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New stable semi-explicit Runge-Kutta methods

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ABSTRACT. Semi-explicit Runge-Kutta methods of order 3 with four stages and order 4 with five stages are discussed, from stability point of view. Some A-stable and L-stable subclasses of such methods are highlighted.

1. INTRODUCTION

For initial value problem

(1.1)
$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0,$$

where $f : [a, b] \times \mathbb{R}^m \longrightarrow \mathbb{R}^m$, $x_0 = a$, $y_0, y \in \mathbb{R}^m$, we consider the numerical solution obtained by special implicit Runge-Kutta methods, called semi-explicit or diagonally-implicit (see [2], [3]).

Many authors have investigated such methods: J.C. Butcher [2], [3], E. Hairer, C. Lubich, G, Wanner [7], [8], P.J. Houwen van der and B.P. Sommeijer [9], K. Burrage [1] etc.

In this paper we will construct some subclasses of semi-explicit Runge-Kutta schemes of order 3 with four stages and order 4 with five stages for problem (1.1). These methods will be A-stable or L-stable thus they are suitable for solving stiff problems.

Without loss of generality, the analysis will be performed when (1.1) is a scalar problem.

2. Preliminaries

Let x_n , n = 0, 1, 2, ..., N be, equal spaced points from interval [a, b], with $x_0 = a$, $x_n - x_{n-1} = h$, $n = 0, 1, 2..., x_N = x_0 + Nh = b$, and let y_n be, the approximate value of exact solution y(x) of (1.1) at the point x_n , n = 0, 1, 2..., N.

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Definition 2.1. A semi-explicit or diagonally-implicit Runge-Kutta method with s stages for numerical solution of the problem (1.1) is defined by the relations

(2.1)
$$k_{i,n} = hf\left(x_n^i, y_n + \sum_{j=1}^s a_{ij}k_{j,n}\right), \quad i = 1, 2, \dots, s$$

(2.2)
$$y_{n+1} = y_n + \sum_{i=1}^s b_i k_{i,n}; \ n = 0, 1, 2 \dots,$$

where $x_n^i = x_n + c_i h$, and $b_i, a_{ij}, c_i, i, j = 1, 2, ..., s$ are real parameters such that

$$a_{ij} = 0$$
, for $j > i$ and $a_{ii} = \lambda$, for all $i, j = 1, 2, \dots, s$.

A semi-explicit Runge-Kutta method is usually displayed in the Butcher's array

$$(2.3) \qquad \qquad \frac{c}{b^T}$$

where $c = (c_1, c_2, \dots, c_s)^T$, $b^T = (b_1, b_2, \dots, b_s)$,

(2.4)
$$A = \begin{pmatrix} \lambda & 0 & 0 & \cdots & 0 \\ a_{21} & \lambda & 0 & \cdots & 0 \\ a_{31} & a_{32} & \lambda & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{s1} & a_{s2} & a_{s3} & \cdots & \lambda \end{pmatrix},$$

should satisfy

$$(2.5) c = A \cdot e,$$

with $e = (1, 1, ..., 1)^T \in \mathbb{R}^s$.

We will focus our attention only to methods with s = 4 stages and s = 5 stages. For s = 4 and s = 5 stages the Runge-Kutta methods are generated respectively by the arrays

The stability function for such methods, depends only on parameter λ (see [9]) and it is given by

(2.7)
$$R(z,\lambda) = \frac{P(z,\lambda)}{Q(z,\lambda)}, \quad z \text{ complex},$$

where

$$P(z,\lambda) = 1 + (1-4\lambda)z + \left(\frac{1}{2} - 4\lambda + 6\lambda^2\right)z^2 + (2.8) + \left(\frac{1}{6} - 2\lambda + 6\lambda^2 - 4\lambda^3\right)z^3 + \left(\frac{1}{24} - \frac{2}{3}\lambda + 3\lambda^2 - 4\lambda^3 + \lambda^4\right)z^4,$$

(2.9)
$$Q(z,\lambda) = (1-\lambda z)^4,$$

for s = 4, and

$$P(z,\lambda) = 1 + (1-5\lambda)z + \left(\frac{1}{2} - 5\lambda + 10\lambda^2\right)z^{\lambda} + \left(\frac{1}{6} - \frac{5}{2}\lambda + 10\lambda^2 - 10\lambda^3\right)z^3 + \left(\frac{1}{24} - \frac{5}{6}\lambda + 5\lambda^2 - 10\lambda^3 + 5\lambda^4\right)z^4 + \left(\frac{1}{120} - \frac{5}{24}\lambda + \frac{5}{3}\lambda^2 - 5\lambda^3 + 5\lambda^4 - \lambda^5\right)z^5,$$
(2.10)

(2.11)
$$Q(z,\lambda) = (1-\lambda z)^5,$$

if the methods have s = 5 stages.

A-stability of the semi-explicit Runge-Kutta methods generated by the arrays (2.6) is equivalent (see [4]) to requirements that the polynomial Q should have no zeros in the left half-plane, that is $\lambda > 0$, and E-polynomial of Nørsett, [10],

(2.12)
$$E(y^2, \lambda) := |Q(iy, \lambda)|^2 - |P(iy, \lambda)|^2,$$

should satisfy

(2.13)
$$E(y^2, \lambda) \ge 0, \quad \forall \ y \in \mathbb{R},$$

for some $\lambda > 0$.

For L-stability, the stability function should satisfy the A-stability, requirements and more

(2.14)
$$\lim_{|z| \to +\infty} R(z, \lambda) = 0.$$

3. The construction of A-stable and L-stable methods of ORDER 3

To obtain semi-explicit methods of order 3 with s = 4 stages, we impose the order conditions (see [2]), together with (2.5), which, in case of semiexplicit methods, become

$$(3.1) b_1 + b_2 + b_3 + b_4 = 1,$$

(3.2)
$$b_1c_1 + b_2c_2 + b_3c_3 + b_4c_4 = \frac{1}{2},$$

(3.3)
$$b_1c_1^2 + b_2c_2^2 + b_3c_3^2 + b_4c_4^2 = \frac{1}{3},$$

$$(3.4) \quad b_2a_{21}c_1 + b_3(a_{31}c_1 + a_{32}c_2) + b_4(a_{41}c_1 + a_{42}c_2 + a_{43}c_3) = \frac{1}{6} - \frac{\lambda}{2},$$

(3.5)
$$c_1 = \lambda, \ c_2 = a_{21} + \lambda, \ c_3 = a_{31} + a_{32} + \lambda,$$

$$(3.6) c_4 = a_{41} + a_{42} + a_{43} + \lambda.$$

So, we are seeking values of parameters from the tableaux (2.6), usually

 $0 < c_i \leq 1, i = 1, 2, 3, 4$, that is $0 < \lambda \leq 1$, such that the equations (3.1) -(3.6) be satisfied and also (2.13) or (2.13) and (2.14). We can state

Lemma 3.1. The solutions of the system (3.1) - (3.6) are depending on the free parameters $\lambda, c_2, c_3, c_4 \in (0, 1]$, pairwise distinct and on the free parameters $b_1, a_{31}, a_{41}, a_{42}$, arbitrary real numbers. The solutions are given by

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$$b_{2} = A_{2}/6(c_{3} - c_{2})(c_{4} - c_{2}),$$

$$b_{3} = -A_{3}/6(c_{3} - c_{2})(c_{4} - c_{3}),$$

$$b_{4} = A_{4}/6(c_{4} - c_{2})(c_{4} - c_{3}),$$

$$a_{43} = c_{4} - a_{41} - a_{42} - \lambda,$$

$$a_{32} = c_{3} - a_{31} - \lambda, \ a_{21} = c_{2} - \lambda, \ c_{1} = \lambda,$$

where

$$(3.8) \quad A_2 = 2 - 3(c_3 + c_4) + 6c_3c_4 - 6b_1 \left[\lambda^2 - \lambda(c_3 + c_4) + c_3c_4\right],$$

$$(3.9) \quad A_3 = 2 - 3(c_2 + c_4) + 6c_2c_4 - 6b_1 \left[\lambda^2 - \lambda(c_2 + c_4) + c_2c_4\right],$$

$$(3.10) \quad A_4 = 2 - 3(c_2 + c_3) + 6c_2c_3 - 6b_1 \left[\lambda^2 - \lambda(c_2 + c_3) + c_2c_3\right]$$

and the free parameters $\lambda, c_2, c_3, c_4, b_1, a_{31}, a_{41}, a_{42}$ should satisfy

$$A_{2}\lambda(c_{2}-\lambda)(c_{4}-c_{3}) - A_{3}[a_{31}\lambda + c_{2}(c_{3}-a_{31}-\lambda)](c_{4}-c_{2}) + A_{4}[a_{41}\lambda + a_{42}c_{2} + c_{3}(c_{4}-a_{41}-a_{42}-\lambda)](c_{3}-c_{2}) = (1-3\lambda)(c_{3}-c_{2})(c_{4}-c_{3}).$$
(3.11)

Proof. By solving the equations (3.1), (3.2) and (3.3) as a linear system with respect to b_2, b_3, b_4 and replacing the expressions of b_2, b_3, b_4 into the equation (3.4), and taking into account (3.5) and (3.6), after a long computation, we obtain the conclusions (3.7) and (3.11).

Remark 3.2. The formulas (3.7) provide the class of all semi-explicit Runge-Kutta methods of order 3, with four stages, depending on 8 free parameters $\lambda, c_2, c_3, c_4 \in (0, 1]$ distinct each other and $b_1, a_{31}, a_{41}, a_{42} \in \mathbb{R}$.

Example 3.3. We can check that the array

represents a family of semi-explicit methods of order 3 with four stages depending on one free parameter $\lambda \in (0, 1]$, belonging to the class specified in the Remark 3.2.

Now we will delimit two subsets of the class of semi-explicit Runge-Kutta methods of order 3 with four stages, namely the subclass of A-stable methods, and the subclass of L-stable methods. We have

Theorem 3.4. For every $\lambda \in [\alpha, 1], c_2, c_3, c_4 \in (0, 1]$, distinct each other and every $b_1, a_{31}, a_{41}, a_{42}$ arbitrary real numbers, where $\alpha = \frac{3 + \sqrt{3}}{12} =$ 0.3943375673..., the solutions (3.7) provide a subclass of A-stable semiexplicit Runge-Kutta methods of order 3 with four stages. Moreover, for the value $\lambda = \lambda^* = 0.5728160625...$, and the rest of free

Moreover, for the value $\lambda = \lambda^* = 0.5728160625...$, and the rest of free parameters as above, the solutions (3.7) provide a subclass of L-stable semi-explicit Runge-Kutta methods of order 3 with s = 4 stages.

Proof. We seek values for λ such that the inequality (2.13) be satisfied. If we write the polynomial E in the form

(3.13)
$$E(y^2, \lambda) = A(\lambda)y^6 + B(\lambda)y^8,$$

where A and B are the polynomials in λ

(3.14)
$$A(\lambda) = \frac{1}{72} - \frac{1}{3}\lambda + \frac{17}{6}\lambda^2 - \frac{32}{3}\lambda^3 + 17\lambda^4 - 8\lambda^5,$$

$$(3.15) \ B(\lambda) = -\frac{1}{576} + \frac{1}{18}\lambda - \frac{25}{36}\lambda^2 + \frac{13}{3}\lambda^3 - \frac{173}{12}\lambda^4 + \frac{76}{3}\lambda^5 - 22\lambda^6 + 8\lambda^7,$$

and then, solve numerically the equations $A(\lambda) = 0$ and $B(\lambda) = 0$, we obtain the real roots. $A(\lambda)$ has the real roots

$$\lambda_1 = 0.0939962451\ldots; \ \lambda_2 = 0.3486234981\ldots, \ \lambda_3 = 1.2805797610\ldots,$$

and $B(\lambda)$ has the real roots:

$$\begin{split} \lambda_1' &= 0.1056624327\ldots, \ \lambda_2' = 0.1072789060\ldots \ \lambda_3' = 0.2038425244\ldots, \\ \lambda_4' &= \frac{1}{4}; \ \lambda_5' = 0.3943375673\ldots \end{split}$$

The polynomials A and B take the factorized forms

(3.16)
$$A(\lambda) = -8(\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3)(\lambda^2 - a\lambda + b),$$

$$(3.17) \quad B(\lambda) = 8(\lambda - \lambda_1')(\lambda - \lambda_2')(\lambda - \lambda_3')(\lambda - \lambda_4')(\lambda - \lambda_5')(\lambda^2 - a'\lambda + b'),$$

where $\lambda^2 - a\lambda + b$ and $\lambda^2 - a'\lambda + b'$ have no real roots, that is, they take only positive values.

We can now solve the system of inequalities

(3.18)
$$A(\lambda) \ge 0, \quad B(\lambda) \ge 0, \quad 0 < \lambda \le 1,$$

by studding the sign of $A(\lambda)$ and $B(\lambda)$.

We obtain that (3.18) are satisfied if and only if $\lambda \in [\lambda'_5, 1]$.

Putting $\lambda'_5 = \alpha = 0.3943375673...$ it follows the first conclusion of the theorem. If we take for λ the value $\lambda = \lambda^* = 0.5728160625...$, we see that the coefficient of z^4 in the numerator P of stability function (2.7), vanishes, so the degree of P is less than the degree of Q and then we have (2.14). Because $\lambda^* \in [\alpha, 1]$ we can say that the subclass of semi-explicit methods with $\lambda = \lambda^*$ are L-stable.

We have used the Maple 6 and Mathematica 5 packages for numerical solving of equations $A(\lambda) = 0$ and $B(\lambda) = 0$.

Example 3.5. We present five example of semi-explicit Runge-Kutta methods of order 3 with four stages, the first four methods are A-stable and the last, L-stable.

(3.19)

(3.20)

$\frac{1}{2}$ $\frac{1}{5}$ $\frac{2}{3}$ 1	$\begin{vmatrix} 1\\ -\frac{3}{10}\\ -\frac{3}{10}\\ -\frac{1}{9}\\ -\frac{4}{5}\\ -\frac{22}{2} \end{vmatrix}$	$\begin{array}{c} 0\\ \frac{1}{2}\\ \frac{5}{18}\\ 1\\ \frac{5}{9} \end{array}$	$\begin{array}{c} 0\\ 0\\ \frac{1}{2}\\ \frac{3}{10}\\ 9 \end{array}$	$\begin{array}{c} 0\\ 0\\ \frac{1}{2}\\ 1 \end{array}$
	$ ^{-}\overline{45}$	$\overline{9}$	$\overline{10}$	$\overline{30}$

(3.21)

30Iulian Coroian $\frac{3}{51}$ $\frac{5}{52}$ $\frac{5}{54}$ $\frac{5}{5}$ 3 0 $\overline{5}_{2}$ 0 0 3 00 $\overline{\overline{5}}_{3}$ $\overline{5}$ $\frac{3}{5}$ 1 (3.22)0 $\begin{array}{r}
10\\
3\\
\overline{5}\\
\overline{5}\\
\overline{9}\\
\end{array}$ $\overline{10}$ 3 1 $\overline{5}$ $\frac{\overline{5}}{13}$ $\overline{5}$ 1 1 $\overline{4}$ $\overline{3}$ $\overline{36}$ 0.5730.5730.400-0.1730.5730.6000.072-0.0450.573(3.23)1.0000 1.281-0.854 0.573 5 10 11 0 9 $\overline{12}$ $\overline{36}$

4. The construction of A-stable and L-stable methods of oreder 4

Now, we are focusing on semi-explicit Runge-Kutta methods, generated by the second tableau of (2.6), having order p = 4 and s = 5 stages. The order conditions become, in this case (see [2, p.170])

(4.1)
$$\sum_{i=1}^{5} b_i c_i^{k-1} = \frac{1}{k}, \quad k = 1, 2, 3, 4$$

(4.2)
$$\sum_{i=2}^{5} b_i \sum_{j=1}^{i-1} a_{ij} c_j = \frac{1}{6} - \frac{\lambda}{2},$$

(4.3)
$$\sum_{i=2}^{5} b_i c_i \sum_{j=1}^{i-1} a_{ij} c_j = \frac{1}{8} - \frac{\lambda}{3},$$

(4.4)
$$\sum_{i=2}^{5} b_i \sum_{j=1}^{i-1} a_{ij} c_j^2 = \frac{1}{12} - \frac{\lambda}{4},$$

(4.5)
$$\sum_{i=3}^{5} b_i \sum_{j=2}^{i-1} a_{ij} \sum_{k=1}^{j-1} a_{jk} c_k = \frac{1}{24} - \frac{\lambda}{3} + \frac{\lambda^2}{2},$$

with additional conditions (2.5), that is

$$(4.6) c_1 = \lambda, c_2 = a_{21} + \lambda, c_3 = a_{31} + a_{32} + \lambda,$$

$$(4.7) c_4 = a_{41} + a_{42} + a_{43} + \lambda,$$

$$(4.8) c_5 = a_{51} + a_{52} + a_{53} + a_{54} + \lambda.$$

We are seeking for values of parameters $b_i, c_i, a_{ij}, \lambda$, usually $0 < c_i \leq 1$ i = 1, 2, 3, 4, 5, so $0 < \lambda \leq 1$, distinct, such that the equations (4.1)-(4.8) be satisfied and also the conditions (2.13) for A-stability or (2.13) and (2.14) for L-stability satisfied.

The complete solutions of the nonlinear algebraic system (4.1)-(4.8) is not an easy problem, but every solution of this system, provides one semiexplicit (diagonally implicit) Runge-Kutta method of order 4 with s = 5stages.

We will not give the complete solutions of the system (4.1)-(4.8) because it has a very complicated form.

We can state

Theorem 4.1. The solution of the system (4.1)-(4.8) provide A-stable Runge-Kutta methods of order 4 with five stages if and only if

$$\lambda \in [\alpha, \beta] \cup [\gamma, \delta],$$

where

$$\begin{aligned} \alpha &= 0.0701257\ldots, \quad \beta &= 0.0726521\ldots, \\ \gamma &= 0.2402928\ldots, \quad \delta &= 0.4732683\ldots. \end{aligned}$$

Moreover for $\lambda = \lambda_1 = 0.07075122...$ or $\lambda = \lambda_2 = 0.2780538...$, the corresponding solutions of the system (4.1)-(4.8) provide two subclasses of L-stable Runge-Kutta methods of order 4 with five stages.

Proof. The *E*-polynomial (2.12) for methods with s = 5 stages can be written, using (2.10) and (2.11), as

(4.9)
$$E(y^2, \lambda) = A_1(\lambda)y^6 + A_2(\lambda)y^8 + A_3(\lambda)y^{10},$$

where

(4.10)
$$A_1(\lambda) = -\frac{1}{360} + \frac{1}{12}\lambda - \frac{5}{6}\lambda^2 + \frac{10}{3}\lambda^3 - 5\lambda^4 + 2\lambda^5,$$

(4.11)
$$A_{2}(\lambda) = \frac{1}{960} - \frac{1}{24}\lambda + \frac{47}{72}\lambda^{2} - \frac{31}{6}\lambda^{3} + \frac{265}{12}\lambda^{4} - \frac{151}{3}\lambda^{5} + 55\lambda^{6} - 20\lambda^{7},$$

$$(4.12) \qquad A_3(\lambda) = -\frac{1}{14400} + \frac{1}{288}\lambda - \frac{41}{576}\lambda^2 + \frac{56}{9}\lambda^3 - \frac{89}{18}\lambda^4 + \frac{563}{30}\lambda^5 - \frac{505}{12}\lambda^6 + \frac{160}{3}\lambda^7 - 35\lambda^8 + 10\lambda^9.$$

If we find numerically the real roots of the polynomials $A_1(\lambda)$, $A_2(\lambda)$, $A_3(\lambda)$, then we can solve the inequalities

(4.13)
$$A_1(\lambda) \ge 0, \quad A_2(\lambda) \ge 0, \quad A_3(\lambda) \ge 0, \quad 0 < \lambda \le 1,$$

by studding the sign of $A_1(\lambda)$, $A_2(\lambda)$, $A_3(\lambda)$.

We obtain that (4.13) hold for $\lambda \in [\alpha, \beta] \cup [\gamma, \delta]$, where $\alpha = 0.0701257...$, $\beta = 0.072652...$, $\gamma = 0.2402928404...$, and $\delta = 0.4732683912...$, and then with (4.9)

(4.14)
$$E(y^2, \lambda) \ge 0, \quad y \in \mathbb{R}, \quad \lambda \in [\alpha, \beta] \cup [\gamma, \delta].$$

The last condition is sufficient for A-stability of every method, solution of the system (4.1)-(4.8), which ensures the order p = 4 of the method.

If we take $\lambda = \lambda_1 = 0.075122... \in [\alpha, \beta]$ and $\lambda = \lambda_2 = 0.2780538411 \in [\gamma, \delta]$, then we can check that the coefficient of z^5 of the polynomial $P(z, \lambda)$ from (2.10), vanishes. In this case the condition (2.14) is fulfilled, so every solution of the system (4.1)-(4.8) with $\lambda = \lambda_1$ or $\lambda = \lambda_2$ provides one *L*-stable semi-explicit Runge-Kutta method of order p = 4 with s = 5 stages.

Again, we mention that we used the Maple 6 and Mathematica 5 packages for numerical root finding for polynomials (4.10), (4.11), (4.12).

In the next we will give only two particular solutions of the system (4.1)-(4.8), i.e. two particular A-stable or L-stable methods. \Box

Example 4.2. We present two semi-explicit Runge-Kutta methods of order 4 with five stages i.e. two solutions of the system (4.1)-(4.8), the first method (4.15) is A-stable and the last, (4.16), L-stable.

It is clearly that the coefficients of the Runge-Kutta methods (3.23) and (4.16) can be given with arbitrary accuracy.

(4.15)	$\frac{2}{5}$ $\frac{3}{5}$ $\frac{4}{5}$ $\frac{1}{5}$ 1	$ \begin{array}{c c} 2\\ \overline{5}\\ 1\\ \overline{5}\\ 1\\ \overline{5}\\ 1\\ \overline{19}\\ 1337\\ \overline{435}\\ -\overline{55}\\ -\overline{72}\\ \end{array} $	$ \begin{array}{r} \frac{2}{5} \\ \frac{1}{5} \\ -\frac{8}{19} \\ -\frac{1934}{435} \\ \frac{5}{4} \\ \end{array} $	$ \begin{array}{r} 2\\ \overline{5}\\ 16\\ \overline{95}\\ 454\\ \overline{261}\\ -\frac{25}{72}\end{array} $	$ \frac{2}{5} \\ \frac{304}{1305} \\ \frac{95}{144} $	$\frac{2}{\overline{5}}$ $\frac{29}{144}$	_	
(4.16)								
0.278053	0.2	278053						
0.200000	-0.078053		0.278053					
0.600000	-0.340512		0.667068		0.278053			
0.800000	0.905887		0		-0.383939		0.278053	
1.000000	20.8	323214	-13.830	0951	-9.962	345	3.692028	0.278053
	-4.2	221747	3.262	2906	4.168	667	-2.926083	0.916683

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