2y_3 - \mu'y_2/r_1^3 - \mu y_2/r_2^3, & y_4(0) &= -1.0493575098304, \end{aligned} \quad (4.5)$$

where

$$r_1 = [(y_1 + \mu)^2 + y_2^2]^{\frac{1}{2}}, \quad r_2 = [(y_1 - \mu)^2 + y_2^2]^{\frac{1}{2}}$$

and

$$\mu = 1/82.45, \quad \mu' = 1-\mu.$$

The solution $(y_1(t), y_2(t))$ is known to describe a closed orbit with period $P=6.192169331396\dots$. We integrated over one period and compared the results with the initial values. The errors are given in Table 3. For the methods of order 2, 3 and 4 the global errors are reduced by a factor 2.5, 3 and 1.5, respectively.

Table 3. Global errors in the maximum norm for problem (4.5)

Σf	RKE(1,2,2)	Impr. Euler method	RKE(1,3,3)	Kutta's third-order method	RKE(2,4,4)	RK4 method
12000	$.94_{10^{-1}}$.47	.17	.95	$.15_{10^{-1}}$	$.26_{10^{-1}}$
24000	$.17_{10^{-1}}$	$.43_{10^{-1}}$	$.19_{10^{-1}}$	$.61_{10^{-1}}$	$.47_{10^{-3}}$	$.77_{10^{-3}}$
48000	$.35_{10^{-2}}$	$.75_{10^{-2}}$	$.24_{10^{-2}}$	$.71_{10^{-2}}$	$.13_{10^{-4}}$	$.21_{10^{-4}}$
96000	$.77_{10^{-3}}$	$.15_{10^{-2}}$	$.29_{10^{-3}}$	$.88_{10^{-3}}$	$.54_{10^{-6}}$	$.81_{10^{-6}}$

5. CONCLUSIONS

It has been indicated how RK-type(RKE) schemes can be constructed which require less evaluations of the right-hand side function of the differential equation to achieve a certain order than classical RK schemes do.

Several possible ways to exploit the free parameters are discussed: to decrease the local truncation error (as is done in the second- and third-order case), to increase the stability boundaries (third-order case) or to obtain a scheme with simple rational values for the parameters (fourth-order case).

When comparing RKE schemes and classical RK schemes, the former class turns out to be more efficient. For the test problems we used, the global errors are reduced by a factor, varying from 1.5 up to 7; or, equivalently, requiring the same accuracy for both type of methods (and taking the order of consistency into account), the RKE schemes are more efficient by a factor 1.15 up to 2.65.

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