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EXPLICIT RUNGE-KUTTA METHODS FOR THE NUMERICAL SOLUTION OF INITIAL VALUE PROBLEMS.

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Abstract

Explicit Runge-Kutta pairs are the most popular methods for integrating non-stiff initial value problems. Basic theory concerning its accuracy, stability and other properties is presented here as long as with implementation issues. Finally a new pair of orders 5(4) suitable for oscillatory problems is presented and tested.
Keywords: order conditions, truncation error, stability, embedded pairs, phase-lag.
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1 Introduction.

The general class of initial value problems of first order can be written as:

$$y' = f(x, y), \quad y(x_0) = y_0 \in \Re^m, \quad x \in [x_0, x_e], \tag{1}$$

where $f : \Re \times \Re^m \to \Re^m$.

Explicit Runge-Kutta (RK) pairs are widely used for the numerical solution of the initial value problem (1). These pairs are characterized by the extended Butcher tableau [2, 3]:

$$\begin{array}{c|c} c & A \\ \hline & b \\ & \hat{b} \end{array}$$

with b^T, $\hat{b}^T$, $c \in \Re^s$ and $A \in \Re^{s \times s}$ is strictly lower triangular. The procedure that advances the solution from (x_n, y_n) to $x_{n+1} = x_n + h_n$ computes at each step two approximations y_{n+1}, $\hat{y}_{n+1}$ to $y(x_{n+1})$ of algebraic orders p and $p-1$ respectively, given by

$$y_{n+1} = y_n + h_n \sum_{i=1}^{s} b_i f_{ni} \tag{2}$$

and

$$\hat{y}_{n+1} = y_n + h_n \sum_{i=1}^{s} \hat{b}_i f_{ni},$$

with

$$f_{ni} = f(x_n + c_i h_n, y_n + h_n \sum_{j=1}^{i-1} a_{ij} f_{nj}) \tag{3}$$

for $i = 1, 2, .., s \geq p$. In the following we use letters with cups to denote quantities pertaining to the lower-order method of a pair. The methods studied in this article obey the simplifying assumption $A \cdot e = c$, $e = (1, 1, \ldots, 1)^T \in \Re^s$.

From this embedded form (called RK$p(p-1)$) we can obtain an estimate

$$E_{n+1} = \|y_{n+1} - \hat{y}_{n+1}\|$$

of the local truncation error of the $p-1$ order formula. So the step-size control algorithm

$$h_{n+1} = 0.9 \cdot h_n \cdot (\frac{\text{TOL}}{E_{n+1}})^{1/p}, \tag{4}$$

is in common use, with TOL being the requested tolerance. The above formula is used even if TOL is exceeded by E_{n+1}, but then h_{n+1} is simply the recomputed current step. See [25] for more details on the implementation of these type of step size policies.

2 Trees theory for RK methods

2.1 Taylor series expansions

Setting $x' = 1$, then problem (1) reduces, without loss of generality, to the more convenient autonomous problem $y' = f(y)$. When advancing the

$p-$order RK method (2-3), applied to the latter problem, we actually try to approximate the corresponding Taylor method of the form

$$y(x_{n+1}) \approx y(x_n) + hy'(x_n) + \frac{1}{2!}h^2 y''(x_n) + \cdots + \frac{1}{p!}h^p y^{(p)}(x_n), \qquad (5)$$

On the other hand we may expand f_{ni} around the point (x_n, y_n) and derive from (2) the expression

$$y_{n+1} = y_n + hq_{11}y'_n + h^2 q_{21}y''_n + h^3\left(q_{31}f'f + q_{32}f''f^2\right) + \cdots, \qquad (6)$$

with q_{ij} depending exclusively on the coefficients A, b, c.

Verify now,

$$\begin{aligned}
y'' &= \frac{\partial f(y(x))}{\partial x} = \frac{\partial f}{\partial y}f = f'f,\\
y''' &= \frac{\partial^2 f}{\partial y^2}\cdot(f,f) + \frac{\partial f}{\partial y}\cdot\frac{\partial f}{\partial y}\cdot f = f''(f,f) + f'f'f,\\
y^{(4)} &= \frac{\partial^3 f}{\partial y^3}\cdot(f,f,f) + \frac{\partial f}{\partial y}\cdot\frac{\partial f}{\partial y}\cdot\frac{\partial f}{\partial y}\cdot f +\\
&\quad \frac{\partial f}{\partial y}\cdot\frac{\partial^2 f}{\partial y^2}\cdot(f,f) + 3\cdot\frac{\partial^2 f}{\partial y^2}\cdot\left(\frac{\partial f}{\partial y}\cdot f, f\right)\\
&= f'''(f,f,f) + f'f'f'f + f'f''(f,f) + 3f''(f'f,f),\\
&\quad \cdots
\end{aligned}$$

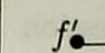
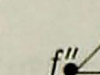
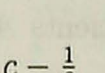
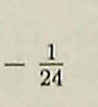
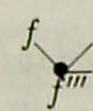
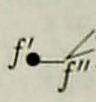
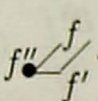
where the elementary differentials $f''(f,f)$, $f'''(f,f,f)$, $f'f''(f,f)$, $f''(f'f, f)$ are Frechet derivatives, [9, pg 158].

After matching (5) and (6) we arrive at

$$\begin{aligned}
&y(x_{n+1}) - y_{n+1} = h(q_{11}-1)f + h^2\left(q_{21}-\tfrac{1}{2}\right)\tfrac{\partial f}{\partial y}f +\\
&h^3\left(\left(q_{31}-\tfrac{1}{6}\right)f^T\cdot\tfrac{\partial^2 f}{\partial y^2}\cdot f + \left(q_{32}-\tfrac{1}{6}\right)\tfrac{\partial f}{\partial y}\cdot\tfrac{\partial f}{\partial y}\cdot f\right) + \cdots
\end{aligned} \qquad (7)$$

So requiring $t_{11} = q_{11} - 1 = 0$, $t_{21} = q_{21} - \frac{1}{2} = 0$, $t_{31} = q_{31} - \frac{1}{6} = 0$, $t_{32} = q_{32} - \frac{1}{6} = 0$ we conclude to the order conditions we have to satisfy for constructing a third order method. The order conditions up to fourth

Table 1: The equations of condition of Runge-Kutta methods, for orders 1-4.

equation	equation tree – form	elementary differential
$t_{11} = b \cdot e - 1$		
$t_{21} = b \cdot c - \frac{1}{2}$		
$t_{31} = \frac{1}{2} b \cdot c^2 - \frac{1}{6}$		
$t_{32} = b \cdot A \cdot c - \frac{1}{6}$		
$t_{41} = \frac{1}{6} b \cdot c^3 - \frac{1}{24}$		
$t_{42} = \frac{1}{2} b \cdot A \cdot c^2 - \frac{1}{24}$		
$t_{43} = b \cdot C \cdot A \cdot c - \frac{1}{8}$		
$t_{44} = b \cdot A^2 \cdot c - \frac{1}{24}$		

order are listed in first column of Table 1. In this table we denote by c^i the componentwize multiplication $c \cdot c \cdots c$ (i-times, assuming $c^0 = e$), for which we allow a higher order of precedence over the regular (matrix-to-matrix or matrix-to-vector) multiplication (dot product). Moreover, the same symbol will be used here to denote both types of multiplication. Whenever both types of multiplication are found simultaneously in a relation and there is a possible conflict, we distinguish the order of precedence, by the proper use of parenthesis. We also define $C = \text{diag}\,(c)$.

2.2 Trees and Rooted trees

Equation (7) has the form

$$y(x_{n+1}) - y_{n+1} = \sum_{i=1}^{\infty} \sum_{\tau \in T_i} h^i \frac{1}{\sigma(\tau)} \left(\Phi(\tau) - \frac{1}{\gamma(\tau)} \right) F(\tau)$$

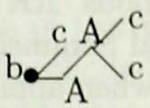
where T_i is the set of rooted trees of order i [18], σ, γ are integer-valued functions of τ, Φ is a certain composition of A, b, c, the skeleton of which depends only on τ and F is an elementary differential [4].

We then consider that a Runge-Kutta method is of order p if and only if

$$X(\tau) = \frac{1}{\sigma(\tau)} \left(\Phi(\tau) - \frac{1}{\gamma(\tau)} \right) = 0, \text{ for every } \tau \in T_i, \text{ for } i = 1(1)p,$$

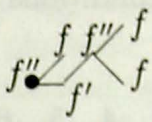
The above relation defines a set of order conditions, which are linear in the components of b and nonlinear in the components of A, c (see, for example, Hairer, Nrsett and Wanner [7] or Butcher [4]). In the following the symbol $T^{(i)}$ denotes a vector whose elements are all the elements of the set $X(T_i)$ in some prescribed (but otherwise arbitrary) order.

The unique matching between a rooted tree τ and an order condition, comes clear after putting b at root, A at internal nodes c at leaves and using a prefix multiplication. Then we produce the single $\Phi(\tau)$ from the order conditions. For example using the following tree τ we name its nodes



and we produce $\Phi(\tau) = bCA^2c^2$.

In the same sense we derive the corresponding elementary differential. We put at every node (including root and the leaves) $f^{(k)}$ where k is the number of successors of the node. Using the same tree and putting the derivatives



we conclude to the elementary differential $F(\tau) = f''(f, f'f''(f, f))$.

The two columns at right of table 1, show this relation for order conditions up to four.

The number of equations of condition (equals the number of rooted trees) for orders up to ten are given in the first row of table 2.

Now observe that $F(t_{42}) = f'f''(f,f) \neq f''(f'f,f) = F(t_{43})$ for systems of ODEs enforcing two separate equations t_{42} and t_{43}. But this is not necessary in the scalar case since $f' \cdot f''(f,f) = f'' \cdot f' \cdot f^2 = f''(f' \cdot f, f)$, and these equations may combine in $t_{42} + t_{43}$. The enumeration of order conditions is based in the relevant theory of unrestricted partitions of a number [18, pg 122]. The number of order conditions up to tenth order, for the scalar autonomous problem, are listed in the last row of 2.

3 Runge-Kutta methods for Periodic Problems

In a previous work [11] we have considered the problem of the construction of specially designed methods for periodic initial value problems. The methods were designed in such a way that for linear systems with $f(x,y) = Ay + g(x)$, where A is a matrix with pure imaginary eigenvalues, the phase error of the free oscillations in the numerical solution is small. A second class of problems with a solution described by free oscillations of high frequency and forced oscillations of low frequency can be efficiently integrated by these methods also. In all other cases the greater the ratio $\min_x |Ay(x)/g(x)|$ the better the efficiency of the methods. RK methods for problems of this type were introduced by Houwen and Sommeijer in [8].

The study of RK behavior when applied to oscillatory problems is analyzed through the scalar test problem,

$$y' = i\omega y, \quad \omega \in \Re, \; i = \sqrt{-1}, \tag{8}$$

Table 2: The number of order conditions for systems and scalar autonomus equation.

order	1	2	3	4	5	6	7	8	9	10
system	1	1	2	4	9	20	48	115	286	719
scalar aut.	1	1	2	3	5	7	11	15	22	30

which yields the numerical solution $y_n = (P(v) + iQ(v))^n y_0 = R^n(v) y_0$, with $v = \omega h$. The polynomials P, Q are

$$P(v) = \sum_{j=0}^{\infty} (-1)^j v^{2j} t'_{2j}, \quad Q(v) = \sum_{j=0}^{\infty} (-1)^j v^{2j+1} t'_{2j+1}$$

where $t'_{-1} = 0$, $t'_0 = 1$ and $t'_j = bA^{j-1}e$. So the numbers t'_j depend only on the coefficients of the method. Actually t's are parts of order conditions since $t'_1 = \Phi(t_{11})$, $t'_2 = \Phi(t_{21})$, $t'_3 = \Phi(t_{32})$, $t'_4 = \Phi(t_{44})$, $t'_5 = \Phi(t_{59})$, etc. It must be observed that for explicit methods (that is for A lower triangular), the summation in the determination of $P(v)$ and $Q(v)$ above is finite (specifically, j runs from 0 through s).

The phase-lag (or dispersion) order of a RK method is defined as the order of approximation of the argument of the exponential function by the argument of R along the imaginary axis. Symbolically, the phase-lag order of a method is q, whenever $\delta(v) = O(v^{q+1})$, for $\delta(v) = v - \arg(R(v))$. For RK methods this notion has been introduced in [8]. The imaginary stability interval of a RK method $I_I = (0, v_0)$ is defined by the relations $|R(v)| < 1$ and $|R(v_0 + \theta)| > 1$, for every $v \in I_I$ and every suitably small positive θ. A method characterized by a non-vanishing imaginary stability interval is called dissipative. High order methods of this type can be found in [23, 24].

Although for a RK method the phase-lag property is defined for the special problem (8), as it was shown by the numerical tests presented in [11, 15] RK pairs of high phase-lag order exhibit a remarkable numerical performance on a much wider class of test problems. This results was recently extended even for multistep methods [26]. It seems that for a certain class of initial value problems (as those whose solutions are described by free oscillations or free oscillations of high frequency with forced oscillations of low frequency superimposed, over long integration intervals), it might be advantageous to use pairs of methods of high phase-lag order with minimized leading truncation error coefficients instead of pairs of the same algebraic order as the latter, but with a phase-lag order equal to the minimal allowed by the number of stages and their algebraic order.

The dissipation order of a RK method (see Houwen and Sommeijer [8]) is defined as the order of approximation of the modulus of the exponential function by the modulus of the characteristic function $P(v)$ of the method along the imaginary axis. That is the dissipation order is q, *iff* $\alpha(v) = O(v^{q+1})$, for $\alpha(v) = 1 - |P(v)|$. For higher dissipation order RK pairs see

Table 3: Phase lag order conditions for a fourth or fifth order method.

order	phase lag equation
6	$1/120 - t'_5 = 0$
8	$1/840 - t'_6 + t'_7 = 0$
10	$1/2268 - t'_6/3 + t'_8 - t'_9 = 0$
12	$221/1247400 - t'_{10} + t'_{11} - 2t'_6/15 + t'_8/3 = 0$
14	$349/4864860 - t'_{10}/3 + t'_{12} - t'_{13} - 17t'_6/315 + 2t'_8/15 = 0$
16	$74251/2554051500 - 2t'_{10}/15 + t'_{12}/3 - 62t'_6/2835 + 17t'_8/315 = 0$

[23]. In practical situations one is interested in estimating the phase-lag and dissipation order of a pth algebraic-order RK method. Explicit formulas for both these quantities are offered by the following theorem.

Phase-lag and dissipation order conditions for RK methods. A RK method is of phase-lag order $2r_p$ *iff* for every $k = 1, \ldots, r_p$,

$$X_p(k) = 0 \text{ and } X_p(r_p + 1) \neq 0$$

where

$$X_p(k) = \sum_{n=1}^{k} \frac{2^{2(k-n+1)}\left(2^{2(k-n+1)} - 1\right)}{(2(k-n+1))!} B_{2(k-n+1)} t'_{2n-2} - t'_{2k-1},$$

and $B_{2n} = B_{2n}(0)$ are the Bernoulli numbers. Moreover a method is of dissipation order $r_d \geq 2$ *iff* for every $k = 2, \ldots, r_d$, $\tilde{X}_d(k) = 0$ and $\tilde{X}_d(r_d + 1) \neq 0$, where $\tilde{X}_d(k) = \sum_{n=1}^{k} \left(t'_{2n-2} t'_{2(k-n)} + t'_{2n-1} t'_{2(k-n)-1}\right)$.

Proof: The proof concerning phase lag order conditions has been given in [11]. The proof concerning dissipation order conditions can be found in [15].

If a specific method is of algebraic-order p, then one should take into account in the previous theorem, that from the algebraic order conditions it is $t'_j = \frac{1}{j!}$, for $0 \leq j \leq p$.

Interpreting the theorem above we conclude to the phase-lag order conditions listed in Table 3, [8].

Actually a fifth algebraic order method satisfies phase-lag order six since $1/120 = t'_5$ is an order condition.

4 Stability for Runge-Kutta methods

There are two kinds of stability when dealing with numerical methods for ODEs. Zero stability and Absolute stability. We use them for the investigation of the behavior of methods when selecting very small or large step sizes respectively.

Zero stability is tested to the model problem $y' = 0$, with analytic solution $y(x) = y(x_0) =$ constant. Runge-Kutta methods are zero stable by construction. It is easy to confirm that the sequence we produce applying a RK method to the test problem is $y_0 = y_1 = \cdots = y_n$ which is in accordance with the theoretical solution. Zero stability and first order of accuracy ensure the convergence of the method to the solution.

Absolute stability is tested to the problem

$$y' = \lambda y, \quad \mathrm{Re}\lambda < 0. \tag{9}$$

This problem has a stable fixed point at $y = 0$. When a discrete numerical scheme is applied to (9), $y_{n+1} < y_n$ is expected to hold.

Applying an explicit RK method to (9), we observe that

$$y_{n+1} = R(H) \cdot y_n$$

where $R(H) = 1 + \sum_{j=1}^{j=s} t'_j H^j$, with $H = \lambda h$. It is natural to ask for $|R(H)| < 1$ then. The latter equation defines a region in the complex plane which is desirable to be as large as possible. Another measure of stability is the length of negative real axis in that region.

For example, the two stages second order RK method

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

has $R(H) = 1 + H + \frac{1}{2}H^2$. We can easily verify that $|R(H)| < 1$ for $H \in (-2, 0)$, which is the stability interval.

5 Runge-Kutta pairs of orders 5(4)

It is known that the minimal number of stages required for the construction of a fifth-order RK method and a 5(4) pair is six. It is the lowest number

of stages that can supply as many coefficients as we need for solving the 25 equations arriving after the expansion of (4) for such a pair. In general, some norm (usually the Euclidean or the maximum) of the truncation error coefficients of that formula of the pair that propagates the numerical solution is regarded as a good indication of its numerical performance. Among families of pairs of the same order and of the same number of effective function evaluations, usually the best pair that can be constructed belongs to the family with the greater number of free parameters.

The most popular RK pairs currently in use are those constructed by Fehlberg [6] and by Dormand and Prince [5]. The FE4(5)#2 pair of Fehlberg belongs to a two-parameter family of pairs. Fehlberg selected the values of these free parameters in order to minimize the truncation error coefficients of the fourth-order method of the pair. It can be shown that the restriction $c_5 = 1$ that Fehlberg imposed on the pairs of the family he proposed is not essential, and it seems that the only reason for its use was the simplification of the otherwise very laborious, at that time, necessary calculations. After performing extensive numerical testing, Shampine in [19] suggested that, from the numerical point of view, it is advantageous to propagate the higher-order solution of a pair (*Local Extrapolation or Higher Order Mode*). Later on, Dormand and Prince proposed a family that uses the first function evaluation from the next step in order to embed a fourth-order method to the fifth-order one, at effectively no additional cost (FSAL device). An individual pair DP5(4), of their four-parameter family, with minimized truncation error coefficients of its fifth-order method, is until now widely regarded as the best fifth-order pair. This pair is undoubtedly better than FE4(5)#2, when both pairs are applied in local extrapolation mode.

Recently Papakostas and Papageorgiou [13], presented a very interesting new family of orders 5(4). They reduced the number of simplifying assumptions and they gained one free parameter more. As a consequence they obtained the pair PP5(4) with the minimal value of the Euclidean norm of the truncation error $\left\|T^{(6)}\right\|_2$, so far. The latter pair is clearly more efficient than FE4(5)#2 and DP5(4).

During the last decade some authors proposed an alternative approach for deriving optimal pairs. They construct seven stages pairs hoping to overcome the extra cost by the reduction of $\left\|T^{(6)}\right\|_2$. Shampine [20], sug-

gests as efficiency measure the quantity $eff = \text{stages} \cdot \left(\left\|T^{(6)}\right\|_2\right)^{1/5}$. The lower the eff the higher the efficiency of a pair. So Bogacki and Shampine [1], proposed the pair BS5(4) while in Sharp and Smart [22], the pair SS5(4) was appeared. These pairs were clearly more efficient than FE5(4)#2 and DP5(4). Interpreting the results in [13], they are more efficient than PP5(4) also.

The New pair: The new method NEW5(4) can be based on 13 stages 8(7) pairs appeared in [25, 17]. We prefer here the PD8(7) pair [17], which is more common to the numerical analysis community. We use the same coefficients c, A which mean that we use the same 13 stages. The weight coefficients b and $\widehat{b}$ need to be determined for the new pair. These weights are of fifth and fourth order of accuracy respectively.

Choosing $b_i = 0$, $i = 2, 3, 4, 5$ we may only solve five of the order conditions:

$$be = 1, bc = 1/2, bc^2 = 1/3, bc^3 = 1/4, bc^4 = 1/5.$$

All the other equations of condition are automatically satisfied by the special properties of matrix A, such as $Ac = \frac{c^2}{2}$, $Ac^2 = \frac{c^3}{3}$, $Ac^3 = \frac{c^4}{4}$, $Ac^4 = \frac{c^5}{5}$, [17]. For example we may drop equation t_{42} since $t_{42} = \frac{1}{2}b \cdot A \cdot c^2 - \frac{1}{24} = \frac{1}{2}b \cdot \frac{c^3}{3} - \frac{1}{24} = \frac{1}{6}bc^3 - \frac{1}{24} = t_{41}$. We may also satisfy another four equations from the phase-lag conditions of orders 8, 10, 12 and 14. So we form a linear system of nine equations in nine unknowns. The resulting weights can be found in Table 4.

The fourth order weights are derived after we set $\widehat{b}_i = 0$, $i = 2, 3, 13$. Then we solve four order conditions

$$\widehat{be} = 1,\ \widehat{bc} = 1/2,\ \widehat{bc^2} = 1/3,\ \widehat{bc^3} = 1/4,$$

and the six phase-lag conditions of orders 6, 8, 10, 12, 14 and 16, for the ten unknowns weights. The values of $\widehat{b}$ can be found in Table 4 also.

The characteristics of the pairs under discussion in this paper are listed in Table 5. The values $\left\|T^{(6)}\right\|_2$ and eff are small enough and ensure increased efficiency. The values $B_2, C_2, E_1, E_2, D_\infty$ concern the reliability of the pairs and ought to be small. NEW5(4) has comparable values with other pairs and it is expected to outperform them on periodic or oscillatory problems. The value $E_2 = \infty$, is due to the requirement $\widehat{t}_5 = \frac{1}{120}$, so the denominator of E_2, $\min_{1<i<9} \left|\widehat{T}_i^{(5)}\right| = 0$. This could cause problems when integrating constant

Table 4: Weights for 5th and 4th order formulas.

$b_1 = 0.02099749076290023$	$b_2 = 0$
$b_3 = 0$	$b_4 = 0$
$b_5 = 0$	$b_6 = -1.38741197813366512$
$b_7 = 0.36651164304019813$	$b_8 = 3.62247827293689219$
$b_9 = -3.52372952792910932$	$b_{10} = 1.77767824900707695$
$b_{11} = 0.08981523715148630$	$b_{12} = -0.03399030685898095$
$b_{13} = 0.06765092002320157$	
$\widehat{b}_1 = -0.11906526797642945$	$\widehat{b}_2 = 0$
$\widehat{b}_3 = 0$	$\widehat{b}_4 = 2.9554898331075603$
$\widehat{b}_5 = 0.6677202916703168$	$\widehat{b}_6 = -2.4061660499314006$
$\widehat{b}_7 = -2.8259627323720786$	$\widehat{b}_8 = 5.58262049082311$
$\widehat{b}_9 = -5.506915501533943$	$\widehat{b}_{10} = 2.548169078914484$
$\widehat{b}_{11} = 0.061438759844964615$	$\widehat{b}_{12} = 0.04267109745341627$
$\widehat{b}_{13} = 0$	

coefficients linear systems of ODEs, since only truncation errors of the form $\widehat{t}'_j = \frac{1}{j!}$ and $t'_j = \frac{1}{j!}$ do not vanish then. So $\widehat{t}'_j = t'_j = \frac{1}{j!}$, $j = 1, 2, 3, 4, 5$ and $\widehat{t}'_j \neq \frac{1}{720}$, $t'_j \neq \frac{1}{720}$ forms two formulas of fifth order for such type of problems and must be avoided in general. Here we could simply avoid this using the seventh algebraic order companion formula of the underlying 8(7) pair.

6 Numerical results

The most widely used RK pair is DP5(4), [10]. So we tested this pair as well as the new method on a set of five oscillatory test problems that we have used many times in relevant papers, see [11, 24, 15].

Model problem

$$y''(x) = -25\, y(x)$$

with initial conditions $y(0) = 1$, $y'(0) = 0$, for $x \in [0, 1000]$, and theoretical solution of this problem is $y(x) = \cos 5x$.

Inhomogeneous equation

$$y'' = -100y + 99\sin x,$$

with $y(0) = 1$, $y'(0) = 11$ for $x \in [0, 500]$. Its theoretical solution is $y(x) = \cos 10x + \cos x + \sin x$.

Hyperbolic problem

The hyperbolic PDE,

$$\begin{aligned} \frac{\vartheta u}{\vartheta x} &= \frac{\vartheta u}{\vartheta r},\ u(x,0) = 0,\ u(0,r) = \sin \pi^2 r^2, \\ 0 &\le r \le 1,\ x \ge 0 \end{aligned}$$

is discretisized by symmetric differences (with $\Delta r = 1/50$) to the system of ODEs

$$\begin{bmatrix} y_1' \\ y_2' \\ \\ \\ y_{50}' \end{bmatrix} = \frac{1}{2 \cdot 50} \begin{bmatrix} 0 & -1 & & & \\ 1 & 0 & -1 & & \\ & & 1 & 0 & -1 \\ & & -1 & 4 & -3 \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ \\ \\ y_{50} \end{bmatrix}.$$

Its theoretical solution was approximated by another internal integration, with much smaller step than the one used for the actual integration.

Bessel equation

$$y'' = -\left(100 + \frac{1}{4x^2}\right) y,$$

with initial conditions $y(1) = -0.2459357644513483$, $y'(1) = -0.5576953439142885$, for $x \in [1, 500]$. The theoretical solution of this problem is $y(x) = \sqrt{x} J_0(10x)$.

Duffing equation

$$y'' = -y - y^3 + .002\cos 1.01x,$$

with $y(0) = 0.200426728067$, $y'(0) = 0$, for $x \in [0, 1000]$.

Theoretical solution, [27] (the rest coefficients are smaller than 10^{-12}):

$$\begin{aligned} y(x) &= 0.200179477536\cos 1.01x + 2.46946143 \cdot 10^{-4} \cos 3.03x \\ &\quad + 3.04014 \cdot 10^{-7} \cos 5.05x + 3.74 \cdot 10^{-10} \cos 7.07x + \cdots \end{aligned}$$

Table 5: The main characteristics of the pairs appeared in this paper.

	$\|T^{(6)}\|_2$	stages	eff	phase lag	B_2	C_2	E_1	E_2	D_∞	S_R
FE54	$3.3 \cdot 10^{-3}$	6	1.91	6	3.2	1.4	1.8	64	8	-3.6
DP54	$4.0 \cdot 10^{-4}$	6	1.25	6	1.5	1.7	0.3	74	11.6	-3.3
PP54	$6.5 \cdot 10^{-5}$	6	0.87	6	1.8	1.8	0.02	28	13.7	-3.5
BS54	$2.2 \cdot 10^{-5}$	7	0.82	6	0.6	0.6	.0003	6	1.2	-3.9
SS54	$7.1 \cdot 10^{-5}$	7	1.03	6	1.1	1.1	0.09	27	0.9	-3.9
NEW54	$5.1 \cdot 10^{-5}$	13	1.80	14	1.2	1.3	0.1	∞	16.7	-6.0

$B_2 = \left\|\hat{T}^{(6)}\right\|_2 / \left\|\hat{T}^{(5)}\right\|_2$, $C_2 = \left\|T^{(6)} - \hat{T}^{(6)}\right\|_2 / \left\|\hat{T}^{(5)}\right\|_2$ [17],
$E_1 = \left\|T^{(6)}\right\|_2 / \left\|\hat{T}^{(5)}\right\|_2$, $E_2 = \max_{1<i<9} \left|\hat{T}^{(5)}\right| / \min_{1<i<9} \left|\hat{T}_i^{(5)}\right|$ [28],
$D_\infty = \max\left(\max_{i,j} |a_{ij}|, \|b\|_\infty, \|c\|_\infty\right)$, S_R: Left point of Stability Interval.

The pairs were tested for tolerances 10^{-3}, 10^{-4},..., 10^{-9}. The stepsize control algorithm (4) was used for both pairs. According to the interpretation for tests of this type used in [16], we notify the percentage difference (among the two methods being tested) by the number of function evaluations required for achieving a given maximum global error over the range of integration. This percentage is called efficiency gain and it is recorded for each problem and accuracy in Table 6 in units of 1%. In this table positive numbers mean that the first of the two methods is superior. The final row gives the mean value of efficiency gain for each problem. The final row's first number is the average efficiency gain for all problems. The empty places are due to unavailability of data for the respective errors. Since DP5(4) uses about 80% more time for achieving a prescribed accuracy, we can easily verify the clear superiority in efficiency of the new pair in comparison to the other pair.

7 Conclusion

Runge-Kutta pairs are the most widely used methods for the numerical integration of Initial Value Problems. Its main competitor are multistep methods especially implemented as Predictor Corrector schemes. The basic

Table 6: Efficiency gains of NEW5(4) relative to DP5(4)a, for the range of tolerances 10^{-3}, 10^{-4}, ..., 10^{-9}.

log global error	model	inhomog.	Hyperb.	Bessel	Dufing
−1	140	100		126	
−2	131	92	−10	113	19
−3	122	85	5	101	34
−4	113	78	22	90	51
−5	104	71	41	79	70
−6	96	64	63	69	92
−7			89		116
−8					143
81	118	82	35	96	75

disadvantage of the latter methods is that they do not leave as many free parameters as RK methods in order to deal special type of problems. These problems may have oscillatory solutions, Hamiltonian nature, stiffness etc. RK are suitable for fulfilling such properties then.

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