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Explicit Runge-Kutta Formulas with Increased Stability Boundaries

P. J. van der Houwen

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Abstract. A survey of the main results is given of our work of the last years on explicit Runge-Kutta methods for the integration of ordinary or partial differential equations. Three classes of integration formulas are presented which have second, third and fourth order accuracy, respectively. These methods are characterized by their limited storage requirements and by the possibility to adapt the characteristic root of the method to the problem under consideration. They may be used for the integration of parabolic, of hyperbolic and of stiff differential equations.

1. Definitions

Let

$$\frac{dy}{dx} = f(x, y) \tag{1.1}$$

represent a set of differential equations of which the real vector function $f(x, y)$ belongs to a class of sufficient differentiability. In order to solve an initial value problem for this equation we consider explicit m-point single-step Runge-Kutta formulas, i.e. formulas of the type

$$\begin{aligned} y_{n+1} &= y_n + \sum_{j=0}^{m-1} \theta_j k_j, \\ k_j &= h_n f\left(x_n + \mu_j h_n, y_n + \sum_{l=0}^{j-1} \lambda_{j,l} k_l\right), \\ \mu_0 &= \lambda_{0,0} = \lambda_{0,-1} = 0. \end{aligned} \tag{1.2}$$

Here, h_n is the step length $x_{n+1} - x_n$. Using the condensed representation of Runge-Kutta methods, introduced by Butcher, we may represent (1.2) by the array form

$$\begin{array}{c|c} M & \Lambda \\ \hline & \Theta \end{array} \tag{1.2'}$$

where M is the column vector $(\mu_0, \ldots, \mu_{m-1})$, Λ the lower triangular matrix containing the parameters $\lambda_{j,l}$ and Θ the row vector $(\theta_0, \ldots, \theta_{m-1})$.

When scheme (1.2) is applied to the scalar equation

$$\frac{dy}{dx} = \delta y,$$

we obtain

$$y_{n+1} = P_m(h_n \delta) y_n,$$

where $P_m(z)$ is a polynomial of the form

$$P_m(z) = \beta_0 + \beta_1 z + \cdots + \beta_m z^m, \tag{1.3}$$

of which the coefficients β_j can be expressed in terms of the Runge-Kutta parameters. The polynomial $P_m(z)$ will be called the stability polynomial associated to formula (1.2′). As is well-known, the stability polynomial is compatible with a Runge-Kutta formula of order p, provided that

$$\beta_j = \frac{1}{j!}, \quad j = 0, 1, \ldots, p. \tag{1.4}$$

When (1.4) is satisfied, the polynomial $P_m(z)$ will be called p-th order exact.

Furthermore, the region S defined by

$$S = \{z \,|\, |P_n(z)| < 1\} \tag{1.5}$$

will be called the stability region of the Runge-Kutta formula.

In this paper, scheme (1.2) applied to equation (1.1) is said to be stable when the set of points $h_n \delta$, where δ is an eigenvalue of the Jacobian matrix of (1.1), belongs to the stability region S of the stability polynomial.

2. Some special Runge-Kutta formulas

We propose three classes of Runge-Kutta formulas of which the stability polynomials can be chosen freely, apart from the condition that these polynomials are in agreement with the order of accuracy of the formulas (condition (1.4)). A further characteristic of our formulas are the limited storage requirements when used in a computer.

The first class of formulas is of the type

$$\begin{array}{l|lllll}
0 & & & & & \\
\lambda_{1,0} & \lambda_{1,0} & & & & \\
\lambda_{2,1} & 0 & \lambda_{2,1} & & & \\
\cdot & \cdot & & \cdot & & \\
\cdot & \cdot & & & \cdot & \\
\cdot & \cdot & & & & \cdot \\
\lambda_{m-1,m-2} & 0 & \ldots & 0 & \lambda_{m-1,m-2} & \\
\hline
 & 0 & \ldots & & 0 & 1
\end{array} \tag{2.1}$$

This scheme generates a Runge-Kutta method which is at least of first order. In case that

$$\lambda_{m-1,m-2} = \tfrac{1}{2} \tag{2.2}$$

we even have second order accuracy.

By putting

$$\lambda_{j,j-1} = \frac{\beta_{m+1-j}}{\beta_{m-1}}, \quad j = 1, 2, \ldots, m-2; \quad \lambda_{m-1,m-2} = \beta_2 \tag{2.3}$$

the stability polynomial assumes the form

$$P_m(z) = 1 + z + \beta_2 z^2 + \cdots + \beta_m z^m. \tag{2.4}$$

The second class of formulas is given by

$$\begin{array}{c|ccccccc}
0 & & & & & & & \\
\lambda_{1,0} & \lambda_{1,0} & & & & & & \\
\lambda_{2,1}+\frac{1}{4} & \frac{1}{4} & \lambda_{2,1} & & & & & \\
\lambda_{3,2}+\frac{1}{4} & \frac{1}{4} & 0 & \lambda_{3,2} & & & & \\
\cdot & \cdot & \cdot & & \cdot & & & \\
\cdot & \cdot & \cdot & & & \cdot & & \\
\cdot & \cdot & \cdot & & & & \cdot & \\
\frac{8}{15} & \frac{1}{4} & 0 & \cdots & 0 & \frac{17}{60} & & \\
\frac{2}{3} & \frac{1}{4} & 0 & \cdots & 0 & 0 & \frac{5}{12} & \\
\hline
 & \frac{1}{4} & 0 & \cdots & 0 & 0 & 0 & \frac{3}{4}
\end{array} \tag{2.5}$$

For $m > 3$ (2.5) is third order exact. When we put

$$\begin{aligned}
\lambda_{j,j-1} &= \frac{\beta_{m-j+1}}{\beta_{m-j-1}}\left(1+\frac{1}{4\lambda_{j+1,j}}\right)-\frac{1}{4}, \qquad j=2,3,\ldots,m-3,\\
\lambda_{1,0} &= \frac{\beta_m}{\beta_{m-1}}\left(1+\frac{1}{4\lambda_{2,1}}\right),
\end{aligned} \tag{2.6}$$

the stability polynomial becomes

$$P_m(z) = 1 + z + \tfrac{1}{2}z^2 + \tfrac{1}{6}z^3 + \beta_4 z^4 + \cdots + \beta_m z^m. \tag{2.7}$$

The third class of formulas considered in this paper is generated by the array form

$$\begin{array}{c|cccccccccc}
0 & & & & & & & & & & \\
\frac{1}{2} & \frac{1}{2} & & & & & & & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & & & & & & & \\
\lambda_{3,1}+\lambda_{3,2} & 0 & \lambda_{3,1} & \lambda_{3,2} & & & & & & & \\
\lambda_{4,1}+\lambda_{4,3} & 0 & \lambda_{4,1} & 0 & \lambda_{4,3} & & & & & & \\
\lambda_{5,4} & 0 & 0 & 0 & 0 & \lambda_{5,4} & & & & & \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & \\
\cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & & & & \\
\cdot & \cdot & \cdot & \cdot & \cdot & & & \cdot & & & \\
\lambda_{m-4,m-5} & 0 & 0 & 0 & 0 & \cdots & 0 & \lambda_{m-4,m-5} & & & \\
\frac{1}{2} & 0 & \lambda_{m-3,1} & 0 & 0 & \cdots & 0 & 0 & \lambda_{m-3,m-4} & & \\
\frac{1}{2} & 0 & \lambda_{m-2,1} & 0 & 0 & \cdots & 0 & 0 & 0 & \lambda_{m-2,m-3} & \\
1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 1 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \quad \frac{1}{6}
\end{array} \tag{2.8}$$

where

$$\begin{aligned}
\lambda_{m-3,1} &= 0 \quad \text{for} \quad m \geqq 8,\\
\lambda_{m-2,1} &= 0 \quad \text{for} \quad m \geqq 7.
\end{aligned}$$

Table 2.1. Parameters $\lambda_{j,1}$ expressed in terms of β_j

	$m=5$	$m=6$	$m=7$	$m=8$	$m \geqq 9$
$\lambda_{3,1}$	$\frac{1}{2}-24\beta_5$	$\frac{1}{2}-\frac{\beta_6}{\beta_5}$	$\frac{48(\beta_6-2\beta_7)}{1-48(\beta_5-2\beta_6)}$	$\frac{2(\beta_{m-1}-2\beta_m)}{\beta_{m-3}-2\beta_{m-2}+4\beta_{m-1}}$	
$\lambda_{3,2}$	$24\beta_5$	$\frac{\beta_6}{\beta_5}$	$\frac{96\beta_7}{1-48(\beta_5-2\beta_6)}$	$\frac{4\beta_6}{\beta_{m-3}-2\beta_{m-2}+4\beta_{m-1}}$	
$\lambda_{4,1}$	0	$\frac{1}{2}-24\beta_5$	$24(\beta_5-2\beta_6)$	$48(\beta_6-2\beta_7)$	$2\frac{\beta_{m-2}-2\beta_{m-1}}{\beta_{m-4}}$
$\lambda_{4,3}$	1	$24\beta_5$	$\frac{1}{2}-24(\beta_5-2\beta_6)$	$24(\beta_5-2\beta_6+4\beta_7)$	$\frac{\beta_{m-3}-2\beta_{m-2}+4\beta_{m-1}}{\beta_{m-4}}$
$\lambda_{5,4}$		1	$\frac{1}{2}$	$\frac{1}{2}$	$\lambda_{j,j-1}=\frac{\beta_{m+1-j}}{\beta_{m-j}}$
$\lambda_{6,5}$			1	$\frac{1}{2}$	$j=5, 6, \ldots, m-5,\ m \geqq 10.$
$\lambda_{7,6}$				1	
$\lambda_{m-4,m-5}$					$24\beta_5$
$\lambda_{m-3,m-4}$					$\frac{1}{2}$
$\lambda_{m-2,m-3}$					$\frac{1}{2}$
$\lambda_{m-1,m-2}$					1

Formula (2.8) is fourth order exact. By expressing the parameters $\lambda_{j,l}$ in terms of $\beta_5, \ldots, \beta_m$, as listed in Table 2.1, we obtain a stability polynomial of the form

$$P_m(z)=1+z+\tfrac{1}{2}z^2+\tfrac{1}{6}z^3+\tfrac{1}{24}z^4+\beta_5 z^5+\cdots+\beta_m z^m. \tag{2.9}$$

The derivation of the formulas (2.1), (2.5), (2.8) and of the expressions of the Runge-Kutta parameters $\lambda_{j,l}$ in terms of the stability coefficients β_j may be found in [9].

In the subsequent sections several types of stability polynomials will be given which are appropriate for the integration of parabolic, of hyperbolic and of stiff differential equations, respectively.

3. Stability Polynomials for Parabolic Differential Equations

Many parabolic differential equations lead after discretization of the space variables to a set of ordinary differential equations of type (1.1) of which the Jacobian matrix has negative eigenvalues δ with the property

$$|\delta|_{\min} \ll |\delta|_{\max}.$$

Let $[-\beta, 0]$ be the segment of the real axis which belongs to the stability domain S of the Runge-Kutta formula to be used. Then, the stability condition becomes

$$h_n < \frac{\beta}{|\delta|_{\max}}. \tag{3.1}$$

Hence, we are looking for polynomials $P_m(z)$ of type (2.4), (2.7) or (2.9), which have a real stability boundary β as large as possible.

The optimal polynomials of type (2.4) are well-known; one has

$$P_m(z) = T_m\left(1 + \frac{z}{m^2}\right), \quad \beta = 2m^2, \tag{3.2}$$

where $T_m(z)$ denotes the Chebyshev polynomial of degree m in z. These polynomials were already used by Franklin [3] in 1959 in connection with the integration of linear diffusion problems.

In [4] a strongly stable version of such first order polynomials is given, namely

$$P_m(z) = \frac{T_m(w_0 + w_1 z)}{T_m(w_0)},$$
$$w_0 = \frac{s+1}{s-1}, \quad w_1 = \frac{2\sqrt{s}}{m(s-1)\,\mathrm{th}\left[m \ln \frac{\sqrt{s}+1}{\sqrt{s}-1}\right]}, \quad s = \frac{|\delta|_{\max}}{|\delta|_{\min}}. \tag{3.3}$$

This polynomial has the property that, if the real stability boundary is chosen according to

$$\beta = \frac{w_0 + 1}{w_1}. \tag{3.4}$$

the characteristic roots of the Runge-Kutta formula have absolute values less than 1, i.e.

$$|P_m(h_n \delta)| = T_m^{-1}\,(w_0) < 1. \tag{3.5}$$

Furthermore, it is proved that of all first order polynomials satisfying condition (3.5), polynomial (3.3) allows the largest integration steps.

The optimization of polynomials of type (2.4) with the additional condition $\beta_2 = \frac{1}{2}$, was studied by Lomax [15]. He gave a set of second order polynomials with considerably increased stability boundaries. However, in his paper he makes no attempt to find the optimal polynomials. Our starting point in constructing polynomials with a maximal real stability boundary is based on the following theorem (cf. [16]):

Theorem 3.1. Of all polynomials $P_m(x)$ of the form

$$P_m(x) = 1 + z + \cdots + \frac{1}{p!} z^p + \beta_{p+1} z^{p+1} + \cdots + \beta_m z^m,$$

where p and m are given numbers, the polynomial which has $m - p$ alternating points of tangency to the lines $y = \pm 1$, $x < 0$, maximizes (if it exists) the real stability boundary.

Table 3.1. Coefficients of the optimal polynomials for $p = 2$, $m = 3, \ldots, 12$

m	$\beta(m)/m^2$	$10^9\beta_3$	$10^{10}\beta_4$	$10^{11}\beta_5$	$10^{12}\beta_6$	$10^{14}\beta_7$	$10^{16}\beta_8$	$10^{18}\beta_9$	$10^{20}\beta_{10}$	$10^{23}\beta_{11}$	$10^{25}\beta_{12}$
3	0.6956	62500000									
4	0.7529	78084485	36084541								
5	0.7782	84608499	55271248	12219644							
6	0.7917	87994019	66169168	22176071	2731156						
7	0.7998	89985021	72877550	29298151	5723751	4336799					
8	0.8050	91257740	77281768	34366789	8297337	10298268	5148095				
9	0.8085	92121645	80322777	38043289	10373348	16275261	13652347	4743119			
10	0.8111	92735331	82508285	40773070	12021734	21658644	23378958	13887849	3490930		
11	0.8130	93187123	84130659	43846249	13332017	26301736	33046921	25627575	11181948	20999782	
12	0.8144	93529476	85367612	44453441	14381440	30237000	42045847	38385258	22126214	73028416	10518942

Table 3.2. Coefficients of the optimal polynomials for $p = 3$, $m = 4, \ldots, 13$

m	$\beta(m)/m^2$	$10^9\beta_4$	$10^{10}\beta_5$	$10^{11}\beta_6$	$10^{13}\beta_7$	$10^{14}\beta_8$	$10^{16}\beta_9$	$10^{18}\beta_{10}$	$10^{20}\beta_{11}$	$10^{22}\beta_{13}$	$10^{25}\beta_{13}$
4	0.3767	18455702									
5	0.4214	23721832	11118724								
6	0.4457	26054057	17697690	4284125							
7	0.4604	27315880	21688644	8124209	11539864						
8	0.4699	28083307	24265433	11058382	25241896	2302144					
9	0.4765	28587698	26020933	13252127	37998480	5734468	3543546				
10	0.4811	28938153	27269677	14905913	48724828	9395275	9857520	4339861			
11	0.4846	29192093	28189409	16172622	57582581	12857102	17520203	13321234	4332017		
12	0.4873	29382258	28886366	17159628	64852101	15962684	15508353	25524232	14532165	3593250	
13	0.4894	29528506	29427153	17941422	70830830	18681545	33239933	39414755	29855892	13070917	25165030

Table 3.3. Coefficients of the optimal polynomials for $p = 4$, $m = 5, \ldots, 14$

m	$\beta(m)/m^2$	$10^{10}\beta_5$	$10^{11}\beta_6$	$10^{12}\beta_7$	$10^{13}\beta_8$	$10^{15}\beta_9$	$10^{16}\beta_{10}$	$10^{18}\beta_{11}$	$10^{20}\beta_{12}$	$10^{23}\beta_{13}$	$10^{25}\beta_{14}$
5	0.2424	40869614									
6	0.2770	53034307	24047305								
7	0.2978	58522914	38959287	9614737							
8	0.3114	61530756	48271897	18665099	2802424						
9	0.3207	63380802	54415671	25823024	6324541	6241238					
10	0.3274	64609566	58675260	31318718	9676950	16017061	1098880				
11	0.3324	65471686	61750557	35551748	12603033	26853219	3154281	1569873			
12	0.3362	66102156	64045172	38852969	15078409	37424775	5747862	4976600	1857672		
13	0.3392	66578336	65804031	41465210	17151510	47156774	8539768	9788891	6438509	18516202	
14	0.3409	66949337	67189660	43572346	18894332	55903927	11327608	15470573	13617834	69780353	15817898

The proof of this theorem follows the lines along which the minimax property of the Chebyshev polynomials is proved. Although we did not succeed to prove the existence of a polynomial with $m-p$ tangent points, theorem 3.1 gives us the equations for the coefficients β_j if such a polynomial indeed exists. We have, in fact,

$$\begin{aligned} P_m(z_j) &= (-1)^{p+j} \\ P'_m(z_j) &= 0 \end{aligned}, \quad j=1,2,\ldots,m-p, \tag{3.6}$$

where for each j, z_j represents the point where $P_m(z)$ touches the line $y=(-1^{p+j})$. In [8] the solution of system (3.6) is discussed. In Table 3.1 the results for $p=2$, $m=3,4,\ldots,12$ are listed.

Note that for large values of m the stability limit β is approximately proportional to m^2 which means that the effective step length h/m has an upper bound which increases linearly with m.

In the same manner the polynomials of type (2.7) and (2.9) can be optimized. Some results are given in Table 3.2 and 3.3.

4. Stability Polynomials for Hyperbolic Differential Equations

Cauchy problems for symmetric hyperbolic equations reduce by discretization of the space variables to sets of ordinary differential equations of which the Jacobian has purely imaginary values. As in the case of parabolic equations the value of $|\delta|_{\max}$ is usually very large. When $[-i\beta, i\beta]$ is the stability interval on the imaginary axis we have the stability condition

$$h_n < \frac{\beta}{|\delta|_{\max}}. \tag{4.1}$$

The standard Runge-Kutta formulas of orders 1 until 4 have imaginary stability boundaries 0, 1, 1.7, 2.8, respectively. As in the real eigenvalue case we have tried to construct Runge-Kutta formulas with larger stability intervals but now on the imaginary axis.

For $p=1$ we found (cf. [4])

$$P_2(z) = 1 + z + z^2 \tag{4.2}$$

with the imaginary stability boundary $\beta=1$.

It turned out that for $m>2$ the optimal polynomials are at least second order exact, i.e. $p \geqq 2$.

Putting $p=2$ we found for odd values of m (cf. [5])

$$P_m(z) = T_{\frac{m-1}{2}}\left(\frac{(m-1)^2+2z^2}{(m-1)^2}\right) + 2z\,\frac{(m-1)^2+z^2}{(m-1)^3}\,U_{\frac{m-3}{2}}\left(\frac{(m-1)^2+2z^2}{(m-1)^2}\right) \tag{4.3}$$

with $\beta = m-1$.

In Table 4.1 coefficients of the optimal polynomials of degree 3, 5, 7, and 9 are given.

Table 4.1. Coefficients of the optimal polynomials for $p=2$, $m=3, 5, 7, 9$

m	β_3	β_4	β_5	β_6	β_7	β_8	β_9
3	$\frac{1}{4}$						
5	$\frac{3}{16}$	$\frac{1}{32}$	$\frac{1}{128}$				
7	$\frac{19}{108}$	$\frac{1}{27}$	$\frac{2}{243}$	$\frac{1}{1458}$	$\frac{1}{2187}$		
9	$\frac{11}{64}$	$\frac{5}{128}$	$\frac{17}{2048}$	$\frac{1}{1024}$	$\frac{5}{32768}$	$\frac{1}{1048576}$	$\frac{1}{8388608}$

Note that the coefficients β_j tends to $1/j!$ as $m \to \infty$.

For even values of m we only solved the case $m=4$. The optimal polynomial turned out to be of fourth order accuracy:

$$P_4(z) = 1 + z + \tfrac{1}{2}z^2 + \tfrac{1}{6}z^3 + \tfrac{1}{24}z^4 \tag{4.4}$$

with $\beta = 2\sqrt{2}$. Thus, for $m=4$ polynomials of lower order of accuracy do not exist.

We did not consider the general third and fourth order cases.

5. Stability Polynomials for Stiff Differential Equations

The third type of equations to be considered in this paper belong to the class of stiff differential equations. These equations are characterized by the fact that the real parts of the eigenvalues of the Jacobian matrix which lie in the left half plane, are widely separated. We restrict our considerations to the case where these eigenvalues are located in three clusters, one of which being centered at a point δ_0 near the origin, the other two being centered at points δ_1 and δ_2 far from the origin.

In order to integrate such equations, the stability polynomial $P_m(z)$ should be such that its stability region contains neighbourhoods of the origin and of the points $z_1 = h_n \delta_1$, $z_2 = h_n \delta_2$. This means that the stability polynomial changes when h_n varies.

Suppose that the polynomial

$$R_r(z) = 1 + z + \beta_2 z^2 + \cdots + \beta_r z^r \tag{5.1}$$

has an appropriate stability region at the origin. In addition, let $R_r(z)$ satisfy the consistency conditions. Then, for large values of $|z_1|$ and $|z_2|$, we are looking for a polynomial of the form

$$P_m(z) = R_r(z) + z^{r+1} L_l(z), \tag{5.2}$$

where $L_l(z)$ is a polynomial of degree l in z of which the stability region contains neighbourhoods of z_1 and z_2 as large as possible.

Furthermore, we require that the coefficients of $L_l(z)$ are real and uniformly bounded functions of z_1 and z_2. Note that $P_m(z)$ and $R_r(z)$ have the same behaviour as $z \to 0$, and therefore, have a comparable stability region near the origin.

For small values of $|z_1|$ and $|z_2|$, $P_m(z)$ should behave as

$$\sum_{j=0}^{m} \frac{1}{j!} z^j \tag{5.3}$$

in order to approximate $\exp(z)$ as close as possible in the neighbourhood of the origin.

Polynomials of the type just described, were considered in [12]. It was pointed out that for large values of $|z_1|$ and $|z_2|$ the optimal polynomial $P_m(z)$ satisfies relations of the type

$$\begin{aligned} P_m^{(j)}(z_1) &= 0, \quad j = 0, 1, \ldots, m_1 \\ P_m^{(j)}(z_2) &= 0, \quad j = 0, 1, \ldots, m_2. \end{aligned} \tag{5.4}$$

When $z_2 = \bar{z}_1$ and $z_2 \neq z_1$ we have to choose odd values for l with $m_1 = m_2 = (l-1)/2$; when $z_1 = z_2$ we choose $m_1 = m_2 = l$, and finally, when z_1 and z_2 are real and $z_1 \neq z_2$ we choose $m_1 + m_2 = l - 1$.

The polynomials defined by (5.3) and (5.4), which are optimal for small and large values of $|z_1|$ and $|z_2|$, respectively, can be matched together by a technique called "exponential fitting". The principle on which this technique is based, was already used by several authors. We mention Pope [16] and Liniger and Willoughby [14]. In our case, exponential fitting amounts to the relations

$$\begin{aligned} P_m^{(j)}(z_1) &= \exp(z_1), \quad j = 0, 1, \ldots, m_1 \\ P_m^{(j)}(z_2) &= \exp(z_2), \quad j = 0, 1, \ldots, m_2. \end{aligned} \tag{5.5}$$

For large values of $|z_1|$ and $|z_2|$ these relations reduce to (5.4). For small values of $|z_1|$ and $|z_2|$ we obtain from (5.5) a polynomial approximating (5.3), provided that $R_r(z)$ is a r-th degree Taylor-expansion of $\exp(z)$, i.e. $r = p$. When $r > p$ relations (5.5) give rise to singular coefficients in $L_l(z)$. In order to remove these singularities we replace the coefficients β_j, $j = p+1, \ldots, r$, in a neighbourhood of the origin, e.g. $\max(|z_1|, |z_2|) < 1$, by continuous functions $c_j(z_1, z_2)$ such that $c_j(0, 0) = 1/j!$ and $c_j(z_1, z_2) = \beta_j$ when $\max(|z_1|, |z_2|) = 1$.

For large values of $|z_1|$ and $|z_2|$ the left hand stability region is given by (cf. [11])

$$\begin{aligned} |z - z_1| &< \beta_r^{-\frac{1}{m_1+1}} |z_1|^{\frac{m_1+1-r}{m_1+1}} \left| \frac{z_2}{z_2 - z_1} \right|^{\frac{m_2+1}{m_1+1}} \\ |z - z_2| &< \beta_r^{-\frac{1}{m_2+1}} |z_2|^{\frac{m_2+1-r}{m_2+1}} \left| \frac{z_1}{z_1 - z_2} \right|^{\frac{m_1+1}{m_2+1}} \end{aligned} \tag{5.7a}$$

if $z_2 \neq z_1$, and by

$$|z - z_1| < \beta_r^{-\frac{1}{l+1}} |z_1|^{\frac{l+1-r}{l+1}} \tag{5.7b}$$

if $z_2 = z_1$.

In order to illustrate the results given above we consider the case $l=1$. We then have

(5.8)
$$P_m(z) = R_r(z) + [z_2 g(z_1, z_2) + z_1 g(z_2, z_1)]\, z^{r+1} - [g(z_1, z_2) + g(z_2, z_1)]\, z^{r+2}$$

where

$$g(z_1, z_2) = \frac{1}{z_1^{r+1}} \, \frac{\exp(z_1) - R_r(z_1)}{z_2 - z_1}.$$

The left hand stability regions are given by

$$|z - z_1| < \beta_r^{-1} |z_1|^{1-r} \left| \frac{z_2}{z_2 - z_1} \right|, \qquad |z - z_2| < \beta_r^{-1} |z_2|^{1-r} \left| \frac{z_1}{z_2 - z_1} \right|$$

if $z_2 \neq z_1$, and by

$$|z - z_1| < \beta_r^{-\frac{1}{2}} |z_1|^{1-r}$$

if $z_2 = z_1$.

The right hand stability region is given by

$$\{z \,\|\, R_r(z)| < 1\}.$$

6. Applications

In this section some stabilized Runge-Kutta formulas are explicitly given. For numerical results obtained by these integration methods we refer to [10, 11] and Section 7.

Firstly, we give a formula which is appropriate for the integration of parabolic equations when high accuracy is not descired. In such cases we may use shifted Chebyshev polynomials, for example

$$T_6\left(1 + \frac{z}{36}\right) = 1 + z + \frac{35}{216} z^2 + \frac{7}{729} z^3 + \frac{1}{3888} z^4 + \frac{1}{314928} z^5 + \frac{1}{68024448} z^6.$$

The real stability boundary is 72. Substitution of the coefficients of this polynomial into (2.1), (2.3) yields the generating array form

(6.1)
$$\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{216} & \frac{1}{216} & & & & & \\
\frac{1}{81} & 0 & \frac{1}{81} & & & & \\
\frac{3}{112} & 0 & 0 & \frac{3}{112} & & & \\
\frac{8}{135} & 0 & 0 & 0 & \frac{8}{135} & & \\
\frac{35}{216} & 0 & 0 & 0 & 0 & \frac{35}{216} & \\
\hline
 & 0 & 0 & 0 & 0 & 0 & 1
\end{array}$$

The corresponding Runge-Kutta formula has first order accuracy.

When a highly accurate discretization with respect to the time variable is desired, one may use the fourth order exact stability polynomials listed in Table 3.3. For $m=6$ we have

$$P_6(z) = 1 + z + \tfrac{1}{2} z^2 + \tfrac{1}{6} z^3 + \tfrac{1}{24} z^4 + 0.0053034307\, z^5 + 0.00024047305\, z^6$$

with real stability boundary $\beta \sim 10$. According to Table 2.1 this polynomial can be associated to the fourth order exact scheme

$$(6.2)\qquad \begin{array}{l|llllll} 0 & & & & & & \\ 0.5 & 0.5 & & & & & \\ 0.5 & 0 & 0.5 & & & & \\ 0.5 & 0 & 0.4546571 & 0.0453429 & & & \\ 0.5 & 0 & 0.3727177 & 0 & 0.1272823 & & \\ 1 & 0 & 0 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & \frac{1}{6} \end{array}$$

Secondly, we give a second order scheme which is appropriate for the integration of hyperbolic systems:

$$(6.3)\qquad \begin{array}{c|ccccc} 0 & & & & & \\ \frac{1}{4} & \frac{1}{4} & & & & \\ \frac{1}{6} & 0 & \frac{1}{6} & & & \\ \frac{3}{8} & 0 & 0 & \frac{3}{8} & & \\ \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & \\ \hline & 0 & 0 & 0 & 0 & 1 \end{array}$$

Here, the stability polynomial is given in Table 4.1, $m=5$; the imaginary stability boundary equals 4.

Finally, we give a formula which can be used for the integration of stiff equations of the type described in Section 5:

$$\begin{array}{c|ccc} 0 & & & \\ \dfrac{16\beta_3}{16\beta_2-3} & \dfrac{16\beta_3}{16\beta_2-3} & & \\ \dfrac{16\beta_2-3}{12} & 0 & \dfrac{16\beta_2-3}{12} & \\ \hline & \dfrac{1}{4} & 0 & \dfrac{3}{4} \end{array}$$

where β_2 and β_3 are defined according to (5.8) with $r=1$ and $R_r(z)=1+z$. The right hand stability region is given by

$$|z+1|<1,$$

the left hand stability regions by

$$|z-z_1|<\left|\frac{z_2}{z_2-z_1}\right|, \quad |z-z_2|<\left|\frac{z_1}{z_2-z_1}\right|$$

and by

$$|z-z_1|<\sqrt{|z_1|}$$

in the cases $z_2 \neq z_1$ and $z_2 = z_1$, respectively.

This integration formula is first order exact and "almost" third order exact when $h_n \to 0$.

7. Numerical Examples

The integration formulas given in Section 6 will be applied to a parabolic, a hyperbolic and a stiff differential equation, respectively. We shall concentrate on the experimental verification of the theoretically derived stability conditions. The experiments were carried out on an Electrologica EL X8 computer.

Our first problem is a non-linear diffusion problem which proceeds from Fehlberg [2]:

$$\frac{\partial u}{\partial t}=d(x,u)\frac{\partial^2 u}{\partial x^2},\quad 0\leqq x\leqq 1,\quad t\geqq 0,$$

$$u(x,0)=2[1-\ln(1-x^2)],\quad 0\leqq x\leqq 1,$$

(7.1) $$\frac{\partial u}{\partial x}=0,\quad x=0,\quad t\geqq 0,$$

$$u(1,t)=2+\ln(1+t),\quad t\geqq 0,$$

$$d(x,u)=\frac{\exp(2-u)}{4(2+x^2)}.$$

The exact solution of this problem is given by

(7.2) $$u(x,t)=2+\ln(1+t)-2\ln(2-x^2).$$

By using the method of lines we can replace (7.1) by a set of ordinary first order differential equations. Following Fehlberg we write

$$\frac{du_0}{dt}=2d_0\frac{1}{\Delta^2 x}(u_1-u_0),$$

(7.1′) $$\frac{du_j}{dt}=d_j\frac{1}{\Delta^2 x}(u_{j-1}-2u_j+u_{j+1}),\quad j=1,2,\ldots,14,$$

$$\frac{du_{15}}{dt}=d_{15}\frac{1}{\Delta^2 x}\left(u_{14}-2u_{15}+2+\ln(1+t)\right).$$

Here, $\Delta x=1/16$, $d_j=d(j\Delta x,u_j)$ and u_j denotes an approximation to the exact solution $u(x,t)$ at $x=j\Delta x$.

The Jacobian matrix J of (7.1′) is given by a product of a diagonal and a tridiagonal matrix:

$$J=\frac{1}{\Delta^2 x}\begin{pmatrix} d_0 & & & 0\\ & \cdot & & \\ & & \cdot & \\ 0 & & & d_{16}\end{pmatrix}\begin{pmatrix} a_0 & 2 & & & 0\\ 1 & a_1 & 1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & 1 & a_{14} & 1\\ 0 & & & 1 & a_{15}\end{pmatrix};$$

the entries a_j are defined by

$$a_0=-2(1-u_0+u_1),$$

$$a_j=-(2+u_{j-1}-2u_j+u_{j+1}),\quad j=1,2,\ldots,14,$$

$$a_{15}=-\left(2+u_{14}-2u_{15}+2+\ln(1+t)\right).$$

Since the off-diagonal entries of J are positive, its eigenvalues are real. Furthermore, by Gerschgorin's theorem, the eigenvalues are situated in the interval

$$\left[-4, \frac{1}{\Delta^2 x} \max_j (d_j, 0)\right].$$

This suggests to apply an integration formula generated by polynomials of the type discussed in Section 3. In fact, we have used the first order formula defined by (6.1). The corresponding stability condition is

$$\Delta t \leqq \frac{72 \Delta^2 x}{4 \max_j d_j}. \tag{7.3}$$

By integrating with the maximal step allowed by this condition we reached the point $t = 100$ in 35 steps with a maximal absolute error

$$\max_j |u_j - u(j \Delta x, 100)| = 3 \cdot 10^{-2},$$

or, relatively, an error of about 0.5%.

It may be interesting to calculate the number of integration steps which are theoretically required to integrate from $t=0$ to $t=100$ with the maximal step length allowed by condition (7.3). Substitution of the exact solution (7.2) into the diffusion coefficient $d(x, u)$ yields

$$d = \frac{1}{1+t} \frac{(2-x^2)^2}{4(2+x^2)} \leqq \frac{1}{2(1+t)}.$$

Hence, by (7.3)

$$\Delta t = 36 \Delta^2 x (1+t) = \tfrac{1}{7}(1+t).$$

From this relation it follows that the number of integration steps at $t=100$ is approximately given by

$$7 \int_0^{100} \frac{dt}{1+t} = 7 \ln 101 \cong 33.$$

The second problem is the Cauchy problem for a non-linear hyperbolic equation (cf. Richtmyer and Morton [17, p. 128]):

$$\begin{aligned} \frac{\partial u}{\partial t} &= -u \frac{\partial u}{\partial x}, \quad -\infty \leqq x \leqq \infty, \quad t \geqq 0, \\ u(x, 0) &= x, \quad -\infty \leqq x \leqq \infty. \end{aligned} \tag{7.4}$$

The exact solution is given by

$$u(x, t) = \frac{x}{1+t}. \tag{7.5}$$

Problem (7.4) can be approximated by an initial value problem for the set of equations

$$\frac{du_j}{dt} = -\frac{1}{2} u_j \frac{1}{\Delta x} (u_{j+1} - u_{j-1}), \quad j = 0, \pm 1, \ldots. \tag{7.4'}$$

The Jacobian matrix can be represented in the form

$$J = -\frac{1}{2} \frac{1}{\Delta x} \left(-u E_- + (E_+ - E_-) u + u E_+\right),$$

where $E_{\pm}$ are the usual shift operators and u represents the vector with components u_j. By splitting J into a symmetric and a skew-symmetric part it is seen that J is "almost" skew-symmetric and that the spectral radius is approximately bounded by

$$\frac{1}{\Delta x} \max_j |u_j|.$$

Hence, one of the polynomials given in Section 4 seems to be an appropriate stability polynomial. We have chosen the second order exact fifth degree polynomial which generates formula (6.3).

The solution u was required in the region

$$-\tfrac{1}{2} \leqq x \leqq \tfrac{1}{2}, \quad 0 \leqq t \leqq \tfrac{1}{2}$$

with

$$\Delta x = 0.008.$$

The time steps Δt were chosen as large as allowed by stability, i.e.

$$\Delta t = \frac{4 \Delta x}{\max_j |u_j|}. \tag{7.6}$$

After 10 integration steps the process reached $t = \frac{1}{2}$ with a maximal error

$$\max_j |u_j - u(j \Delta x, \tfrac{1}{2})| = 7_{10} - 6.$$

Finally, we consider a stiff equation which is of interest in biochemistry:

$$\begin{aligned} \frac{dS}{dt} &= (C-1) S + 0.99 C, \\ \frac{dC}{dt} &= 1000 (S - C - SC), \\ S(0) &= 1, \quad C(0) = 0. \end{aligned} \tag{7.7}$$

Since we did not obtain an analytical solution the results from a fifth order Runge-Kutta process with $\Delta t = 0.001$ were taken as the exact solution. At $t = 50$ this process produced the values

$$\begin{aligned} S &= 0.76587 83202 487, \\ C &= 0.43371 03535 768. \end{aligned} \tag{7.8}$$

The Jacobian matrix of (7.7) is given by

$$J = \begin{pmatrix} C-1 & S+0.99 \\ 1000(1-C) & -1000(S+1) \end{pmatrix}.$$

The eigenvalues of J are given by

$$\delta_{0,1} = -\tfrac{1}{2} b \pm \sqrt{\tfrac{1}{4} b^2 + 10(C-1)}, \quad b = 1000(S+1) + (1-C),$$

or approximately,

$$\delta_0 \cong \frac{1}{100} \frac{C-1}{S+1}, \quad \delta_1 \cong -1000(S+1).$$

Obviously, the polynomials discussed in Section 5 are suitable for the integration of Eq. (7.7). For instance, we may apply scheme (6.4). Since the left hand eigenvalue cluster consists of just one eigenvalue the corresponding stability condition does not limit the integration step; the right hand stability condition becomes in this case (cf. Section 6)

$$\Delta t < \frac{2}{|\delta_0|} \cong 200 \frac{S+1}{|C-1|},$$

which is not a real restriction of Δt. In Table 7.1 some results are listed obtained by formula (6.4).

Table 7.1. Absolute errors at $t = 50$

Δt	N	$\|S(50) - S_N\|$	$\|C(50) - C_N\|$
5	10	$10^{-2.8}$	$10^{-3.4}$
2	25	$10^{-3.2}$	$10^{-3.7}$
1	50	$10^{-3.5}$	10^{-4}
0.5	100	$10^{-3.8}$	$10^{-4.3}$
0.2	250	$10^{-4.2}$	$10^{-4.7}$
0.1	500	$10^{-4.5}$	10^{-5}

Note that the standard fourth order Runge-Kutta method with real stability limit 2.8 requires at least $50/(2.8/|\delta_1|) > 3000$ steps for the integration of this problem.

8. Concluding Remarks

The aim of our study is to arrive at a unified treatment of the integration of differential equations. The results presented in this paper are only partial. For example, a topic as local truncation error estimates based on the first neglected Taylor terms (instead of the last Taylor terms taken into account) is still subject of investigation. Some first results are given in [9]. Furthermore, a strategy which matches stabilized formules of low accuracy to non-stabilized formulas of high accuracy can easily be applied to the formulas described here (cf. [7]).

An extension of stabilized Runge-Kutta formulas can be obtained when we allow the Runge-Kutta coefficients to be functions of the Jacobian matrix of the differential equation. Such formulas require less function evaluations than the formulas considered here and, therefore, may be advantageous. The semi-implicit formulas of Rosenbrock [18] and Calahan [1] belong to this class. In [13] an explicit and a semi-implicit formula based on two function evaluations are given. Both formulas are third order exact and can be fitted exponentially.

References

1. Calahan, D. A.: A stable, accurate method of numerical integration for non-linear systems. Proc. IEEE **56**, 744–746 (1968).
2. Fehlberg, E.: Klassische Runge-Kutta-Formeln vierter und niedrigerer Ordnung mit Schrittweiten-Kontrolle und ihre Anwendung auf Wärmeleitungsprobleme. Computing **6**, 61–71 (1970).

3. Franklin, J. N.: Numerical stability in digital and analogue computation for diffusion problems. J. Math. Phys. **37**, 305–315 (1959).
4. Houwen, P. J. van der: Finite difference methods for solving partial differential equations. MC Tract 20, Mathematisch Centrum, Amsterdam (1968).
5. Houwen, P. J. van der: Difference schemes with complex time steps. Report MR 105, Mathematisch Centrum, Amsterdam (1969), 16 pp.
6. Houwen, P. J. van der: One-step methods for linear initial value problems I, Polynomial methods. Report TW 119/70, Mathematisch Centrum, Amsterdam (1970), 36 pp.
7. Houwen P. J. van der: One-step methods for linear initial value problems II, applications to stiff equations. Report TW 122/70, Mathematisch Centrum, Amsterdam (1970), 42 pp.
8. Houwen, P. J. van der, Kok, J.: Numerical solution of a minimax problem Report TW 123/71, Mathematisch Centrum, Amsterdam (1971), 25 pp.
9. Houwen, P. J. van der: Stabilized Runge-Kutta methods with limited storage requirements. TW 124/71, Mathematisch Centrum, Amsterdam (1971), 33 pp.
10. Houwen, P. J. van der: One-step methods for linear initial value problems. ZAMM **51**, T58–59 (1971).
11. Houwen, P. J. van der, Beentjes, P., Dekker, K., Slagt, E.: One-step methods for linear initial value problems, Numerical results. Report TW 130/71, Mathematisch Centrum, Amsterdam (1971), 83 pp.
12. Houwen, P. J. van der: A survey of stabilized Runge-Kutta formulas. MC Tract 37, chapter 5, Mathematisch Centrum, Amsterdam (1971).
13. Houwen, P. J. van der: Explicit and semi-implicit Runge-Kutta formulas for the integration of stiff equations. Report TW 132/72, Mathematisch Centrum, Amsterdam (1972), 20 pp.
14. Liniger, W., Willoughby, R. A.: Efficient integration methods for stiff systems of ordinary differential equations. SIAM J. Numer. Anal **7**, 47–66 (1970).
15. Lomax, H.: On the construction of highly stable, explicit, numerical methods for integrating coupled ordinary differential equations with parasitic eigenvalues. NASA Technical Note, NASATN D-4547 (1968), 45 pp.
16. Pope, D. A.: An exponential method of numerical integration of ordinary differential equations. Comm. ACM, **6**, 491–493 (1963).
17. Richtmyer, R. D., and Morton, K. W.: Difference methods for initial-value problems. Interscience Publishers, John Wiley, New York 1967.
18. Rosenbrock, H. H.: Some general implicit processes for the numerical solution of differential equations. Comput. J. **5**, 329–330 (1963).

P. J. van der Houwen
Mathematisch Centrum,
2e Boerhaavestraat 49
Amsterdam, Netherlands