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VOLTERRA EQUATIONS BY IMBEDDING TECHNIQUES

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Analysis of numerical methods for second kind Volterra equations by
imbedding techniques^{*)}

by

P.H.M. Wolkenfelt, P.J. van der Houwen & C.T.H. Baker^{**)}

ABSTRACT

Our purpose, in this paper, is to gain insight into the properties of a wide class of numerical methods for second kind Volterra integral equations with an arbitrary smooth (non-linear) kernel function. The main tool in the analysis proposed here is the imbedding of the integral equation in a differential equation containing a parameter. The solution of the integral equation is then related to the solution of the differential equation and this connection suggests a technique for deriving numerical methods, many of which prove to be classical. Introductory sections are devoted to exploring this connection, which we exploit by pursuing the stability approach for numerical methods applied to differential equations.

KEY WORDS & PHRASES: *numerical analysis, Volterra integral equations of the second kind, stability, imbedding.*

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1. INTRODUCTION

In this paper we propose a possible approach for the investigation of error propagation in numerical methods for non-linear Volterra integral equations of the form

$$(1.1) \quad f(x) = g(x) + \int_0^x K(x,y,f(y))dy, \quad 0 \leq x \leq X,$$

where $g(x)$ and $K(x,y,f)$ are arbitrary given vector functions belonging to a class of sufficiently differentiable functions, and $f(x)$ is the unknown function.

Recently, several papers have been published in which stability results are stated for particular classes of methods and kernel functions varying from simple linear functions such as

$$(1.2) \quad K(x,y,f) = af \quad \text{and} \quad K(x,y,f) = (ax+b)f, \quad a \text{ and } b \text{ constant}$$

(cf. BAKER and KEECH [4], VAN DER HOUWEN [7]) to rather general kernel functions of the form (cf. VAN DER HOUWEN & WOLKENFELT [8], BAKER [3])

$$(1.3) \quad K(x,y,f) = \sum_{i=1}^r X_i(x)Y_i(y,f).$$

In essence, the approach presented in these papers turns out to be the analysis of a numerical method for ordinary differential equations to which the integral equation method is more or less equivalent when applied to kernel functions of the form (1.2) or (1.3).

This suggests that we start directly by converting the integral equation into a differential equation without restricting the kernel function K . By identifying the integral equation method to an integration method for this (rather unusual) differential equation and by carrying out a stability analysis of the integration method it is possible to derive the characteristic equation corresponding to the integration method for general kernel functions. In VAN DER HOUWEN & WOLKENFELT [9] this approach is described for a class of direct quadrature methods. (Quadrature methods which may be

obtained by applying quadrature rules of the form

$$\int_0^{nh} \phi(y) dy \approx h \sum_{j=0}^n \omega_{nj} \phi(jh)$$

to discretize (1.1), yield equations of the form

$$\tilde{f}_n = g(nh) + h \sum_{j=0}^n \omega_{nj} K(nh, jh, \tilde{f}_j)$$

for values \tilde{f}_n approximating $f(nh)$, $n = 1, 2, \dots$, with given $\tilde{f}_0 = f(0) = g(0)$.

In the present paper the analysis outlined in [9] is developed and extended to a larger class of methods using the formalism developed in BAKER [3].

Thus, *the investigation into stability proposed here applies to a very wide class of methods applied to a general nonlinear equation (1.1)*. At the same time, and as a bonus, the relationship to imbedding reveals that classical methods for (1.1) can be viewed in a new light and also *suggests the construction of new classes of numerical methods*.

In the following sections we give the analysis for a scalar integral equation (1.1). The generalization to systems of equations is straightforward and requires little modification of the analysis.

1.1. Derivation of the differential equation

Let the definition of the kernel function $K(x, y, f)$ be extended for $y > x$ (e.g. by interpolation or by defining $K(x, y, f) = K(y, x, f)$ if $y > x$) and define the function

$$(1.4) \quad \Psi(t, x) = g(x) + \int_0^t K(x, y, f(y)) dy, \quad 0 \leq t, x \leq X$$

where $f(x)$ satisfies the integral equation (1.1). Since we obviously have

$$(1.5) \quad f(x) = \Psi(x, x)$$

we may write (1.4) as

$$(1.6) \quad \Psi(t, x) = g(x) + \int_0^t K(x, y, \Psi(y, y)) dy.$$

This equation contains $f(x)$ as a part of its solution. Differentiation of (1.6) with respect to t , leads to the initial value problem (cf. POUZET [12, §V])

$$(1.7) \quad \begin{aligned} \frac{d}{dt} \Psi(t, x) &= K(x, t, \Psi(t, t)) \\ \Psi(0, x) &= g(x) \end{aligned} \quad , \quad 0 \leq x, t \leq X.$$

Equation (1.7) can be regarded as a partial differential equation. However, it is more convenient to treat it as an ordinary differential equation, where x is considered as a parameter and t as the independent variable.

2. SOLUTION OF THE INITIAL VALUE PROBLEM

Formally, any integration method for ordinary differential equations may be applied to the initial value problem (1.7). In this section we discuss the application of linear multistep methods and Runge-Kutta methods.

The convergence of these methods (which is not the subject of the present investigation) requires careful consideration because of the unconventional form of the initial value problem (1.7). In fact, it appears that convergence is not trivially implied by the convergence of methods for ordinary differential equations. However, in cases where the integration method can be identified with a *direct* solution method for Volterra integral equations we may apply the convergence conditions holding for these direct methods (compare §§ 2.1.2 and 2.2.2). When such an identification is not possible (see e.g. § 2.3) then convergence must be established by other means. In WOLKENFELT [14] this is done by constructing quadrature rules from convergent linear multistep methods and by verifying the conditions of a general convergence theorem for VIEs (see BAKER [1, chapter 6]).

2.1.1. Integration by linear multistep methods

Suppose that (1.7) is integrated with a uniform stepsize h by a linear k -step method (LAMBERT [10, p.11]) with coefficients $\{a_j, b_j\}_{j=0}^k$ (with the normalization $a_0 = 1$). Then we obtain a scheme of the form

$$(2.1) \quad \sum_{j=0}^k [a_j \tilde{\psi}_{n+1-j}(x) + b_j h K(x, \eta_{n+1-j}, \tilde{\psi}_{n+1-j}(\eta_{n+1-j}))] = 0, \\ n = k-1, k, \dots, N-1,$$

where $\eta_n = nh$ and $\tilde{\psi}_n(x) = \tilde{\Psi}(\eta_n, x)$ denotes the numerical approximation to $\Psi(\eta_n, x)$, $n = 0, 1, \dots, N$. In order to start scheme (2.1) we need, apart from $\tilde{\psi}_0(x) = g(x)$, the functions $\tilde{\psi}_1(x), \dots, \tilde{\psi}_{k-1}(x)$. Methods for computing these starting functions may be found in § 2.2.1 (see also (2.6)). The functions $\tilde{\psi}_{n+1}(x)$, $n = k-1, k, \dots$, can be computed by first finding $\tilde{\psi}_{n+1}(\eta_{n+1})$ from the equation

$$(2.2) \quad \tilde{\psi}_{n+1}(\eta_{n+1}) + b_0 h K(\eta_{n+1}, \eta_{n+1}, \tilde{\psi}_{n+1}(\eta_{n+1})) = - \sum_{j=1}^k [a_j \tilde{\psi}_{n+1-j}(\eta_{n+1}) + \\ + b_j h K(\eta_{n+1}, \eta_{n+1-j}, \tilde{\psi}_{n+1-j}(\eta_{n+1-j}))],$$

and then writing

$$(2.3) \quad \tilde{\psi}_{n+1}(x) = - \left\{ \sum_{j=1}^k a_j \tilde{\psi}_{n+1-j}(x) + h \sum_{j=0}^k b_j K(x, \eta_{n+1-j}, \tilde{\psi}_{n+1-j}(\eta_{n+1-j})) \right\}$$

Finally, by putting $\tilde{f}_{n+1} = \tilde{\psi}_{n+1}(\eta_{n+1})$ a numerical approximation to $f(\eta_{n+1})$ is obtained. Since we are only interested in \tilde{f}_{n+1} it suffices to evaluate (2.3) for $x = \eta_{n+1}, \eta_{n+2}, \dots, \eta_N$. Thus, scheme (2.1) requires roughly the solution of N equations of the form (2.2) and $N^2/2$ evaluations of the kernel function K .

2.1.2. Relation with direct quadrature methods

In this section we indicate a relation between the scheme (2.1) and the direct quadrature methods frequently used for the integration of (1.1), that is formulae of the form

$$(2.4) \quad \tilde{f}_{n+1} = g(\eta_{n+1}) + h \sum_{j=0}^{n+1} \omega_{n+1,j} K(\eta_{n+1}, \eta_j, \tilde{f}_j), \quad \eta_j = jh, \quad j = 0, 1, \dots, N,$$

where ω_{nj} ($j = 0, 1, \dots, n$; $n = 0, 1, \dots, N$) are given weight parameters and \tilde{f}_n denotes the numerical approximation to $f(\eta_n)$. We have the following theorem.

THEOREM 2.1. *If there exist constants a_i and b_i ($i = 0, \dots, k$) such that (for $n \geq k-1$)*

$$(2.5) \quad \sum_{i=0}^k a_i \omega_{n+1-i, j} = \begin{cases} 0 & (j = 0, 1, \dots, n-k), \\ -b_{n+1-j} & (j = n-k+1, \dots, n+1), \end{cases}$$

$$\sum_{i=0}^k a_i = 0,$$

Then $\tilde{\psi}_{n+1}(\eta_{n+1})$ defined by (2.1) and \tilde{f}_{n+1} defined by (2.4) can be identified with each other, provided that the starting functions $\tilde{\psi}_n(x)$ are defined by

$$(2.6) \quad \tilde{\psi}_n(x) = g(x) + h \sum_{j=0}^n \omega_{nj} K(x, \eta_j, \tilde{\psi}_j(\eta_j)), \quad n = 0, 1, \dots, k-1.$$

PROOF. The proof is straightforward on verifying by substitution that

$$(2.7) \quad \tilde{\psi}_{n+1}(x) = g(x) + h \sum_{j=0}^{n+1} \omega_{n+1, j} K(x, \eta_j, \tilde{\psi}_j(\eta_j)), \quad (n \geq k-1)$$

yields a solution of (2.1) provided that (2.5) is satisfied. From (2.7) and (2.6) it is immediate that $\tilde{\psi}_{n+1}(\eta_{n+1})$ satisfies the same scheme as \tilde{f}_{n+1} so that \tilde{f}_{n+1} can be identified with $\tilde{\psi}_{n+1}(\eta_{n+1})^*$.

EXAMPLE 2.1. Consider a Gregory scheme of order 3 which is generated by the matrix of quadrature weights

$$(2.8) \quad (\omega_{nj}) = \frac{1}{12} \begin{bmatrix} 6 & & & & & & & & \\ 5 & 14 & 5 & & & & & & \\ 5 & 13 & 13 & 5 & & & & & \\ 5 & 13 & 12 & 13 & 5 & & & & \\ & & \dots & & & & & & \\ 5 & 13 & 12 & 12 & \dots & 12 & 12 & 13 & 5 \end{bmatrix}$$

*) Indeed, $\tilde{f}_{n+1} = \tilde{\psi}_{n+1}(\eta_{n+1})$ if either is unique.

Evidently, conditions (2.5) are satisfied when we choose $k=2$, $a_0=-1$, $a_1=1$, $a_2=0$, $b_0 = 5/12$, $b_1 = 8/12$ and $b_2 = -1/12$. These coefficients are easily recognized as those of the third order Adams-Moulton formula for ordinary differential equations. The starting function $\tilde{\psi}_1(x)$ is given by the trapezoidal rule. It can be shown that a k -th order Gregory scheme for the integral equation (1.1) may be identified with a k -th order Adams-Moulton method for equation (1.7) provided that the required starting functions are properly chosen. Of course, this correspondence is a consequence of the well-known link between Gregory quadrature rules and the Adams-Moulton integration methods. For further details of the relation between direct quadrature formulae and linear multistep methods we refer to WOLKENFELT [14]. \square

EXAMPLE 2.2. Consider an integration scheme based on the repeated Simpson rule and using the trapezoidal rule for the first interval when n is odd. The matrix of weights then becomes

$$(2.9) \quad (\omega_{nj}) = \frac{1}{6} \begin{bmatrix} 3 & 3 & & & & & & & & & \\ 2 & 8 & 2 & & & & & & & & \\ 3 & 5 & 8 & 2 & & & & & & & \\ 2 & 8 & 4 & 8 & 2 & & & & & & \\ & & & & \dots & & & & & & \\ 3 & 5 & 8 & 4 & 8 & 4 & 8 & \dots & 4 & 8 & 2 \\ 2 & 8 & 4 & 8 & 4 & 8 & 4 & \dots & 8 & 4 & 8 & 2 \end{bmatrix}$$

For all values of $n \geq 1$ condition (2.5) can be satisfied by $k = 2$, $a_0 = -1$, $a_1 = 0$, $a_2 = 1$, $b_0 = 1/3$, $b_1 = 4/3$ and $b_2 = 1/3$. These coefficients define the (weakly stable) fourth order Milne method (HENRICI [6, p.201,241]). \square

2.2.1. Integration by Runge-Kutta methods

In order to motivate a Runge-Kutta method for (1.7) we first consider the equation

$$(2.10) \quad \frac{d}{dt} \Psi(t, x) = K(x, t, \Psi(t, x)),$$

(parametrized by x) which is a slight modification of (1.7). If (2.10) is integrated by a p -stage Runge-Kutta method we obtain a scheme which may be written in the form

$$(2.11) \quad \begin{cases} \tilde{\psi}_{n+1}^{(r)}(x) = \tilde{\psi}_n(x) + h \sum_{s=0}^{p-1} \beta_{rs} K(x, nh + \theta_s h, \tilde{\psi}_{n+1}^{(s)}(x)), & r = 0, 1, \dots, p-1 \\ \tilde{\psi}_{n+1}(x) = \tilde{\psi}_n(x) + h \sum_{s=0}^{p-1} c_s K(x, nh + \theta_s h, \tilde{\psi}_{n+1}^{(s)}(x)), & n = 0, 1, \dots, N-1 \end{cases}$$

for each x , where the parameters θ_s , β_{rs} and c_s specify the Runge-Kutta method (a survey of all kind of formulae can be found in LAMBERT [10], LAPIDUS & SEINFELD [11]).

Returning to the problem (1.7), the scheme (2.11) suggests we define a Runge-Kutta scheme for (1.7) by the formulae

$$(2.12a) \quad \tilde{\psi}_{n+1}^{(r)}(x) = \tilde{\psi}_n(x) + h \sum_{s=0}^{p-1} \beta_{rs} K(x, nh + \theta_s h, \tilde{\psi}_{n+1}^{(s)}(nh + \theta_s h)),$$

$r = 0, 1, \dots, p-1$

$$(2.12b) \quad \tilde{\psi}_{n+1}(x) = \tilde{\psi}_n(x) + h \sum_{s=0}^{p-1} c_s K(x, nh + \theta_s h, \tilde{\psi}_{n+1}^{(s)}(nh + \theta_s h)),$$

$n = 0, 1, \dots, N-1.$

In order to compute $\tilde{\psi}_{n+1}(x)$ we substitute $x = nh + \theta_r h$ in (2.12a) to obtain a system of p equations for the values $\tilde{\psi}_{n+1}^{(r)}(nh + \theta_r h)$. When these equations are solved we find $\tilde{\psi}_{n+1}(x)$ from (2.12b) and a numerical approximation to $f((n+1)h)$ from $\tilde{\psi}_{n+1}((n+1)h)$.

If we define $\theta_p = 1$ and

$$(2.13) \quad \begin{aligned} \beta_{ps} &= c_s, & s &= 0, 1, \dots, p-1, \\ \beta_{sp} &= 0, & s &= 0, 1, \dots, p, \end{aligned}$$

then (2.12a-b) can be written

$$(2.14) \quad \begin{cases} \tilde{\psi}_{n+1}^{(r)}(x) = \tilde{\psi}_n(x) + h \sum_{s=0}^p \beta_{rs} K(x, nh + \theta_s h, \tilde{\psi}_{n+1}^{(s)}(nh + \theta_s h)) \\ \tilde{\psi}_{n+1}(x) = \tilde{\psi}_{n+1}^{(p)}(x), & (r = 0, 1, \dots, p, \quad n = 0, 1, \dots, N-1). \end{cases}$$

Without the restriction (2.13) for the parameters β_{rs} the scheme (2.14) even comprises a larger class of methods (see BAKER [2] for a motivation).

Therefore, we will analyze (2.14) rather than (2.12).

Note that (2.14) requires only the function $\tilde{\psi}_0(x) = g(x)$ to start the integration so that it can be used to provide the required starting functions for the linear multistep methods discussed in §2.1.1.

2.2.2. Equivalence with Runge-Kutta type quadrature methods

From (2.14) one derives that

$$\tilde{\psi}_n(x) = g(x) + h \sum_{j=0}^{n-1} \sum_{s=0}^P \beta_{ps} K(x, jh + \theta_s h, \tilde{\psi}_{j+1}^{(s)}(jh + \theta_s h)).$$

Substituting this expression into (2.14) and introducing the meshpoints η_j numbered according to

$$(2.15) \quad \eta_{i(p+1)+r} = ih + \theta_r h$$

yields the scheme

$$(2.16) \quad \begin{aligned} \tilde{f}_{n(p+1)+r} = & g(\eta_{n(p+1)+r}) + h \sum_{j=0}^{n-1} \sum_{s=0}^P \beta_{ps} K(\eta_{n(p+1)+r}, \eta_{j(p+1)+s}, \\ & \tilde{f}_{j(p+1)+s}) \\ & + h \sum_{s=0}^P \beta_{rs} K(\eta_{n(p+1)+r}, \eta_{n(p+1)+s}, \tilde{f}_{n(p+1)+s}), \end{aligned}$$

where $\tilde{f}_{n(p+1)+r} \simeq f(\eta_{n(p+1)+r})$.

This formula is easily recognized as a Runge-Kutta type quadrature method for the integral equation (1.1). It is generally referred to as an extended Runge-Kutta method (BAKER [1]). The mixed Runge-Kutta methods ([1]) do not fall within the class considered in §2.2.1, but they are included in the general setting which is presented in section 3.

2.3. New methods by imbedding

The numerical methods of extended Runge-Kutta type are derived directly from the corresponding Runge-Kutta method for solving ordinary differen-

tial equations. Therefore, the imbedding technique (which produces an ordinary differential equation) does not generate any new methods of this kind. However, in case of linear multistep methods the relation with quadrature methods is more interesting, in the sense that new methods may arise. The relation of linear multistep methods for ordinary differential equations and quadrature methods for solving integral equations is discussed in WOLKENFELT [14]. As an example, we quote here the interesting class of multistep methods which are based on backward differentiation formulae (also known as Curtiss-Hirschfelder formulae). These formulae are amongst those recommended^{*)} in the literature when stability considerations are paramount (LAMBERT [10]).

Since stability may be a problem in the integration of Volterra integral equations, we give some attention to the use of backward differentiation formulae for the integration of (1.1). The coefficients of these formulae are defined by

$$a_0 = 1, \quad \sum_{r=1}^q (1-r)^j a_r + j b_0 = -1, \quad j = 0(1)q.$$

The corresponding scheme of the form (2.4) may be found by generating the weights according to (2.5). However, explicit knowledge of the weights is not necessary and from a practical point of view, it may be more convenient to base the implementation of the algorithm on (2.1) instead of (2.4).

3. CLASSICAL BLOCK-BY-BLOCK AND STEP-BY-STEP METHODS

The literature (see BAKER [1]) contains a variety of numerical methods for (1.1); many such methods reduce to extensions of the quadrature and Runge-Kutta methods indicated in §§ 2.1 and 2.2. Such extensions yield equations of the form

$$(3.1) \quad \tilde{f}_{n+1} = g(\eta_{n+1}) + h \sum_{j=0}^{m(n+1)} \Omega_{n+1,j} K(\eta_{n+1}, \eta_j, \tilde{f}_j), \quad n \geq 0$$

^{*)} However, one should bear in mind the possibility of "over-stability".

where $\tilde{f}_n \simeq f(\eta_n)$ and, for example, $\eta_0 = 0$, $\tilde{f}_0 = g(0)$, $\eta_j = ih + \theta_r h$ ($i = 0, 1, \dots, N-1$; $r = 0, 1, \dots, p$), with $i = [(j-1)/(p+1)]$, $r \equiv (j-1) \bmod (p+1)$ ($[z]$ denotes the integer part of z). For (semi-) explicit methods $m(n+1) = n+1$, whilst for block-by-block methods typified by those of Linz and those of de Hoog and Weiss (BAKER [1, §6.7]) we have $m(n+1) = (p+1)\{[n/(p+1)]+1\}$. (We note that different methods of defining $K(x, y, f(y))$ when $y > x$ yield the differing versions of these block methods.) BAKER [2] indicated methods for choosing the parameters $\{\Omega_{nj}, \eta_j\}$ given quadrature rules and/or a tableau of Runge-Kutta parameters (e.g. the mixed Runge-Kutta methods); further similar prescriptions are also possible. If we set, in (3.1), $\eta_j = jh$ and $\Omega_{nj} = \omega_{nj}$ (the weights of quadrature rules based on equidistant abscissae) we obtain a wide class of quadrature methods, in particular those considered by BAKER and KEECH [4].

3.1. Extension of the analysis

We shall consider methods associated with a scheme (3.1) of the form outlined above.

If we assume that the kernel $K(x, y, f(y))$ has the form $F(y, f(y))$, independent of x , and $g(x)$ is constant, then equation (1.1) reduces to an initial value problem of the form

$$(3.2) \quad f'(x) = F(x, f(x)), \quad f(0) = g(0).$$

In this case the quadrature methods considered in §2.1.2 reduce to linear multistep methods for solving (3.2). Hence, it is not surprising that the equations (3.1) frequently simplify, under the same assumption, to recognizable methods for (3.2). A condition for this phenomenon is given in theorem 3.1. In the interim we suppose that if $K(x, y, f(y)) = F(y, f(y))$ then (3.1) may be reduced to the following form

$$(3.3) \quad \sum_{j=0}^k \{A_j \tilde{\phi}_{n+1-j} + h B_j \tilde{\kappa}_{n+1-j}\} = \vec{0}.$$

Here, the vectors $\tilde{\phi}_j$ and $\tilde{\kappa}_j$ have the form

$$(3.4) \quad \vec{\phi}_j = [\tilde{f}_m, \dots, \tilde{f}_{m+p}]^T, \quad m = j(p+1),$$

and

$$(3.5) \quad \vec{\kappa}_j = [F(\eta_m, \tilde{f}_m), \dots, F(\eta_{m+p}, \tilde{f}_{m+p})]^T, \quad m = j(p+1),$$

and the matrices $\{A_j, B_j\}_{j=0}^k$ are fixed independently of h and are generated by the parameters Ω_{nj} in (3.1).

We note that (3.3) is a generalization of the linear multistep method

$$\sum_{j=0}^k \{a_j \tilde{f}_{n+1-j} + hb_j F(\eta_{n+1-j}, \tilde{f}_{n+1-j})\} = 0,$$

(compare, for example, the cyclic linear multistep methods of DONELSON & HANSEN [5, p.138]; see also STETTER [13, §4.3]).

Let us now apply the method associated with (3.3) to the equation (1.7) in which x is a parameter and t is the integration variable. That is, we replace $F(\eta_i, \tilde{f}_i)$ in (3.5) by $K(x, \eta_i, \tilde{\psi}_i(\eta_i))$ and \tilde{f}_i in (3.4) by $\tilde{\psi}_i(x)$, where x is a parameter and $\tilde{\psi}_i(x) = \tilde{\Psi}(\eta_i, x)$ denotes the numerical approximation to $\Psi(\eta_i, x)$. We find

$$(3.6) \quad \sum_{j=0}^k \{A_j \vec{\phi}_{n+1-j}(x) + hB_j \vec{\kappa}_{n+1-j}(x)\} = \vec{0}, \quad (n \geq k-1),$$

where the components of $\vec{\phi}_j(x)$ are values $\tilde{\psi}_i(x)$ and those of $\vec{\kappa}_j(x)$ are values $K(x, \eta_i, \tilde{\psi}_i(\eta_i))$, ($i = m, m+1, \dots, m+p$). Thus, equation (3.6) provides a generalization of (2.1). Starting values for $\tilde{\psi}_n(x)$ may be defined by setting $n = 0, 1, \dots, k(p+1)-1$ in

$$(3.7) \quad \tilde{\psi}_n(x) = g(x) + h \sum_{j=0}^{m(n)} \Omega_{nj} K(x, \eta_j, \tilde{\psi}_j(\eta_j))$$

together with $\tilde{\psi}_0(x) = g(x)$, and such values provide components for the starting vectors $\vec{\phi}_0(x), \dots, \vec{\phi}_{k-1}(x)$ for (3.6).

Now we assumed that when $K(x, y, f(y)) = F(y, f(y))$ then (3.1) reduces to (3.3). It is not difficult to see that the inclusion of x as a parameter in the equations

$$(3.8) \quad \tilde{\psi}_n(x) = g(x) + h \sum_{j=0}^{m(n)} \Omega_{nj} K(x, \eta_j, \tilde{\psi}_j(\eta_j))$$

permits the reduction of these equations, *pari passu*, to (3.6). Hence the values \tilde{f}_n defined by (3.1) can be identified with values $\tilde{\psi}_n(\eta_n)$ generated by the components $\tilde{\psi}_n(x)$ of the vectors $\tilde{\phi}_j(x)$ satisfying (3.6). Informally, this result generalizes Theorem 2.1.

The structure of the equations (3.1) sufficient to yield the properties required above can be formalized. By assumption, the non-zero coefficients Ω_{nj} ($n \geq 0$) form a block-lower triangular array; let us first suppose that the partitioned submatrices of this array are denoted $V_{n,j}$ so that equations (3.8) may be written in vector form as

$$(3.9) \quad \tilde{\phi}_{n+1}(x) = g(x)\vec{e} + h \sum_{j=0}^{n+1} V_{n+1,j} \tilde{\phi}_j(x)$$

where $\vec{e} = [1, 1, \dots, 1]^T$. We have the following result

THEOREM 3.1. *If there exist fixed matrices $\{A_j, B_j\}_{j=0}^k$ such that (for $n \geq k-1$)*

$$(3.10) \quad \begin{aligned} \sum_{i=0}^k A_i V_{n+1-i,j} &= 0 & (j = 0, 1, \dots, n-k) \\ \sum_{i=0}^k A_i V_{n+1-i,j} &= -B_{n+1-j} & (j = n-k+1, \dots, n+1) \\ \sum_{i=0}^k A_i &= 0 \end{aligned}$$

then (3.6) follows from (3.9).

To illustrate, it frequently occurs, in practice, that

$$[\Omega_{nj}] = \begin{bmatrix} \vdots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ w & w_0 & w_1 & \cdot & \dots & w_{k-1} & w_k & \cdot & \cdot & \cdot \\ w & w_0 & w_0 & w_1 & \dots & w_{k-2} & w_{k-1} & w_k & \cdot & \cdot \\ w & w_0 & w_0 & w_0 & \dots & w_{k-3} & w_{k-2} & w_{k-1} & w_k & \cdot \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

where w, w_0, w_1, \dots, w_k are fixed matrices, so that for $n = k, k+1, \dots$

$$V_{n+1,r} = \begin{cases} \omega_{k+r-n-1}, & \text{if } n+1-k \leq r \leq n+1 \\ \omega_0, & \text{if } 1 \leq r \leq n-k \\ \omega, & \text{if } r = 0. \end{cases}$$

Then appropriate matrices $\{A_j, B_j\}_{j=0}^k$ can be found to satisfy (3.10).

3.2. Imbedding of the numerical method

We take the opportunity here to emphasize a certain aspect of the preceding analysis. In §3.1, equation (3.6) results from discretizing equation (1.7) with an appropriate method and equation (1.7) results from imbedding (1.1) in (1.6). We may instead take as our starting point equation (3.1) in the form

$$(3.11) \quad \tilde{f}_{n+1} = g(\eta_{n+1}) + h \sum_{j=0}^{m(n+1)} \Omega_{n+1,j} K(\eta_{n+1}, \eta_j, \tilde{f}_j)$$

and imbed this equation in

$$(3.12) \quad \tilde{\psi}_{n+1}(x) = g(x) + h \sum_{j=0}^{m(n+1)} \Omega_{n+1,j} K(x, \eta_j, \tilde{f}_j)$$

so that $\tilde{\psi}_{n+1}(\eta_{n+1}) = \tilde{f}_{n+1}$.

Since $\tilde{\psi}_{n+1}(x) = \tilde{\Psi}(\eta_{n+1}, x)$ equation (3.12) defines a function $\tilde{\Psi}(t, x)$ for $t = \eta_0, \eta_1, \dots$; instead of differentiating $\tilde{\Psi}(t, x)$ with respect to t (as was undertaken for $\Psi(t, x)$ in §1.1) we can apply a differencing technique (in the variable t) associated with the matrices A_j to form $\sum_{j=0}^k A_j \tilde{\phi}_{n+1-j}(x)$ and obtain (3.6) by virtue of (3.9) and (3.10). This approach shows the analogy between the derivation of (1.7) from (1.1) and the derivation of (3.6) from (3.1).

4. STABILITY

In this section we investigate the recurrence relations between the functions $\tilde{\psi}_n(x)$. In §4.1.1 and 4.1.2 we start by analyzing these relations for the case of linear multistep methods and Runge-Kutta methods, respectively. In §4.2 the ideas are extended to the more general class of methods of section 3.

4.1.1. Linear multistep methods

The first-order variational equation of scheme (2.1) assumes the form

$$(4.1) \quad \sum_{j=0}^k [a_j \Delta \tilde{\psi}_{n+1-j}(x) + h b_j J_{n+1-j}(x) \Delta \tilde{\psi}_{n+1-j}(\eta_{n+1-j})] = 0,$$

where $J_n(x) = (\partial/\partial f)K(x, \eta_n, \tilde{\psi}_n(\eta_n))$ and $\eta_n = nh$.

At each point η_{n+1} we define the linear operators C_j by

$$(4.2) \quad C_j : \phi(x) \rightarrow a_j \phi(x) + b_j h J_{n+1-j}(x) \phi(\eta_{n+1-j}).$$

Evidently, the C_j are operators with domain and range in the space of all bounded real-valued functions defined on the interval $[0, X]$ provided that $J_{n+1-j}(x)$ is a bounded real-valued function defined on $[0, X]$. The inverse of the operator C_0 can be found by solving $C_0 \phi(x) = \chi(x)$ for a given function $\chi(x)$, i.e. by solving

$$(4.3) \quad a_0 \phi(x) + b_0 h J_{n+1}(x) \phi(\eta_{n+1}) = \chi(x).$$

Substitution of $x = \eta_{n+1}$ in (4.3) yields

$$(4.4) \quad \phi(\eta_{n+1}) = [a_0 + h b_0 J_{n+1}(\eta_{n+1})]^{-1} \chi(\eta_{n+1}),$$

unless $[a_0 + h b_0 J_{n+1}(\eta_{n+1})] = 0$ (which is exceptional).

Substitution of (4.4) into (4.3) yields the function $\phi(x)$ and therefore the inverse of C_0 exists, apart from the exceptional case.

Using the operators C_j , (4.1) may be written in the form

$$(4.5) \quad \Delta \tilde{\psi}_{n+1}(x) = - C_0^{-1} \sum_{j=1}^k C_j \Delta \tilde{\psi}_{n+1-j}(x)$$

or equivalently

$$(4.6) \quad \vec{\Delta v}_{n+1}(x) = M_n \vec{\Delta v}_n(x),$$

where $\vec{\Delta v}_{n+1}(x)$ is the vector of functions

$$\vec{\Delta V}_{n+1}(x) = [\tilde{\Delta\psi}_{n+1}(x), \dots, \tilde{\Delta\psi}_{n+2-k}(x)]^T$$

and the amplification operator M_n is given by

$$(4.7) \quad M_n = \begin{bmatrix} -c_0^{-1}c_1 & -c_0^{-1}c_2 & \dots & -c_0^{-1}c_{k-1} & -c_0^{-1}c_k \\ 1 & & & & \\ & 1 & & \bigcirc & \\ & & \bigcirc & & \\ & & & 1 & 0 \end{bmatrix}$$

When the relation (4.6) is discretized with respect to x we obtain a relation of the form

$$\vec{\Delta V}_{n+1} = M_n^* \vec{\Delta V}_n,$$

where

$$\vec{\Delta V}_n = [\tilde{\Delta\psi}_n, \dots, \tilde{\Delta\psi}_{n+1-k}]^T$$

and

$$\tilde{\Delta\psi}_n = [\tilde{\Delta\psi}_n(x_0), \dots, \tilde{\Delta\psi}_n(x_N)]^T.$$

The operator M_n^* is a matrix operator and is obtained by replacing the operators occurring in (4.7) by matrices of order $N+1$: the identity operators are replaced by identity matrices and the operators C_j by the matrices C_j^* , where

$$C_j^* = [a_j \delta_{is} + hb_j J_{n+1-j}(\eta_i) \delta_{i,i+s-(n+1-j)}]_{i,s=0}^N,$$

here, δ_{is} denotes the Kronecker symbol. For such a matrix operator, the location of the eigenvalues of M_n^* gives an indication of the stability behaviour of the scheme. Therefore, the characteristic equation of (4.7) is of importance. We have the following theorem.

THEOREM 4.1. Let $\rho(\zeta)$ be the polynomial defined by

$$\rho(\zeta) = \sum_{j=0}^k a_j \zeta^{k-j},$$

let $R(\zeta)$ be the matrix with elements

$$r_{ij} = \rho(\zeta) \delta_{ij} + b_j h J_{n+1-j}(\eta_{n+1-i}) \zeta^{k-j}, \quad i, j = 0, 1, \dots, k,$$

where δ_{ij} denotes the Kronecker symbol. Then the eigenvalues of the amplification operator M_n of the linear multistep method (2.1) satisfy the characteristic equation

$$(4.8) \quad \det\{R(\zeta)\} = 0.$$

PROOF. Let $\vec{e}(x) = [e_1(x), \dots, e_k(x)]^T$ be an eigenfunction of M_n with eigenvalue ζ . We first construct \vec{e} and ζ . The equation

$$M_n \vec{e} = \zeta \vec{e}$$

leads to the following expression for the eigenfunction $\vec{e}(x)$

$$(4.9) \quad \vec{e}(x) = e(x) [\zeta^{k-1}, \zeta^{k-2}, \dots, \zeta, 1]^T,$$

where $e(x)$ satisfies

$$(4.10) \quad \sum_{j=0}^k c_j \zeta^{k-j} e(x) = 0.$$

Substitution of (4.2) yields

$$(4.11) \quad \sum_{j=0}^k [a_j e(x) + h b_j J_{n+1-j}(x) e(\eta_{n+1-j})] \zeta^{k-j} = 0.$$

This relation determines $e(x)$ (provided that $\sum_{j=0}^k a_j \zeta^{k-j} \neq 0$), and by (4.9) the eigenfunction $\vec{e}(x)$, if we can find ζ and the $e(\eta_{n+1-j})$, $j = 0, 1, \dots, k$. Consider the relations

$$(4.12) \quad \sum_{j=0}^k [a_j e(\eta_{n+1-i}) + h b_j J_{n+1-j}(\eta_{n+1-i}) e(\eta_{n+1-j})] \zeta^{k-j} = 0, \\ i = 0, 1, \dots, k,$$

which are obtained from (4.11) by substituting $x = \eta_{n+1-i}$. These relations represent a linear homogeneous system of $k+1$ equations for the $k+1$ components $e(\eta_{n+1-i})$. A non-trivial solution is obtained if the matrix of coefficients has a zero-determinant, i.e. if the eigenvalue ζ satisfies the "auxiliary" or characteristic equation

$$(4.13) \quad \det\{[\rho(\zeta)\delta_{ij} + hb_j^J \eta_{n+1-j}(\eta_{n+1-i})\zeta^{k-j}]\} = 0,$$

where δ_{ij} is the Kronecker symbol. Finding ζ from this equation and the values $e(\eta_{n+1-i})$ from (4.12), and substituting into (4.11) yields the function $e(x)$ from which $\vec{e}(x)$ can be derived by virtue of (4.9). \square

REMARKS.

- (i) Recall that equation (4.11) was obtained by first writing a k -term recurrence relation as a two-term relation and then solving the associated eigenvalue problem. The following line of approach can also be followed (which is equivalent with the first one). If we replace $\Delta\psi_{n+1-j}(x)$ in (4.1) by $\zeta^{n+1-j}e(x)$, then we obtain equation (4.11). By such a procedure the function $\zeta^{n+1-j}e(x)$ is considered as a trial solution of (4.1) and a condition for existence of such a solution is then given by the solvability of the associated linear system (4.12). In §4.1.2 and §4.2 this approach will be followed.
- (ii) Let $\tilde{R}(\zeta)$ be the $(k+1-\mu) \times (k+1-\mu)$ -matrix obtained from $R(\zeta)$ by omitting the j -th row and the j -th column for those j with $b_j = 0$, μ being the number of vanishing coefficients b_j . It is easily verified that in such cases (4.8) can be written in the form

$$(4.8') \quad \{\rho(\zeta)\}^\mu \det\{\tilde{R}(\zeta)\} = 0.$$

- (iii) Equation (4.8) or (4.8') can be used to derive the conditions under which the eigenvalues of M_n are within or on the unit circle. If $\mu \neq 0$ it is not possible to force all eigenvalues of M_n within the unit circle because of the factor $\rho(\zeta)$ in (4.8'). If we make the (natural) assumption that $\rho(\zeta)$ corresponds to a zero-stable linear multistep method (cf. LAMBERT [10]), then $\rho(\zeta)$ will always have one or more

simple zeros on the unit circle. However, it can be proved (cf. VAN DER HOUWEN & WOLKENFELT [9]) that each eigenvalue of M_n on the unit circle has μ independent eigenvectors.

- (iv) The characteristic equation (4.8) is rather complicated, in general. In certain cases, however, a simplification is possible. If we take the test equation employed by BAKER & KEECH [4], i.e. $K(x,y,f) = \lambda f$, one easily verifies that (4.8) reduces to

$$\rho(\zeta) + h\lambda\sigma(\zeta) = 0,$$

and, therefore, the present analysis is consistent with the "classical" approach.

- (v) If the linear multistep method is such that $b_i \neq 0$, for some i ($0 \leq i \leq k$) and $b_j = 0$ for $j \neq i$ (cf. the midpoint rule, backward differentiation methods), then we obtain from (4.8') the equation

$$\rho(\zeta) + b_i h J_{n+1-i}(\eta_{n+1-i}) \zeta^{k-i} = 0.$$

- (vi) The simplifications above could be obtained due to the fact that we are dealing with a scalar integral equation. When systems are treated we obtain a characteristic equation which is similar to (4.8) with J_n replaced by Jacobian matrices J_n . Only by assuming that these Jacobians can be diagonalized by the same set of eigenvectors a reduction to (4.8) is possible with J_n replaced by an eigenvalue which corresponds to a particular eigenvector.
- (vii) Theorem 4.1 provides us with the characteristic equation corresponding to the perturbation equation (4.1) for arbitrary perturbations $\Delta\tilde{\psi}_{n+1-j}(x)$ with $j = 1, 2, \dots, k$. However, in actual computations we only calculate $\tilde{\psi}_n(x_i)$, $i = n, n+1, \dots, N$; $n = k, k+1, \dots, N$, so that one is inclined to put $\Delta\tilde{\psi}_{n+1-j}(x) = 0$ for $x < x_{n+1-j}$, $j = 1, 2, \dots, k$. This, of course, changes the amplification operator M_n , but it can be verified that its eigenvalues are not changed.

4.1.2. Runge-Kutta methods

The first-order variational equation of scheme (2.14) assumes the form

$$(4.14) \quad \Delta \tilde{\psi}_{n+1}^{(r)}(x) = \Delta \tilde{\psi}_n(x) + h \sum_{s=0}^p \beta_{rs} J_{n+1}^{(s)}(x) \Delta \tilde{\psi}_{n+1}^{(s)}(\xi_{n+1}^s) \quad (r=0,1,\dots,p),$$

where $\xi_{n+1}^s = nh + \theta_s h$ and $J_{n+1}^{(s)}(x) = (\partial/\partial f)K(x, \xi_{n+1}^s, \tilde{\psi}_{n+1}^{(s)}(\xi_{n+1}^s))$.

Following the approach indicated in remark (i) of §4.1.1 we substitute a trial solution of the form $\zeta^{n+1} [e_0(x), \dots, e_p(x)]^T$ and arrive at the equations

$$e_p(x) - \zeta \{ e_r(x) - h \sum_{s=0}^p \beta_{rs} J_{n+1}^{(s)}(x) e_s(\xi_{n+1}^s) \} = 0, \quad (r=0,1,\dots,p).$$

Substituting the values $x = \xi_{n+1}^q$ ($q = 0,1,\dots,p$) we obtain the set of equations

$$\vec{e}_p - \zeta \{ \vec{e}_r - h \sum_{s=0}^p \beta_{rs} P_s \vec{e}_s \} = 0, \quad (r=0,1,\dots,p),$$

where $\vec{e}_r = [e_r(\xi_{n+1}^0), \dots, e_r(\xi_{n+1}^p)]^T$ and where P_s denotes the matrix defined by

$$P_s = [J_{n+1}^{(s)}(\xi_{n+1}^i) \delta_{i,i+j-s}]_{i,j=0}^p.$$

This system of $p+1$ vector equations for the $p+1$ vectors \vec{e}_r has a non-trivial solution if ζ satisfies the equation

$$(4.15) \quad \det\{\zeta[\alpha_{ij} h P_j - \delta_{ij} I_{p+1}] + [\delta_{i,i+j-p} I_{p+1}]\} = 0,$$

where I_{p+1} denotes the unit matrix of order $p+1$.

Thus, we have the following theorem:

THEOREM 4.2. *The eigenvalues of the amplification operator associated with the Runge-Kutta method (2.14) satisfy (4.15).*

4.2. A general result

The first-order variational equation for equation (3.6), in which (we recall) the components of $\vec{\kappa}_j(x)$ are values $K(x, \eta_i, \tilde{\psi}_i(\eta_i))$ may be written

$$(4.16) \quad \sum_{j=0}^k \{ A_j \Delta \tilde{\phi}_{n+1-j}^{(x)} + h B_j J_{n+1-j}^{(x)} R_{n+1-j}(\Delta \tilde{\phi}_{n+1-j}^{(x)}) \} = \vec{0},$$

where $J_j(x)$ is a diagonal matrix whose diagonal elements are values $(\partial/\partial f)K(x, \eta_i, \tilde{\psi}_i(\eta_i))$, ($i = m, m+1, \dots, m+p$, where $m = j(p+1)$) whilst

$$(4.17) \quad \vec{\Delta\phi}_j(x) = [\Delta\tilde{\psi}_m(x), \dots, \Delta\tilde{\psi}_{m+p}(x)]^T$$

and

$$(4.18) \quad R_j(\vec{\Delta\phi}_j(x)) = [\Delta\tilde{\psi}_m(\eta_m), \dots, \Delta\tilde{\psi}_{m+p}(\eta_{m+p})]^T.$$

We observe that (4.18) may be expressed in the form

$$(4.19) \quad R_j(\vec{\Delta\phi}_j(x)) = \sum_{i=1}^{p+1} E_i \vec{\Delta\phi}_j(\eta_{m+i-1}), \quad (m = j(p+1)),$$

where $E_i = \vec{e}_i \vec{e}_i^T$ and \vec{e}_i is the i -th column of the identity matrix of order $p+1$.

A trial solution of the form $\vec{\Delta\phi}_{n+1-j}^{\rightarrow}(x) = \zeta^{n+1-j} \vec{e}(x)$ satisfies (4.16) if

$$(4.20) \quad \sum_{j=0}^k \zeta^{k-j} \{A_j \vec{e}(x) + h B_j J_{n+1-j}(x) \sum_{i=1}^{p+1} E_i \vec{e}(\xi_{n+1-j}^{i-1})\} = \vec{0},$$

where $\xi_{n+1-j}^i = \eta_{(n+1-j)(p+1)+i}$ ($i = 0, 1, \dots, p$; $j = 0, 1, \dots, k$) and $\vec{e}(x)$ is a vector with $(p+1)$ components. A solution of (4.20) may be found if

$$\det\left\{ \sum_{j=0}^k \zeta^{k-j} A_j \right\} \neq 0$$

and

$$(4.21) \quad \sum_{j=0}^k \zeta^{k-j} \{A_j \vec{e}(\xi_{n+1-s}^r) + h B_j J_{n+1-j}(\xi_{n+1-s}^r) \sum_{i=1}^{p+1} E_i \vec{e}(\xi_{n+1-j}^{i-1})\} = \vec{0}$$

$$(r = 0, 1, \dots, p; s = 0, 1, \dots, k).$$

The set of equations (4.21) constitutes a set of $(p+1)(k+1)$ vector equations in as many unknowns, and the criterion for solvability is the vanishing of an associated determinant which is a (matrix) polynomial of degree k in ζ . (This "auxiliary" polynomial is a characteristic polynomial for an amplification matrix occurring in the two-term recurrence relation associated with (4.16).) It may be seen that the root ζ of largest modulus gives some insight into the local amplification of $\vec{\Delta\phi}_j^{\rightarrow}(x)$ in (4.16).

The required polynomial may be written

$$(4.22) \quad \det \left\{ \sum_{j=0}^k \zeta^{k-j} (A_j^* + h B_j^*) \right\} = 0,$$

where A_j^* and B_j^* are matrices of order $(p+1)^2(k+1)$. If we partition A_j^* and B_j^* into blocks of order $p+1$ and treat each block as a single matrix element, we may write

$$A_j^* = \text{diag}(A_j, \dots, A_j),$$

and

$$B_j^* = \text{diag}(B_j^{J_{n+1-j}(\xi_{n+1-k}^0)}, \dots, B_j^{J_{n+1-j}(\xi_{n+1-k}^p)}, \dots, \\ B_j^{J_{n+1-j}(\xi_{n+1}^0)}, \dots, B_j^{J_{n+1-j}(\xi_{n+1}^p)}) \times G_j$$

where G_j is the matrix in which the $(k-j)(p+1)+i$ -th column ($i = 1, \dots, p+1$) has entries E_i , and zeros elsewhere. As an example the matrix G_k has the form

$$G_k = \begin{bmatrix} E_1 & E_2 & \dots & E_{p+1} & \vdots & \vdots & \vdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ E_1 & E_2 & \dots & E_{p+1} & \vdots & \vdots & \vdots \end{bmatrix}$$

4.3. Examples

In order to illustrate the application of the theorems 4.1 and 4.2 we derive the characteristic equation for a few examples. The first example concerns one of the simplest integration formulas, the trapezoidal rule when applied to an integral equation with an arbitrary, non-linear kernel. For the trapezoidal rule which is generated by the multistep coefficients

$$k = 1; \quad a_0 = -a_1 = 1, \quad b_0 = b_1 = -\frac{1}{2},$$

It is easily verified that the characteristic equation (4.8) assumes the form

$$(4.23) \quad [1 - \frac{1}{2}z_{11}] \zeta^2 - [2 + \frac{1}{2}(z_{00} - z_{11}) + \frac{1}{4}(z_{10}z_{01} - z_{00}z_{11})] \zeta + (1 + \frac{1}{2}z_{00}) = 0,$$

where z_{ij} denotes the value of $hJ_{n+i}(\eta_{n+j})$. Thus, by theorem 4.1 the eigenvalues of the amplification matrix M_n are given by the roots of this equation (4.23).

Our second example deals with a general linear multistep method but now the kernel function is restricted to the two-parameter convolution kernel (cf. [8])

$$K(x, y, f) = (\lambda + \mu(x-y))f.$$

In this special case the characteristic equation (4.8) assumes the form

$$\det\{[\rho(\zeta)\delta_{ij} + hb_j\zeta^{k-j} + h^2\mu(j-i)\zeta^{k-j}]\} = 0$$

i and j being the row and column index, respectively. Subtracting successive rows for $i = 0, 1, \dots, k-1$ in the determinant yields

$$(4.24) \quad \det \begin{bmatrix} \rho + \alpha_0 & -\rho + \alpha_1 & \alpha_2 & \dots & \alpha_k \\ \alpha_0 & \rho + \alpha_1 & -\rho + \alpha_2 & & \alpha_k \\ \alpha_0 & \alpha_1 & \rho + \alpha_2 & & \alpha_k \\ \vdots & \vdots & & \ddots & \vdots \\ \alpha_0 & \alpha_1 & \dots & \rho + \alpha_{k-1} & -\rho + \alpha_k \\ \beta_0 & \beta_1 & \dots & \beta_{k-1} & \rho + \beta_k \end{bmatrix} = 0,$$

where

$$\alpha_j = \mu b_j h^2 \zeta^{k-j}, \quad \beta_j = b_j h(\lambda - \mu h(k-j)) \zeta^{k-j}.$$

By again subtracting successive rows for $i = 0, 1, \dots, k-2$ this equation reduces to

$$\det \begin{bmatrix} \rho & -2\rho & \rho & & & \\ & \rho & -2\rho & \rho & & \\ & & \ddots & \ddots & \ddots & \\ & & & \rho & -2\rho & \rho \\ \alpha_0 & \alpha_1 & \dots & \alpha_{k-2} & \rho+\alpha_{k-1} & -\rho+\alpha_k \\ \beta_0 & \beta_1 & \dots & \beta_{k-2} & \beta_{k-1} & \rho+\beta_k \end{bmatrix} = 0$$

Next, we add to the j -th column of this determinant ($j = 1, 2, \dots, k$) the sum of the preceding columns to obtain

$$\det \begin{bmatrix} \rho & -\rho & & & \\ & \rho & -\rho & & \\ & & \ddots & \ddots & \\ & & & \rho & -\rho \\ S_0 & S_1 & & \rho+S_{k-1} & S_k \\ S_0 & S_1 & & S_{k-1} & \rho+S_k \end{bmatrix} = 0,$$

where $S_j = \sum_{i=0}^j \alpha_i$ and $s_j = \sum_{i=0}^j \beta_i$. Finally, by repeating this operation on the columns $j = 1, 2, \dots, k-1$, we arrive at the characteristic equation

$$(4.25) \quad [\rho(\zeta)]^{k-1} [(\rho(\zeta) + S_{k-1}^*(\zeta))(\rho(\zeta) + s_k(\zeta)) - s_{k-1}^*(\zeta)S_k(\zeta)] = 0,$$

where $S_j^* = \sum_{i=0}^j S_i$ and $s_j^* = \sum_{i=0}^j s_i$. The functions $S_j^*(\zeta)$ and $s_j^*(\zeta)$ can be expressed in terms of the characteristic function

$$\sigma(\zeta) = \sum_{j=0}^k b_j \zeta^{k-j}.$$

A straightforward calculation yields

$$S_{k-1}^*(\zeta) = \mu h^2 \zeta \sigma'(\zeta), \quad S_k(\zeta) = \mu h^2 \sigma(\zeta),$$

$$s_{k-1}^*(\zeta) = (\lambda - \mu h) h \zeta \sigma'(\zeta) - \mu h^2 \zeta^2 \sigma''(\zeta),$$

$$s_k(\zeta) = \lambda h \sigma(\zeta) - \mu h^2 \zeta \sigma'(\zeta).$$

Substitution into (4.25) yields the characteristic equation

$$(4.26) \quad \rho^{k-1}(\zeta) \{ \rho(\zeta) [\rho(\zeta) + \lambda h \sigma(\zeta)] + \mu^2 h^4 \zeta [\sigma(\zeta) \sigma'(\zeta) + \sigma(\zeta) \sigma''(\zeta) \zeta - (\sigma'(\zeta))^2 \zeta] \} = 0.$$

Finally, we consider the characteristic equation of the family of Runge-Kutta formulas generated by the tableau

$$\begin{array}{c|ccc} \theta_0 & \beta_{00} & \beta_{01} & 0 \\ \theta_1 & \beta_{10} & \beta_{11} & 0 \\ \hline \theta_2=1 & \beta_{20} & \beta_{21} & 0 \end{array}$$

By theorem 4.2 the characteristic equation of the amplification matrix for this class reduces to

$$(4.27) \quad \zeta^4 (1-\zeta) \det \begin{bmatrix} (\beta_{00} z_{00}^{-1}) \zeta & \beta_{01} z_{10} \zeta & 1 & 0 \\ \beta_{10} z_{01} \zeta & (\beta_{11} z_{11}^{-1}) \zeta & 0 & 1 \\ \beta_{20} z_{00} \zeta & \beta_{21} z_{10} \zeta & 1-\zeta & 0 \\ \beta_{20} z_{01} \zeta & \beta_{21} z_{11} \zeta & 0 & 1-\zeta \end{bmatrix} = 0,$$

where z_{ij} here denotes the value of $hJ_{n+1}^{(i)}(nh+\theta_j h)$. A straightforward calculation leads to the characteristic equation

$$(4.28) \quad \zeta^6 (1-\zeta) \{ D_1 \zeta^2 - (D_2 + 2D_1 - D_4) \zeta + (D_2 + D_1 - D_4 + D_3) \} = 0$$

where the coefficients D_j are determinants defined by

$$D_1 = \det \begin{bmatrix} \beta_{00} z_{00}^{-1} & \beta_{01} z_{10} \\ \beta_{10} z_{01} & \beta_{11} z_{11}^{-1} \end{bmatrix}, \quad D_2 = \det \begin{bmatrix} \beta_{10} z_{01} & \beta_{11} z_{11}^{-1} \\ \beta_{20} z_{00} & \beta_{21} z_{10} \end{bmatrix}$$

$$D_3 = \det \begin{bmatrix} \beta_{20} z_{00} & \beta_{21} z_{10} \\ \beta_{20} z_{01} & \beta_{21} z_{11} \end{bmatrix}, \quad D_4 = \det \begin{bmatrix} \beta_{00} z_{00}^{-1} & \beta_{01} z_{10} \\ \beta_{20} z_{01} & \beta_{21} z_{11} \end{bmatrix}.$$

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