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P.J. van der HOUWEN & J.G. VERWER
GENERALIZED LINEAR MULTISTEP METHODS I
DEVELOPMENT OF ALGORITHMS WITH ZERO-PARASITIC ROOTS

2e boerhaavestraat 49 amsterdam

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ABSTRACT

With this report the authors propose a special class of generalized linear multistep methods. Such integration methods originate from the classical linear multistep method by replacing the coefficients of the integration formula by functions of the Jacobian matrix. We have concentrated on the construction of formulas of which the principal characteristic root (the stability function) can be adapted to the problem under consideration, while the parasitic roots are zero. Moreover, the formulas allow a crude evaluation of the Jacobian. By choosing the stability function appropriately, the integration formulas may be used for efficient integration of parabolic, hyperbolic and stiff differential equations.

CONTENTS

1. INTRODUCTION

In this report we investigate the generalized linear multistep method, which may be used to solve numerically initial value problems for systems of ordinary differential equations of the type

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

Generalized integration methods are characterized by the fact that the coefficients of the integration formula are functions of the Jacobian matrix, a device first proposed by Rosenbrock (see for example [2] and [5]). In recent years several *generalized Runge-Kutta* formulas have been developed at the Mathematical Centre in Amsterdam. A survey of these methods is given in [2]. Special classes of *generalized linear multistep* methods have been proposed by Nørsett [6], van der Houwen [1] and Lambert and Sigurdsson [4].

The integration method investigated in this report originates from the classical linear multistep method by replacing the coefficients of the integration formula by *functions of the Jacobian* matrix J(y). The considered class of formulas may also be regarded as an extension of the class of formulas originating from the implicit linear multistep method by performing one Newton-Raphson iteration with the last computed solution vector as predictor.

This report merely concentrates on the *construction* of the integration formulas.

In section 2 we discuss two types of consistency conditions. The first type requires an *accurate evaluation* of the Jacobian matrix, while the second one allows an *inaccurate evaluation* of the Jacobian. From a practical point of view formulas allowing a crude Jacobian may be preferred to formulas requiring a correct Jacobian.

In section 3 we introduce integration formulas of which the principal root (*the stability function*) can be adapted to the problem under consideration, while the *parasitic roots are zero*. By choosing the stability function appropriately, these integration formulas may be used for efficient integration of parabolic, hyperbolic and stiff differential equations. Van der Houwen [1] already has given a third order two-step formula with prescribed stability function and zero-parasitic root, requiring a correct evaluation of the Jacobian matrix. Applications of this formula on stiff equations turned out to be satisfactory.

Section 4 is devoted to the construction of integration formulas with prescribed stability function and zero-parasitic roots allowing a crude evaluation of the Jacobian matrix. Here we derive consistency equations for a formula using polynomial expressions and a formula using rational expressions.

In the last section we present a worked out example of a set of integration formulas of which the order can be varied without much computational effort.

Summarizing, in this report we have concentrated on the following points:

1. operator coefficients instead of scalar coefficients,
2. zero-parasitic roots,
3. a prescribed stability function,
4. an inaccurate Jacobian matrix.

In a forthcoming paper the authors intend to publish further theoretical and numerical results.

2. CONSISTENCY CONDITIONS

The generalized linear k-step method is defined by the formula

$$(2.1) \qquad y_{n+1} = \sum_{\ell=1}^{k} A_\ell y_{n+1-\ell} + h_n \sum_{\ell=0}^{k} B_\ell f(y_{n+1-\ell}),$$

where A_ℓ and B_ℓ are *rational functions* of $h_n J(y_n)$. In particular, we assume that $B_0 = 0$. By this assumption (2.1) is an explicit formula.

Let us first define the numbers

$$(2.2) \qquad q_\ell = \frac{x_{n-\ell} - x_n}{h_n}, \qquad \ell = -1,0,\ldots,k-1.$$

By representing the multistep method by the formula

(2.3) $$y_{n+1} = E_n(y_n, y_{n-1}, \ldots, y_{n-k+1}), \qquad k \geq 1,$$

we may give the following definition of consistency.

Definition 2.1

Let y be a solution of the differential equation. Then the multistep method (2.1) is said to be *consistent of order* p *at* $x = x_n$ when for any set of fixed numbers q_ℓ, $\ell = 1,2,\ldots,k-1$,

$$y(x_{n+1}) - E_n(y(x_n),\ldots,y(x_{n+1-k})) = O(h_n^{p+1}) \text{ as } h_n \to 0.$$

By substituting a solution y of the differential equation into the right-hand side of (2.1) and by expanding $y(x_{n+1-\ell})$ and $f(y(x_{n+1-\ell}))$ in powers of h_n we may formally derive the series

(2.4) $$E_n(y(x_n),\ldots,y(x_{n+1-k})) = \sum_{j=0} C_j\, h_n^j \frac{d^j}{dx^j}\, y(x)\Big|_{x=x_n}$$

where

(2.5) $$C_j = \frac{1}{j!} \sum_{\ell=1}^{k} A_\ell\, q_{\ell-1}^{j} + j\, B_\ell\, q_{\ell-1}^{j-1},$$

$$C_0 = \sum_{\ell=1}^{k} A_\ell .$$

The C_j are functions of $h_n J(y(x_n))$. Let us introduce the abbreviations

$$c_j^{(i)} = \frac{d^i}{dz^i}\, C_j(z)\Big|_{z=0}.$$

By expanding the operators C_j in Taylor series we write (2.4) in the form

$$(2.4') \qquad E_n(y(x_n),\ldots,y(x_{n+1-k})) =$$

$$= \sum_{j=0} \sum_{i=0} \frac{1}{i!} c_j^{(i)} J^i(y(x)) \frac{d^j}{dx^j} y(x)|_{x=x_n} h_n^{i+j} =$$

$$= \sum_{j=0} \left[\sum_{i=0}^{j} \frac{1}{(j-i)!} c_i^{(j-i)} J^{j-i}(y(x)) \frac{d^i}{dx^i} y(x)|_{x=x_n} \right] h_n^j =$$

$$= \sum_{j=0} c_j^{(0)} \frac{d^j}{dx^j} y(x)|_{x=x_n} h_n^j + \sum_{j=1} \frac{c_0^{(j)}}{j!} J^j(y(x)) \; y(x)|_{x=x_n} h_n^j +$$

$$+ \sum_{j=2} \frac{c_1^{(j-1)}}{(j-1)!} J^{j-1}(y(x)) \frac{d}{dx} y(x)|_{x=x_n} h_n^j +$$

$$+ \sum_{j=3} \frac{c_2^{(j-2)}}{(j-2)!} J^{j-2}(y(x)) \frac{d^2}{dx^2} y(x)|_{x=x_n} h_n^j +$$

$$+ \sum_{j=4} \sum_{i=3}^{j-1} \frac{c_i^{(j-i)}}{(j-i)!} J^{j-i}(y(x)) \frac{d^i}{dx^i} y(x)|_{x=x_n} h_n^j.$$

From this series the terms containing

$$\frac{d^j}{dx^j} y(x)|_{x=x_n} h_n^j$$

are easily selected. By putting the coefficients of these terms equal to $1/j!$ for $j = 0,1,\ldots p$ and by equating to zero all remaining terms of order $j \le p$ in h_n, we find the consistency conditions for the generalized linear multistep formula. In table 2.1 these conditions are listed. For the special case $k = 2$, in [1] the consistency conditions are given in terms of the derivatives of the functions A_ℓ and B_ℓ.

Table 2.1 Consistency conditions for formula 2.1

$p \geq 1$	$c_0^{(0)} = c_1^{(0)} = 1$, $c_0^{(1)} = 0$.
$p \geq 2$	$c_1^{(1)} + c_2^{(0)} = \frac{1}{2}$, $c_0^{(2)} = 0$.
$p_0 \geq 3$	$c_j^{(0)} = \frac{1}{j!}$, $c_0^{(j)} = 0$, $c_1^{(j-1)} + (j-1)\ c_2^{(j-2)} = 0$, $c_i^{(j-i)} = 0$, for $j = 3,4,\ldots,p_0$ and $i = 3,4,\ldots,j-1$.

In the preceding derivation we have made use of the relation

$$(2.6) \qquad y''(x_n) = J(y(x_n))\ y'(x_n).$$

This implies that in actual computation the Jacobian matrix should be given with an order of accuracy $p - 1$. An alternative is to ignore the relation between the first and second derivative. The consistency conditions then reduce to

$$(2.7) \qquad \begin{aligned} c_j^{(0)} &= \frac{1}{j!}, && j = 0,1,\ldots,p, \\ c_i^{(j-i)} &= 0, && j = 1,2,\ldots,p;\ i = 0,1,\ldots,j-1. \end{aligned}$$

This means that the functions C_j are given by

$$(2.8) \qquad C_j(z) = \frac{1}{j!} + O(z^{p+1-j}) \text{ as } z \to 0.$$

Formulas satisfying these conditions *remain consistent of order* p when the Jabocian matrix is inaccurately evaluated. From a practical point of view, such formulas may be preferred to formulas which strongly depend on a correct evaluation of $J(y_n)$. In the remainder of this report we shall concentrate on formulas allowing an inaccurate Jacobian. This section is concluded with the following theorems.

Theorem 2.1

The order of consistency p of formula (2.1) satisfying the conditions corresponding to a *correct evaluation* of the Jacobian matrix is at most 2k.

Proof. If $k \geq 2$ the theorem may be easily proved by counting the number of parameters corresponding to the equations $c_j^{(0)} = \frac{1}{j!}$, $j = 3,4,\ldots,p$, listed in table 2.1. The case $k = 1$ is trivial. □

Theorem 2.2

The order of consistency p of formula (2.1) satisfying the conditions corresponding to a *crude evaluation* of the Jacobian matrix is at most $2k - 1$.

Proof. With conditions (2.7) this theorem is easily proved by counting again parameters corresponding to $c_j^{(0)} = \frac{1}{j!}$, $j = 0,\ldots,p$. □

3. STABILITY CONSIDERATIONS

Let us consider the *test equation*

$$\frac{dy}{dx} = Jy \qquad (3.1)$$

where J is the Jacobian matrix of the differential equation under consideration. When applied to this equation our multistep formula (2.1) will reduce to a linear difference equation of the form

$$y_{n+1} = \sum_{\ell=1}^{k} [A_\ell(z) + z\, B_\ell(z)] \cdot y_{n+1-\ell} \qquad (3.2)$$

where $z = h_n J$. The characteristic equation corresponding to scheme (3.2) is given by

$$\zeta^k - [A_1(z) + zB_1(z)]\zeta^{k-1} - \ldots - [A_\ell(z) + zB_\ell(z)]\zeta^{k-\ell} - \ldots - \ldots - [A_k(z) + zB_k(z)] = 0. \tag{3.3}$$

The coefficients of (3.3) are rational functions of z and are independent of each other. This means that we can make vanish the parasitic roots for all values of z without reducing the method to a one-step method. In the sequel, we shall restrict our considerations to formulas with *zero-parasitic roots*. This approach may be justified by the following reasons. Firstly, in the numerical approximation y_{n+1} the solution components corresponding to the parasitic roots are also parasitic and are not present in the analytical solution. Secondly, *the principal root*, ζ_1, may be identified with a given stability function. This implies that we can adjust our integration formula to the problem to be solved.

By requiring that all parasitic roots of (3.3) are identically zero, we find the relations

$$A_\ell(z) = -zB_\ell(z), \qquad \ell = 2,3,\ldots,k. \tag{3.4}$$

The principal root ζ_1 is given by

$$\zeta_1(z) = A_1(z) + zB_1(z). \tag{3.5}$$

By identifying ζ_1 with a given stability function R we also obtain a relation for A_1 and B_1, i.e.

$$A_1(z) = R(z) - zB_1(z). \tag{3.6}$$

Thus integration formula (2.1) is reduced to

$$y_{n+1} = R(z)y_n + h_n \sum_{\ell=1}^{k} B_\ell(z)[f(y_{n+1-\ell}) - J_n y_{n+1-\ell}] \tag{3.7}$$

We should observe that relation (3.4) implies

$$A_\ell(0) = 0, \qquad \ell = 2,3,\ldots,k.$$

This means that the order of consistency p of those formulas of class (3.7) satisfying the consistency conditions listed in table 2.1 is at most $k + 1$. A third order, two-step scheme of this type is given in [1]. By the same reason, consistency conditions (2.7) allow an order $p \le k$. A modification of Adams-Bashforth methods suggested by Nørsett [6] turns out to be a subclass of (3.7) provided that the exponential terms present in the methods are replaced by $R(z)$.

4. FORMULAS WITH ZERO-PARASITIC ROOTS ALLOWING INACCURATE JACOBIAN MATRICES

Substitution of (3.5) and (3.6) into the expressions for the functions C_j introduced in section 2 yields

$$(4.1)\qquad \begin{aligned} C_0(z) &= R(z) - \sum_{\ell=1}^{k} zB_\ell(z), \\ C_j(z) &= \frac{1}{j!} \sum_{\ell=1}^{k} (j - zq_{\ell-1})q_{\ell-1}^{j-1}B_\ell(z). \end{aligned}$$

Our problem is now reduced to the selection of functions B_ℓ such that the functions C_j given by (4.1) satisfy the conditions (2.8). Substitution of (4.1) into (2.8) leads to the system

$$(4.2)\qquad \begin{pmatrix} z & z & \cdots & z \\ 1 & 1-q_1z & \cdots & 1-q_{k-1}z \\ 0 & (2-q_1z)q_1 & \cdots & (2-q_{k-1}z)q_{k-1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & (p-q_1z)q_1^{p-1} & \cdots & (p-q_{k-1}z)q_{k-1}^{p-1} \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \\ B_3 \\ \cdot \\ \cdot \\ \cdot \\ B_k \end{pmatrix} = \begin{pmatrix} -1 + R(z) + \varepsilon_{p+1} \\ 1 + \varepsilon_p \\ 1 + \varepsilon_{p-1} \\ \cdot \\ \cdot \\ \cdot \\ 1 + \varepsilon_1 \end{pmatrix}$$

where the ε_j are functions of z which may be freely chosen provided that

$$\varepsilon_j = O(z^j) \text{ as } z \to 0.$$

By use of the first row, i.e.

$$\sum_{\ell=1}^{k} B_\ell(z) = \frac{R(z)-1+\varepsilon_{p+1}}{z},$$

it is easily verified that this system can be written in the form

$$(4.3)\qquad \begin{pmatrix} 1 & 1 & \cdots & 1 \\ q_0 & q_1 & \cdots & q_{k-1} \\ q_0^2 & q_1^2 & \cdots & q_{k-1}^2 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ q_0^p & q_1^p & \cdots & q_{k-1}^p \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \\ B_3 \\ \cdot \\ \cdot \\ \cdot \\ B_k \end{pmatrix} = \begin{pmatrix} D_1 \\ D_2 \\ D_3 \\ \cdot \\ \cdot \\ \cdot \\ D_{p+1} \end{pmatrix}$$

where the functions D_j are defined by

$$(4.4)\qquad \begin{aligned} D_1(z) &= \frac{R(z)-1+\varepsilon_{p+1}(z)}{z}, \\ D_{j+1}(z) &= \frac{jD_j(z)-1-\varepsilon_{p+1-j}(z)}{z}, \qquad j = 1,\ldots,p. \end{aligned}$$

This recurrence relation for the function D_j yields

$$(4.5)\qquad D_j(z) = (j-1)!\,\frac{R(z) - P_{j-1,0}(z)}{z^j} + O(z^{p-j+1}), \qquad z \to 0,$$

where

$$P_{j-1,0}(z) = 1 + z + \frac{z^2}{2!} + \ldots + \frac{z^p}{p!}.$$

By assuming that R is consistent of order p, i.e.

$$(4.6)\qquad \frac{d^i}{dz^i} R(z)\Big|_{z=0} = 1, \qquad i = 0,1,\ldots,p,$$

we may derive for $j = 1,2,\ldots,p$,

$$(4.7) \qquad D_j(z) = (j-1)!\left[\frac{1}{j!} + \frac{z}{(j+1)!} + \ldots + \frac{z^{p-j}}{p!}\right] + \delta_{p-j+1}(z),$$

where the δ_j are functions of z satisfying the condition (compare ε_j)

$$\delta_j = O(z^j) \text{ as } z \to 0.$$

Note that condition (4.6) is a necessary condition for each p-th order integration formula.

At the end of section 3 we have noted that the maximal attainable order of the formulas discussed in this section is k. We now show that for $p = k$ system (4.3) has a solution by an appropriate choice of the function D_{k+1}. Let $B_1, B_2, \ldots, B_k$ be the solution of the first k equations of (4.3), i.e.

$$(4.8) \qquad \sum_{\ell=1}^{k} q_{\ell-1}^{j-1} B_\ell = D_j, \qquad j = 1,2,\ldots,k.$$

The (k+1)-st equation of (4.3) is satisfied when D_{k+1} can be chosen such that

$$(4.9) \qquad D_{k+1} = \sum_{\ell=1}^{k} q_{\ell-1}^{k} B_\ell.$$

From (4.5) it follows that for $p = k$ the function D_{k+1} may be any regular function of z. Hence, (4.9) can always be satisfied. This implies that we can explicitly solve the original system (4.2) for $p = k$ by solving the equivalent system (4.3).

We shall illustrate this for two special cases. Firstly, we investigate polynominal functions B_ℓ of the form

$$(4.10) \qquad B_\ell(z) = b_\ell + \gamma_\ell B(z).$$

where the b_ℓ and γ_ℓ are suitably chosen parameters and B is an appropriately chosen polynomial of degree k-1 independent of ℓ, i.e.

$$(4.11) \qquad B(z) = b^{(0)} + b^{(1)}z + \ldots + b^{(k-1)}z^{k-1}.$$

With relations (2.8), (4.7) and (4.8) it is easily verified that it is of no use to investigate polynomials B_ℓ of higher degree than k - 1. Substitution of (4.10) and (4.11) into (4.8) yields the system

$$\sum_{\ell=1}^{k} q_{\ell-1}^{j-1}\left[b_\ell+\gamma_\ell \sum_{i=0}^{k-1} b^{(i)}z^i\right] = (j-1)! \sum_{i=0}^{k-j} \frac{z^i}{(j+i)!} + \delta_{k-j+1}(z), \qquad j = 1,\ldots,k. \tag{4.12}$$

Equating the coefficients of z^i yields the consistency equations

$$\begin{aligned} &\sum_{\ell=1}^{k} q_{\ell-1}^{j-1}\,(b_\ell+\gamma_\ell b^{(0)}) = \frac{1}{j}, \quad j = 1,2,\ldots,k, \\ &\sum_{\ell=1}^{k} q_{\ell-1}^{j-1}\,\gamma_\ell b^{(i)} = \frac{(j-1)!}{(j+i)!}, \quad i = 1,\ldots,k-1 \text{ and } j = 1,\ldots,k-i. \end{aligned} \tag{4.13}$$

When we succeed to solve this system of equations we have found a k-th order integration formula of the form

$$\begin{aligned} y_{n+1} = R(h_nJ^*)y_n &+ h_n \sum_{\ell=1}^{k} b_\ell[f(y_{n+1-\ell}) - J^*y_{n+1-\ell}] + \\ &+ h_nB(h_nJ^*) \sum_{\ell=1}^{k} \gamma_\ell[f(y_{n+1-\ell}) - J^*y_{n+1-\ell}], \end{aligned} \tag{4.14}$$

where J^* is some approximation for the Jacobian matrix $J(y_n)$. One should observe, however, that in this special case, the maximal attainable order is p = 3. To obtain higher order schemes with polynomial operators B_ℓ of type (4.10) one has to add terms $c_\ell^{(i)}z^i$.

For certain types of Jacobian matrices it may be unattractive to compute polynomial operators B_ℓ because of a possible cancellation of digits. This consideration leads us to a second special case. We investigate a rational function of the form

$$B_\ell(z) = b_\ell + c_\ell \frac{(\alpha+\beta z)^t}{(1+\delta z)^s}, \tag{4.15}$$

where $0 \leq t < k-1$ and $s = k-t-1$. The factors $(\alpha+\beta z)^t$ and $(1+\delta z)^{-s}$ may be expanded to obtain

$$(\alpha+\beta z)^t = \sum_{n=0}^{t} d_n z^n$$

and

$$(1+\delta z)^{-s} = \sum_{m=0}^{k-1} e_m z^m + O(z^k), \qquad z \to 0$$

respectively, where

$$d_n = \binom{t}{n} \alpha^{t-n}\beta^n,$$

$$e_m = \frac{(s+m-1)!}{(s-1)!}(-\delta)^m.$$

Substitution of these expressions into (4.15) leads to

$$B_\ell(z) = \sum_{n=0}^{t} \sum_{m=0}^{k-n-1} g_{\ell,m,n} \, z^{m+n} + O(z^k) \text{ as } z \to 0,$$

where

$$g_{\ell,m,n} = \begin{cases} b_\ell + c_\ell d_0 e_0, & n = m = 0, \\ c_\ell e_m d_n, & n > 0 \vee m > 0. \end{cases}$$

Thus, we arrive at a power series expansion of B_ℓ which reads

$$(4.16) \qquad B_\ell(z) = \sum_{i=0}^{k-1} b^{(i)} z^i + O(z^k) \text{ as } z \to 0,$$

where

$$b_\ell^{(i)} = \sum_{n=0}^{\min(i,t)} g_{\ell,i-n,n}.$$

Substitution of (4.16) into (4.8) yields the system

$$\sum_{\ell=1}^{k} q_{\ell-1}^{j-1} \sum_{i=0}^{k-1} b_\ell^{(i)} z^i = (j-1)! \sum_{i=0}^{k-j} \frac{z^i}{(j+i)!} + \eta_{k-j+1}(z), \qquad j = 1,\dots,k,$$

where the η_j are functions of z satisfying the condition (compare δ_j)

$$\eta_j(z) = O(z^j) \text{ as } z \to 0.$$

Equating the coefficients of z^i leads to the equations

$$(4.17) \qquad \sum_{\ell=1}^{k} q_{\ell-1}^{j-1}\, b_\ell^{(i)} = \frac{(j-1)!}{(j+i)!}, \qquad i = 0,1,\dots,k-1 \text{ and } j = 1,\dots,k-i.$$

Expressing the parameters $b_\ell^{(i)}$ in the original parameters of (4.15) leads to the system of consistency equations. When we succeed to solve this system of equations we have found a k-th order integration formula of the form

$$(4.18) \qquad y_{n+1} = R(h_n J^*) y_n + h_n \sum_{\ell=1}^{k} b_\ell [f(y_{n+1-\ell}) - J^* y_{n+1-\ell}] + $$
$$+ h_n \frac{(\alpha+\beta h_n J^*)^t}{(1+\delta h_n J^*)^s} \sum_{\ell=1}^{k} c_\ell [f(y_{n+1-\ell}) - J^* y_{n+1-\ell}],$$

where J^* is some approximation to the Jacobian matrix $J(y_n)$. As in the previous case, the maximal attainable order for formula (4.18) is $p = 3$.

5. A WORKED OUT EXAMPLE

We shall derive the polynomial functions B_ℓ of type (4.10) for $p = k = 1,2$ and 3. It will be shown that it is possible to choose the operator B and the parameters γ_ℓ independent of the order k. This feature provides a set of integration formulas with which order varying may be applied without much computational effort. To that end we write the functions B_ℓ in the form

$$B_\ell^{(k)}(z) = b_\ell^{(k)} + \gamma_\ell B(z),$$

where the index (k) denotes the order. For k = 1,2 and 3 the consistency equations (4.13) reduce to (the parameters $b^{(i)}$ are independent of k)

$$b_1^{(1)} + \gamma_1 b^{(0)} = 1$$

and

$$b_1^{(2)} + \gamma_1 b^{(0)} + b_2^{(2)} + \gamma_2 b^{(0)} = 1,$$

$$q_1(b_2^{(2)} + \gamma_2 b^{(0)}) = \frac{1}{2},$$

$$(\gamma_1+\gamma_2) b^{(1)} = \frac{1}{2}$$

and

$$b_1^{(3)} + \gamma_1 b^{(0)} + b_2^{(3)} + \gamma_2 b^{(0)} + b_3^{(3)} + \gamma_3 b^{(0)} = 1$$

$$q_1(b_2^{(3)} + \gamma_2 b^{(0)}) + q_2(b_3^{(3)} + \gamma_3 b^{(0)}) = \frac{1}{2},$$

$$q_1^2(b_2^{(3)} + \gamma_2 b^{(0)}) + q_2^2(b_3^{(3)} + \gamma_3 b^{(0)}) = \frac{1}{3},$$

$$(\gamma_1 + \gamma_2 + \gamma_3)\, b^{(1)} = \frac{1}{2},$$

$$(q_1\gamma_2 + q_2\gamma_3)\, b^{(1)} = \frac{1}{6},$$

$$(\gamma_1 + \gamma_2 + \gamma_3)\, b^{(2)} = \frac{1}{6},$$

respectively. To meet the requirement of independency of k for the function B we have to put $\gamma_3 = 0$. A simple calculation then yields

$$b^{(1)} = \frac{1}{6\gamma_2 q_1},$$

$$b^{(2)} = \frac{1}{3}\, b^{(1)},$$

$$\gamma_1 = (3q_1-1)\, \gamma_2,$$

where $\gamma_2 \neq 0$ may be chosen freely. A further calculation yields

$$b_1^{(2)} = 1 - \frac{1}{2q_1} + (1-3q_1)\gamma_2\, b^{(0)},$$

$$b_2^{(2)} = \frac{1}{2q_1} - \gamma_2\, b^{(0)}$$

and

$$b_1^{(3)} = 1 - 3\gamma_2 q_1\, b^{(0)} - b_2^{(3)} - b_3^{(3)},$$

$$b_2^{(3)} = \frac{1}{2q_1}\,(1-2q_1\gamma_2\, b^{(0)} - 2q_2 b_3^{(3)}),$$

$$b_3^{(3)} = (2-3q_1)/6(q_2^2-q_1q_2),$$

where $b^{(0)}$ also is a free parameter. By putting

$$\gamma_2 = \frac{1}{6q_1} \text{ and } b^{(0)} = 1$$

the operator $B(z)$ assumes the form

$$B(z) = 1 + z + \frac{z^2}{3}.$$

The free parameters γ_2 and $b^{(0)}$ may also be used to match two of the parameters $b_\ell^{(k)}$. Another possibility is to give the free parameters appropriate values with respect to R. This approach may lead to a further reduction of computational labour. For $k = 1$ we simply have the integration formula

$$y_{n+1} = R(h_n J^*)y_n + h_n[f(y_n) - J^* y_n].$$

The corresponding integration formulas for $k = 2$ and $k = 3$ assume the form

$$y_{n+1} = I_n + h_n \sum_{\ell=1}^{k} b_\ell^{(k)}[f(y_{n+1-\ell}) - J^* y_{n+1-\ell}],$$

where

$$I_n = R(h_n J^*)y_n + h_n B(h_n J^*) \sum_{\ell=1}^{2} \gamma_\ell [f(y_{n+1-\ell}) - J^* y_{n+1-\ell}].$$

To exploit the partial independency of k we have to use a third order consistent stability function R for all k. Note that for k = 2 the quadratic form of B may be omitted.

REFERENCES

[1] Houwen, P.J. van der, *A note on two-step integration formulas of third order accuracy with prescribed stability function*, Mathematical Centre Report NR 26/72, Amsterdam, 1972.

[2] Houwen, P.J. van der, *Construction of integration formulas for initial value problems*, North-Holland Publishing Company, Amsterdam, (to be published).

[3] Lambert, J.D., *Computational methods in ordinary differential equations*, Wiley, New York, 1973.

[4] Lambert, J.D. and Sigurdsson, S.T., *Multistep methods with variable matrix coefficients*, SIAM J. Numer. Anal., Vol 9, No. 4, December 1972.

[5] Lapidus, L. & Seinfeld, J.H., *Numerical integration of ordinary differential equations*, Academic Press, New York, 1971.

[6] Nørsett, S.P., *An A-stable modification of the Adams-Bashforth methods*, Proc. Conference on Numerical Solution of Differential Equations. (Dundee 1969), Springer-Verlag, Berlin, 1969.