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AFDELING TOEGEPASTE WISKUNDE TW TW 132/72 FEBRUARY

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EXPLICIT AND SEMI-IMPLICIT RUNGE-KUTTA FORMULAS FOR THE INTEGRATION OF STIFF EQUATIONS

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Printed at the Mathematical Centre, 49, 2e Boerhaavestraat 49, Amsterdam.

The Mathematical Centre, founded the 11-th of February 1946, is a non-profit institution aiming at the promotion of pure mathematics and its applications. It is sponsored by the Netherlands Government through the Netherlands Organization for the Advancement of Pure Research (Z.W.O.), by the Municipality of Amsterdam, by the University of Amsterdam, by the Free University at Amsterdam, and by industries.

Contents

Abstract

Non-linear one-step formulas are given for the numerical integration of stiff systems of ordinary differential equations. These methods simulate the stiff solution components accurately by taking into account the exponential character of these components. The main results of this paper are two integration formulas of third order accuracy which use only two derivative evaluations per integration step.

1. Definitions

Let

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

represent a set of differential equations of which the (vector) function f(y) belongs to a class of sufficient differentiability. The present paper is concerned with the numerical integration of the initial value problem for this equation by one-step methods of the type

$$y_{n+1} = y_n + \sum_{j=0}^{m-1} \Theta_j \, k_n^{(j)} ,$$

$$k_n^{(j)} = h_n \, f(y_n + \sum_{l=0}^{j-1} \Lambda_{j,l} \, k_n^{(l)}), \tag{1.2}$$

$$\Lambda_{0,0} = \Lambda_{0,-1} = 0 \ , \quad j = 0, 1, \ldots, m - 1.$$

Here, $h_n = x_{n+1} - x_n$ denotes the step length, y_n the numerical approximation to the solution y(x) at $x = x_n$, and Θ_j, $\Lambda_{j,l}$ are polynomials or rational functions of $h_n J_n$, where $J_n = J(y_n)$ is the Jacobian matrix of (1.1) at $y = y_n$.

Formula (1.2) is said to have an order of accuracy p when the expansion of y_{n+1} in powers of h_n agrees within p + 1 terms with the Taylor expansion for the local solution y(x) of (1.1) through the point (x_n, y_n).

When scheme (1.2) is applied to the model equation

$$\frac{dy}{dx} = \delta y \tag{1.1'}$$

it reduces to the form

$$y_{n+1} = R(h_n \delta) y_n , \tag{1.2'}$$

where $R(h_n \delta)$ is a polynomial or rational function of $h_n \delta$. We shall call R(z) the stability function associated to (1.2). Furthermore, we define the stability region S of (1.2) by

(1.3) $$S = \{z \mid |R(z)| < 1\} .$$

Formula (1.2) is called a stable integration formula for equation (1.1) when all points $h_n\delta$, δ being an eigenvalue of J_n with $\mathrm{Re}\,\delta < 0$, belong to the stability region S. When S contains the whole left half-plane, formula (1.2) is said to be A-stable (cf. Dahlquist [6]). Otherwise, the stability condition leads to an upper bound for the step sizes h_n.

In constructing appropriate stability functions for the integration of stiff equations we shall apply a technique called exponential fitting. This technique is frequently used in literature, in particular by Liniger and Willoughby [4]. Essentially, it means that the stability function is required to satisfy a relation of the type

(1.4) $$R(z_0) = e^{z_0}, \quad z_0 = h_n\delta_0 ,$$

where δ_0 is the center of a cluster of eigenvalues of J_n in the left half plane.

Formulas of type (1.2) were already given by Rosenbrock [5]:

(1.5) $$\Theta_0 = 0 , \quad \Theta_1 = (I-(1-\tfrac{1}{2}\sqrt{2})h_nJ_n)^{-1} ,$$
$$\Lambda_{1,0} = (\tfrac{1}{2}\sqrt{2}-1)\ \Theta_1 ,$$

and by Calahan [1]:

(1.6) $$\Theta_0 = \tfrac{3}{4}(I-\tfrac{1}{2}(1+\tfrac{1}{3}\sqrt{3})h_nJ_n)^{-1}, \quad \Theta_1 = \tfrac{1}{3}\ \Theta_0 ,$$
$$\Lambda_{1,0} = -\ \tfrac{8}{9}\ \sqrt{3}\ \Theta_0 .$$

These formulas are second and third order exact, respectively.

In this paper we give further one- and two-point formulas which are based on the Jacobian matrix J_n.

2. Consistency conditions for one- and two-point formulas

In this section the conditions are derived for first, second and third order accuracy of general two-point formulas, i.e. formulas of the type

$$y_{n+1} = y_n + \Theta_0(h_nJ_n)k_n^{(0)} + \Theta_1(h_nJ_n)k_n^{(1)} ,$$

(2.1)

$$k_n^{(0)} = h_n g(y_n) \quad , \quad k_n^{(1)} = h_n f(y_n + \Lambda_{1,0}(h_nJ_n)k_n^{(0)}) .$$

Let us define the operator

$$D = \Lambda_{1,0}\ f(y_n)\ .\ \nabla ,$$

where ∇ denotes the gradient operator with respect to the components of y and let $D^l\ f(y_n)$ denote the vector of which the components are $D^l\ f_j(y_n)$, where $f_j(y_n)$ is the j-th component of the vector $f(y_n)$. We then can write y_{n+1} in the form

$$y_{n+1} = y_n + \Theta_0\ h_n\ f(y_n) + \Theta_1\ h_n[f(y_n) + h_n\ D\ f(y_n) +$$

$$+ \tfrac{1}{2}h_n^2\ D^2\ f(y_n) + \tfrac{1}{6}h_n^3\ D^3\ f(y_n) + O(h_n^4)] .$$

Expansion of the operators $\Theta_0(h_nJ_n)$, $\Theta_1(h_nJ_n)$ and $D(h_nJ_n)$ in powers of h_n leads to the expression

$$y_{n+1} = y_n + [\Theta_0(0) + \Theta_1(0)]h_n\ f(y_n) +$$

$$+ [\Theta_0{}'(0)\ J_n + \Theta_1{}'(0)\ J_n + \Theta_1(0)\ D(0)]h_n^2\ f(y_n) +$$

$$+ [\tfrac{1}{2}\Theta_0{}''(0)\ J_n^2 + \tfrac{1}{2}\Theta_1{}''(0)\ J_n^2 + \Theta_1(0)\ D'(0)J_n +$$

$$+ \Theta_1{}'(0)\ D(0)J_n + \tfrac{1}{2}\Theta_1(0)\ D^2(0)]\ h_n^3\ f(y_n) + O(h_n^4) .$$

where the accent means differentiation with respect to $h_n J_n$.
By observing that

$$D(0)\ f(y_n) = \Lambda_{1,0}(0)\ f(y_n).\ \nabla f(y_n) = \Lambda_{1,0}(0)\ J_n\ f(y_n)$$

and

$$D'(0)\ f(y_n) = \Lambda'_{1,0}(0)\ f(y_n).\ \nabla f(y_n) = \Lambda'_{1,0}(0)\ J_n\ f(y_n)$$

we arrive at the Taylor expansion

$$(2.2)\quad y_{n+1} = y_n + [\Theta_0(0) + \Theta_1(0)]h_n\ f(y_n) +$$
$$+ [\Theta_0'(0) + \Theta_1'(0) + \Theta_1(0)\ \Lambda_{1,0}(0)]h_n^2\ J_n\ f(y_n) +$$
$$+ [\tfrac{1}{2}\Theta_0''(0)+\tfrac{1}{2}\Theta_1''(0)+\Theta_1(0)\Lambda'_{1,0}(0)+\Theta_1'(0)\ \Lambda_{1,0}(0)]h_n^3 J_n^2 f(y_n)$$
$$+ \tfrac{1}{2}\Theta_1(0)\ D^2(0)\ h_n^3\ f(y_n) + O(h_n^4)\ .$$

The Taylor expansion for the local analytical solution $y_n(x)$ about the point $x = x_n$ is given by

$$(2.3)\quad y_n(x_n+h_n) = y_n + h_n\ f(y_n) + \tfrac{1}{2}h_n^2\ J_n f(y_n) + \tfrac{1}{6}h_n^3\ J_n^2\ f(y_n) +$$
$$+ \tfrac{1}{6}h_n^3\ (f(y_n).\nabla)^2\ f(y_n) + O(h_n^4)\ .$$

A comparison of (2.1) and (2.2) reveals that we have first order accuracy when

$$(2.4)\qquad \Theta_0(0) + \Theta_1(0) = 1\ ,$$

second order accuracy, when, in addition,

$$(2.5)\qquad \Theta_0'(0) + \Theta_1'(0) + \Theta_1(0)\ \Lambda_{1,0}(0) = \tfrac{1}{2}\ ,$$

and third order accuracy when, in addition,

$$\Theta_0''(0) + \Theta_1''(0) + 2[\Theta_1(0)\, \Lambda_{1,0}'(0) + \Theta_1'(0)\, \Lambda_{1,0}(0)] = \frac{1}{3}$$

(2.6)

$$\Theta_1(0)\, \Lambda_{1,0}^2(0) = \frac{1}{3}\ .$$

Note that, generally, a one-point formula ($\Theta_1(0)=0$) cannot be third order exact.

3. Exponential fitted stability functions

In addition to satisfying the consistency conditions derived in the preceding section,we have to identify the stability function of the integration formula to a given, appropriately chosen function $R(z)$. Restricting our considerations to one- and two-point formulas we are led to the identity

(3.1) $$R(z) = 1 + z\,[\Theta_0(z) + \Theta_1(z)] + z^2\, \Theta_1(z)\, \Lambda_{1,0}(z)\ .$$

In table 3.1 some stability functions are collected which have in common that they are exponentially fitted at two or three points of the z-plane, i.e. $z = 0$, $z = z_1$ and $z = z_2$. These functions are particularly suited to the integration of stiff equations. For further stability functions we refer to [2, 3] .

It may be remarked that the stability functions of the Rosenbrock and Calahan formula ((1.5) and (1.6), respectively), are special cases of the three-cluster function of Liniger and Willoughby. These functions arise when we put $\alpha_1 = \alpha_2 = 3 - 2\sqrt{2}$ and $\alpha_1 = 1 \pm 2\sqrt{3}/3$, $\alpha_2 = 1/3$, respectively. Furthermore, when we put $z_1 = z_2$, $\alpha_1 = g'(z_1)/3$ and $\alpha_2 = 1/3$ we obtain a two-cluster function of third order,that is a stability function which is compatible with the consistency conditions (2.4) - (2.6).

Table 3.1 Stability functions and stability regions

	R(z)	S
Two-cluster function of first order of Liniger-Willoughby[4]	$\dfrac{1+\beta_1 z}{1-(1-\beta_1)z}$, $\beta_1 = -\dfrac{1}{z_1} - \dfrac{e^{z_1}}{1-e^{z_1}}$	$\mathrm{Re}\ z < 0$
Three-cluster polynomial of first order Reference [3]	$1 + z + [z_2 g(z_1,z_2) + z_1 g(z_2,z_1)]\, z^2$ $- [g(z_1,z_2) + g(z_2,z_1)]\, z^3$ $g(z_1,z_2) = \dfrac{e^{z_1} - 1 - z_1}{z_1^2 (z_2 - z_1)}$	$\|z+1\| < 1$ $\|z-z_1\| < \dfrac{\|\delta_2\|}{\|\delta_2-\delta_1\|}$ $\|z-z_2\| < \dfrac{\|\delta_1\|}{\|\delta_2-\delta_1\|}$ $\|z-z_1\| < \sqrt{\|z_1\|}$ if $z_1 = z_2$
Three-cluster function of second order of Liniger-Willoughby [4]	$\dfrac{1 + \frac{1}{2}(1-\alpha_1)\, z + \frac{1}{4}(\alpha_2-\alpha_1)\, z^2}{1 - \frac{1}{2}(1+\alpha_1)\, z + \frac{1}{4}(\alpha_2+\alpha_1)\, z^2}$ $\alpha_1 = 2\dfrac{g(z_2)-g(z_1)}{z_2 g(z_1) - z_1 g(z_2)}$, $\alpha_2 = \alpha_1 \dfrac{z_2 - z_1}{g(z_2)-g(z_1)}$ $g(z) = z^2 \dfrac{1-e^z}{e^z(2-z) - (2+z)}$	$\mathrm{Re}\ z < 0$ if $\alpha_1 > 0$, $\alpha_2 > 0$
Two-cluster polynomial of third order Reference [3]	$1 + z + \frac{1}{2} z^2 + \frac{1}{6} z^3 +$ $+ \dfrac{e^{z_1} - (1 + z_1 + \frac{1}{2} z_1^2 + \frac{1}{6} z_1^3)}{z_1^4}\, z^4$	$\|z\| < 1.7$ $\|z-z_1\| < \dfrac{1.8}{\|z_1\|^2}$

4. One-point formulas

We recall that one-point formulas are defined by

(4.1) $$y_{n+1} = y_n + \Theta_0 (h_n J_n) h_n f(y_n) .$$

Let R(z) be a given stability function. Then we can identify the stability function of (4.1) with R(z) by putting (cf. (3.1)).

(4.2) $$\Theta_0(z) = \frac{R(z) - 1}{z} ,$$

so that

(4.1') $$y_{n+1} = y_n + J_n^{-1} [R(h_n J_n) - 1] f(y_n).$$

By imposing the consistency conditions (2.4) and (2.5) on (4.1') we deduce that we have a first order formula when

(4.3) $$R(0) = R'(0) = 1$$

and a second order formula when

(4.4) $$R(0) = R'(0) = R''(0) = 1.$$

It is easily verified that all functions R(z) listed in table 3.1 satisfy (4.3) and that, except for the first two functions, condition (4.4) is also satisfied. When the stability functions of Liniger and Willoughby are substituted into (4.1'), we obtain the $F^{(1)}$ and $F^{(2)}$ formulas of Liniger and Willoughby with a single Newton step [4] .

5. Explicit two-point formulas of third order

We shall derive third order exact integration formulas using two function evaluations per integration step.
Let us try operators of the type

$$\Theta_0(z) = \theta_0(1 + \lambda_1 z + \lambda_2 z^2 + \lambda_3 z^2 + \dots \lambda_{m-2} z^{m-2}) ,$$

(5.1) $$\Theta_1(z) = \theta_1 ,$$

$$\Lambda_{1,0}(z) = \frac{\alpha}{\theta_0} \Theta_0 (z) .$$

Substitution of these expressions into the consistency condition (2.4)-(2.6) yields the relations

$$\theta_0 + \theta_1 = 1 ,$$

$$\theta_0\lambda_1 + \alpha\,\theta_1 = \frac{1}{2} ,$$

$$\alpha^2\theta_1 = \frac{1}{3} ,$$

$$2\theta_0\lambda_2 + 2\alpha\theta_1\lambda_1 = \frac{1}{3} .$$

These equations are easily solved leaving $\alpha, \lambda_3, \dots, \lambda_{m-2}$ undetermined:

(5.2) $$\theta_0 = \frac{3\alpha^2-1}{3\alpha^2},\ \theta_1 = \frac{1}{3\alpha^2},\ \lambda_1 = \frac{1}{2}\alpha\,\frac{3\alpha-2}{3\alpha^2-1},\ \lambda_2 = \frac{1}{2}\alpha^2\,\frac{3\alpha^2-3\alpha+1}{(3\alpha^2-1)^2}$$

Formula (2.1), together with (5.1) and (5.2), defines a class of third exact integration formulas.

The stability polynomial of these formulas is easily seen to be

(5.3) $$1 + z + \frac{1}{2} z^2 + \frac{1}{6} z^3 + (\theta_0\lambda_3+\alpha\theta_1\lambda_2)\ z^4 + \ldots + (\theta_0\lambda_{m-2}+\alpha\theta_1\lambda_{m-3})\ z^{m-1} + \alpha\theta_1\lambda_{m-2}\ z^m .$$

Hence, when a stability polynomial is desired of the form

(5.4) $$R(z) = 1 + z + \frac{1}{2} z^2 + \frac{1}{6} z^3 + \beta_4 z^4 + \ldots \beta_m z^m,$$

where $\beta_4, \ldots, \beta_m$ are given coefficients, we have to solve a system of m-3 non-linear equations, that is the system

(5.5) $$\begin{aligned} \theta_0 \lambda_3 + \alpha\, \theta_1 \lambda_2 &= \beta_4 , \\ &\ldots \\ \theta_0 \lambda_{m-2} + \alpha\, \theta_1 \lambda_{m-3} &= \beta_{m-1} , \\ \alpha\, \theta_1 \lambda_m &= \beta_m . \end{aligned}$$

In this paper we restrict our consideration to the case m = 4. Then system (5.5) reduce to the single equation

(5.5') $$\alpha(3\alpha^2-3\alpha+1) - 6\beta_4(3\alpha^2-1)^2 = 0.$$

In figure 5.1 the behaviour of β_4 as a function of α is illustrated.

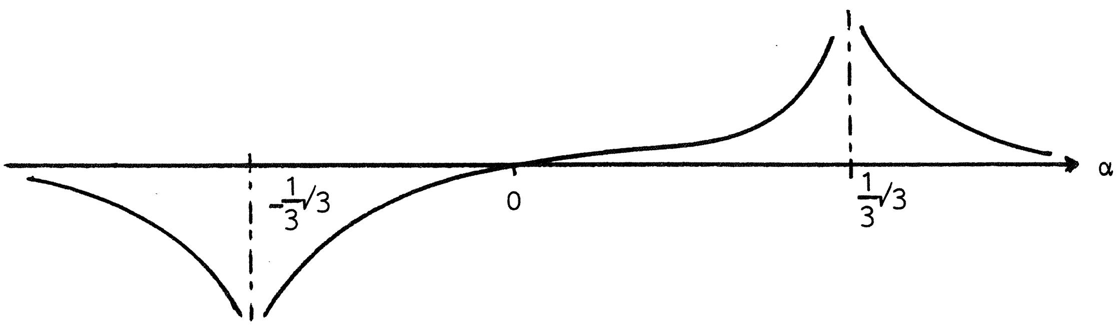

fig.5.1 The function $\beta_4(\alpha)$ defined by (5.5')

From this figure it is seen that for every value of β_4 two real solutions α exist. When $|\beta_4|$ is small we choose that solution of (5.5) which has the larger absolute value in order to avoid large negative and positive values of the paramaters θ_0 and θ_1 (compare (5.2)).

In particular, we may identify (5.3) with the third order, two-cluster polynomial given in table 3.1.

6. A semi-implicit two-point formula of third order

Next we try operators of the type

$$\Theta_0(z) = \theta_0 \frac{1 + \nu z}{1 - \lambda z - \mu z^2} ,$$

(6.1)
$$\Theta_1(z) = \theta_1 ,$$

$$\Lambda_{1,0}(z) = \alpha \frac{1 + \nu z}{1 - \lambda z - \mu z^2} .$$

The consistency conditions (2.4) - (2.6) reduce to the relations

(6.2)
$$\theta_0 + \theta_1 = 1 ,$$

$$\theta_0(\nu+\lambda) + \alpha\theta_1 = \frac{1}{2} ,$$

$$\alpha^2\theta_1 = \frac{1}{3} ,$$

$$\theta_0(\lambda^2+\nu\lambda+\mu) + \alpha\theta_1(\nu+\lambda) = \frac{1}{3} .$$

Furthermore, the stability function assumes the form

(6.3)
$$\frac{1 + (\theta_0+\theta_1-\lambda)z + (\theta_0\nu+\theta_1(\alpha-\lambda)-\mu)z^2 + \theta_1(\alpha\nu-\mu)z^3}{1 - \lambda z - \mu z^2} .$$

We shall try to identify this function with the third order, two-cluster function Liniger-Willoughby and at the same time we try to solve equations (6.2).

The identification process yields the equations

$$\theta_0 + \theta_1 - \lambda = \frac{1}{2}(1-\alpha_1) ,$$

$$\theta_0\nu + \theta_1(\alpha-\lambda) - \mu = \frac{1}{12}(1-3\alpha_1) ,$$

(6.4)
$$\alpha\nu - \mu = 0 ,$$

$$\lambda = \frac{1}{2}(1+\alpha_1) ,$$

$$\mu = -\frac{1}{12}(1+3\alpha_1) ,$$

where α_1 is a free parameter.
It can be easily verified that equations (6.2) and (6.3) are solved by

(6.5)
$$\theta_0 = \frac{3\alpha^2-1}{3\alpha^2} , \quad \theta_1 = \frac{1}{3\alpha^2} , \quad \nu = -\frac{1+3\alpha_1}{12\alpha} , \quad \lambda = \frac{1+\alpha_1}{2} , \quad \mu = -\frac{1+3\alpha_1}{12} ,$$

where α satisfies the equation

(6.6)
$$9\alpha^2 - 6\alpha + 1 + 3\alpha_1(2\alpha-1)(3\alpha^2-1) = 0.$$

In figure 6.1 the behaviour of α_1 as a function of α is given.

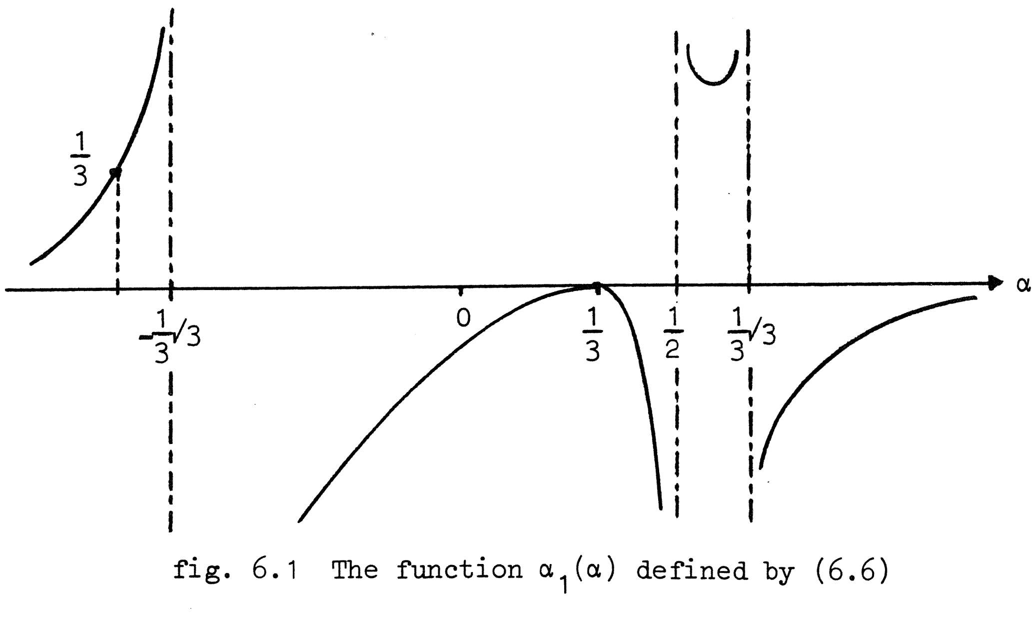

fig. 6.1 The function $\alpha_1(\alpha)$ defined by (6.6)

Clearly, equation (6.6) has for every α_1 at least one real solution. In order to obtain positive weight parameters θ_0 and θ_1 we choose the solution which is larger than $1|\sqrt{3}$ in absolute value.

Formula (2.1), together with (6.1), (6.5) and (6.6), define a one-parameter family of third order two-point formulas. It is easily verified that these formulas are A-stable for every positive value of the parameter α_1. As was proved by Liniger and Willoughby [4], exponentially fitting of these formulas at $z = z_1$ leads to positive values of α_1, and therefore, is compatible with A-stability.

7. Summary of formulas

In this section some of the exponential fitted integration formulas considered in preceding sections are summarized.

$F^{(1)}$ formula of Liniger and Willoughby with a single Newton step

$$(7.1)\quad \begin{cases} y_{n+1} = y_n + h_n[1 - (1-\beta_1)\, h_n J]^{-1}\, f(y_n)\ , \\ \beta_1 = -\dfrac{1}{z_1} - \dfrac{e^{z_1}}{1 - e^{z_1}}\ , \\ p = 1\ ,\quad \text{A-stable}\ ,\quad J = J_n + O(1) \quad \text{as} \quad h_n \to 0\ . \end{cases}$$

Explicit three-cluster formula of first order $(E^{(1)})$

$$(7.2)\quad \begin{cases} y_{n+1} = y_n + h_n\, [1 + (z_2 g(z_1,z_2) + z_1 g(z_2,z_1))\, h_n J \\ \qquad\qquad - (g(z_1,z_2)+g(z_2,z_1))\, h_n^2 J^2]\, f(y_n)\ , \\ g(z_1,z_2) = \dfrac{e^{z_1}-1-z_1}{z_1^2(z_2-z_1)}\ , \\ p = 1\ ,\ |z+1| < 1\ ,\ |z_2-z_1| < \dfrac{|\delta_2|}{|\delta_2-\delta_1|}\ ,\ |z-z_2| < \dfrac{|\delta_1|}{|\delta_2-\delta_1|}\ , \\ |z-z_1| < \sqrt{|z_1|} \ \text{ if } z_2 = z_1\ ,\quad J = J_n + O(h_n) \text{ as } h_n \to 0\ . \end{cases}$$

$F^{(2)}$ formula of Liniger and Willoughby with a single Newton step

(7.3)
$$y_{n+1} = y_n + h_n \left[1 - \tfrac{1}{2} h_n (1+\alpha_1) J + \tfrac{1}{4} h_n^2 (\alpha_2+\alpha_1) J^2\right]^{-1} \cdot$$

$$\cdot \left[1 - \tfrac{1}{2} \alpha_1 h_n J\right] f(y_n) ,$$

$$\alpha_1 = 2 \frac{g(z_2)-g(z_1)}{z_2 g(z_1) - z_1 g(z_2)} ; \alpha_2 = \alpha_1 \frac{z_2-z_1}{g(z_2)-g(z_1)} , g(z) = z^2 \frac{1 - e^z}{e^z(2-z)-(2+z)} ,$$

$p = 2$, A-stable if $\alpha_1 > 0$ and $\alpha_2 > 0$, $J = J_n + O(h_n)$ as $h_n \to 0$.

$F^{(3)}$ formula of Liniger and Willoughby with a single Newton step

(7.4)
Special case of formula (7.2) with

$$\alpha_1 = \frac{1}{3z_1} \frac{e^{z_1}(12-6z_1+z_1^2) - (12+6z_1+z_1^2)}{e^{z_1}(2-z_1) - (2+z_1)} , \alpha_2 = \frac{1}{3} ,$$

$p = 2$, A-stable it Re $z_1 < 0$, $J = J_n + O(h_n)$ as $h_n \to 0$.

Semi-implicit two-cluster formula of third order ($S^{(3)}$)

(7.5)
$$y_{n+1} = y_n + \frac{3\alpha^2-1}{3\alpha^2} k_n^{(0)} + \frac{1}{3\alpha^2} k_n^{(1)} ,$$

$$k_n^{(0)} = h_n \left[1-\tfrac{1}{2}(1+\alpha_1)h_n J + \tfrac{1}{12}(1+3\alpha_1)h_n^2 J^2\right]^{-1} \left[1-\frac{1}{12} \frac{1+3\alpha_1}{\alpha} h_n J\right] f(y_n),$$

$$k_n^{(1)} = h_n f(y_n + \alpha k_n^{(0)}) ,$$

$$9\alpha^2 - 6\alpha + 1 + 3\alpha_1(2\alpha-1)(3\alpha^2-1) = 0 ,$$ α_1 according to (7.4) ,

$p = 3$, A-stable if Re $z_1 < 0$, $J = J_n + O(h_n^2)$ as $h_n \to 0$.

Explicit two-cluster formula of third order ($E^{(3)}$)

$$
(7.6)\begin{cases}
y_{n+1} = y_n + \frac{3\alpha^2-1}{3\alpha^2}\, k_n^{(0)} + \frac{1}{3\alpha^2}\, k_n^{(1)} , \\[2ex]
k_n^{(0)} = h_n[1 + \frac{1}{2}\, \frac{3\alpha-2}{3\alpha^2-1}\, h_n J + \frac{1}{2}\alpha^2\, \frac{3\alpha^2-3\alpha+1}{(3\alpha^2-1)^2}\, h_n^2 J^2]\, f(y_n) , \\[2ex]
k_n^{(1)} = h_n\, f(y_n+\alpha k_n^{(0)}) , \\[2ex]
\alpha(3\alpha^2-3\alpha+1) - 6\,\beta_4(3\alpha^2-1)^2 = 0 , \ \beta_4 = \frac{e^{z_1}-(1+z_1+\frac{1}{2}z_1^2+\frac{1}{6}z_1^3)}{z_1^4} , \\[2ex]
p = 3 , \ |z| < 1.7 , \ |z-z_1| < \frac{1.8}{|z_1|^2} , \ J = J_n + O(h_n^2) \text{ as } h_n \to 0 .
\end{cases}
$$

8. Concluding remarks

Finally, we give in table 8.1 a rough evaluation of the six exponential fitted integration formulas summarized in the preceding section.

Table 8.1 Evaluation of the integration formulas (7.1) - (7.6)

Property	Integration formula
High order of accuracy	$S^{(3)}$, $E^{(3)}$
Little computational work	$E^{(1)}$
Large stability regions	$F^{(1)}$, $F^{(2)}$, $F^{(3)}$, $S^{(3)}$
Two-cluster spectra	$F^{(1)}$, $E^{(1)}$, $F^{(3)}$, $S^{(3)}$, $E^{(3)}$
Three-cluster spectra	$F^{(2)}$, $E^{(1)}$

References

[1] Calahan, D.A., A stable, accurate method of numerical integration for non-linear systems, Proc. IEEE 56, 744 (1968).

[2] Houwen, P.J. van der and J. Kok, Numerical solution of a minimax problem, Report TW 123, Mathematisch Centrum, Amsterdam (1971).

[3] Houwen, P.J. van der, A survey of stabilized Runge-Kutta methods, MC tract 37, Ch.5, Mathematisch Centrum, Amsterdam (1971)

[4] Liniger, W. and R.A. Willoughby, Efficient integration methods for stiff systems of ordinary differential equations, SIAM J., Numer.Anal. 7, 47 (1970).

[5] Rosenbrock, H.H., Some general implicit processes for the numerical solution of differential equations, Comput.J. 5, 329 (1963).

[6] Dahlquist, G.G., A special stability problem for linear multistep problems, BIT 3, 27 (1963).