THE NUMERICAL ANALYSIS OF REDUCIBLE QUADRATURE METHODS FOR VOLTERRA INTEGRAL AND INTEGRO-DIFFERENTIAL EQUATIONS

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TER VERKRIJGING VAN DE GRAAD VAN
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PAULUS HENDRIKUS MARIA WOLKENFELT

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PROMOTOR : PROF.DR. P.J. VAN DER HOUWEN

COPROMOTOR: DR. C.T.H. BAKER

COREFERENT: PROF.DR. H. BRUNNER

Aan Lina

Aan mijn ouders

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Paul Wolkenfelt
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CONTENTS

THE INTRODUCTORY PART

1. INTRODUCTION

The major part of this thesis consists of the six papers [A] to [F], specified in the contents list, dealing with various aspects of the numerical solution of Volterra equations.

Paper [A], written jointly with P.J. van der Houwen, is an adapted version of the report [13] and has been published in condensed form in *COMPUTING* 24 (1980), pp. 341-347. In this paper the emphasis is on the stability analysis of numerical methods. Paper [B] has been written jointly with Chr. T.H. Baker and P.J. van der Houwen, and has appeared in the *Journal of Integral Equations* 3 (1981), pp. 61-82. This paper is concerned with the construction and stability analysis of numerical methods. The papers [C], [D] and [E], each dealing with various aspects of reducible quadrature methods, are detailed elaborations of ideas and results recorded in the technical report [25] and have been submitted for publication. Paper [C], with deletion of the rather long convergence proof, will appear in *BIT* in the course of this year. In paper [F], which is a copy of the prepublication [26] a new class of methods is proposed and analyzed.

In the next sections we give the three important classes of Volterra equations considered in this thesis, and discuss rather concisely numerical methods to solve them. Particular attention is paid to the class of reducible quadrature methods. Furthermore, we touch upon the difficulties encountered in the stability analysis. In addition, we give at the appropriate places a summary of each paper. It should be emphasized that the discussion in this introductory part is not meant to be exhaustive; it is mainly intended to place the six papers in their proper context.

2. VOLTERRA EQUATIONS

In this thesis the emphasis is on the numerical solution of equations of the form

$$f(x) = g(x) + \int_0^x K(x,y,f(y))dy, \qquad x \in J = [0,X]. \tag{2.1}$$

Equation (2.1) is called a (nonlinear) *Volterra integral equation of the second kind* for the unknown function f; the kernel $K = K(x,y,v)$ (with $(x,y) \in T = \{(x,y) \mid 0 \le y \le x \le X\}$ and $v \in \mathbb{R}$) and the forcing function g are given.

Such equations arise from the (repeated) integration of initial value problems for ordinary differential equations (see e.g. TRICOMI [23]), but more significantly, they generally appear in the formulation of problems modelling hereditary phenomena (see the classical work of VOLTERRA [24]). For a discussion of the sources and applications of these equations in scientific and engineering problems, we refer to MILLER [19], TRICOMI [23], SAATY [22], DAVIS [11], NOBLE [20], LONSETH [15].

The theoretical aspects of equation (2.1) constitute a well-established branch of mathematics. A thorough account of this theory, including the questions of the existence, uniqueness and qualitative behaviour of solutions of (2.1) can be found in the text by MILLER [19]. An important basic result is (see also DAVIS [11, p.415], TRICOMI [23, p.42]) that equation (2.1) has a unique continuous solution on J if the following conditions are satisfied:

(i) $g(x)$ is continuous on J;

(ii) $K(x,y,v)$ is uniformly continuous in x and y on T for all finite v;

(iii) $K(x,y,v)$ satisfies the Lipschitz condition

$$|K(x,y,v_1) - K(x,y,v_2)| \leq L|v_1 - v_2|$$

uniformly for $(x,y) \in T$, where L is a positive constant.

Other important classes of Volterra equations considered in this thesis are *Volterra integral equations of the first kind*

$$(2.2) \qquad \int_0^x K(x,y,f(y))dy = g(x), \qquad x \in J,$$

and *Volterra integro-differential equations*

$$(2.3) \qquad f'(x) = F(x,f(x), \int_0^x K(x,y,f(y))dy), \qquad x \in J.$$

In general, the equations mentioned above can not be solved by analytical methods. Approximate solutions, however, can be obtained by numerical techniques.

3. NUMERICAL METHODS

The fact that a Volterra equation can be regarded as a generalization

of the initial value problem for ordinary differential equations (cf. NOBLE [20]) is also reflected in the development of numerical methods. In particular, numerical methods for (2.1), (2.2) and (2.3) generate in a step-by-step or block-by-block fashion, approximate values f_n (n=k(1)N) to the exact solution f(x) on the mesh $\{x_n=nh \mid n=0(1)N,\ x_N=X\}$. If k > 1, starting values f_j, j = 1(1)k-1 must be given, while f_0 is known.

An important class of methods originates on replacing the integral term in (2.1), (2.2) or (2.3) with $x = x_n$ by approximate quadrature rules based on the abscissae x_j, j = 0(1)n, and weights w_{nj} (j=0(1)n, n≥k), i.e. rules of the form

$$\int_0^{x_n} \phi(y)dy \simeq h \sum_{j=0}^{n} w_{nj}\, \phi(x_j). \tag{3.1}$$

For the solution of (2.1) we then obtain the equations

$$f_n = g(x_n) + h \sum_{j=0}^{n} w_{nj}\, K(x_n,x_j,f_j), \qquad n \geq k. \tag{3.2}$$

If the required starting values $f_0,\ldots,f_{k-1}$ are given, then $f_k, f_{k+1},\ldots$, can be computed in a step-by-step fashion. The method (3.2) is called a (step-by-step) *direct quadrature method*. For a discussion of these methods, including their convergence behaviour, we refer to BAKER [2]. This thesis is mainly concerned with the analysis of an important subclass of direct quadrature methods, called (ρ,σ)-reducible quadrature methods. For a discussion of other interesting classes of methods, such as Runge-Kutta methods and collocation methods, see [8,9,4] and the references therein.

Direct quadrature methods for the solution of first kind equations (2.2) have the form

$$h \sum_{j=0}^{n} w_{nj}\, K(x_n,x_j,f_j) = g(x_n), \qquad n \geq k. \tag{3.3}$$

Equation (2.2) is known to be ill-posed and therefore difficulties can be expected when solving such equations numerically. Indeed, not all quadratures rules (3.1) yielding convergent methods for second kind equations, generate convergent direct quadrature methods for first kind equations. To guarantee convergence, rather restrictive assumptions on the quadrature rules are necessary. Difficulties in the numerical treatment of (2.2) are reflected in the convergence proofs which are frequently long and cumbersome, especially if one is interested in proving the order of convergence.

More details on methods of the form (3.3) can be found in BAKER [2], see also the references in paper [C].

Numerical methods for Volterra integro-differential equations originate by applying methods for ordinary differential equations to (2.3) in which the integral term is replaced by numerical quadrature. More details and references can be found in BAKER [3].

3.1. Reducible quadrature methods

If the kernel K is independent of x and if g is constant, that is, if (2.1) has the form

$$f(x) = \gamma + \int_0^x \kappa(y,f(y))dy, \tag{3.4}$$

then (2.1) (or (3.4)) is equivalent to the initial value problem

$$f'(x) = \kappa(x,f(x)), \quad f(0) = \gamma. \tag{3.5}$$

As a consequence, the class of second kind Volterra integral equations includes classical initial value problems as a special case. This implies that in this case the numerical method (3.2) can be regarded as a rather unconventional and inefficient way of solving (3.5), and this observation raises the following question:

> Can a numerical method for (2.1) applied to (3.4) be reduced to a method for solving (3.5) *directly*? (that is a method which yields a finite-term recurrence relation for the approximations f_n).

It turns out that such a reduction is possible if the quadrature weights display a suitable structure. To illustrate this, consider the repeated trapezium rule as a direct quadrature method applied to (3.4). We then obtain the equations

$$f_n = \gamma + h \sum_{j=0}^{n} w_{nj}\, \kappa(x_j,f_j), \tag{3.6}$$

where $w_{n0} = w_{nn} = \frac{1}{2}$ and $w_{nj} = 1$ for $j = 1(1)n-1$. The structure of the quadrature weights is given by the equalities $w_{n+1,j} = w_{nj}$, $j = 0(1)n-1$. Therefore, differencing successive equations (3.6) yields

$$f_{n+1} = f_n + \frac{h}{2}\,[\kappa(x_n,f_n) + \kappa(x_{n+1},f_{n+1})],$$

which is immediately recognized as the trapezoidal rule applied to (3.5). Most of the commonly used quadrature rules display an easily recognizable structure which can be formalized by the concept of *repetition factor*. The repetition factor r associated with the weights in (3.1) is defined (cf. LINZ [14]) as the smallest positive integer such that $w_{nj} = w_{n+r,j}$ for $u \le j \le n-v$, where u and v are fixed numbers independent of n. As an example, the weights of the repeated trapezium rule discussed above have a repetition factor of one.

It should be emphasized here, that the structure of the quadrature weights plays a crucial role in the stability analysis of numerical methods (see §4). There, the structure is also exploited to reduce the direct quadrature method to a finite-term recurrence relation, that is a method for solving ordinary differential equations. However, starting with a set of quadrature rules it is not known in advance which ODE method will result. This, in part, motivates the following question:

> Is it possible to construct a direct quadrature method which, when applied to (3.4), reduces to a *prescribed* (well-known) method for solving (3.5)?

In particular, one may ask for conditions under which equations of the form (3.6) reduce to

$$\sum_{i=0}^{k} a_i f_{n-i} = h \sum_{i=0}^{k} b_i \kappa(x_{n-i}, f_{n-i}), \tag{3.7}$$

where a_i and b_i represent the coefficients of a linear k-step method for ODEs. In this case, a positive answer to the above question is given by identification of (3.6) and (3.7). This procedure yields relations between the quadrature weights w_{nj} and the coefficients a_i and b_i of the form

$$\sum_{i=0}^{k} a_i w_{n-i,j} = \begin{cases} 0 & \text{if } 0 \le j \le n-k-1, \\ b_{n-j} & \text{if } n-k \le j \le n, \end{cases}$$

from which the quadrature weights can be generated. The resulting quadrature rules are called (ρ,σ)-*reducible* where ρ and σ denote the first and second characteristic polynomial defined by

$$\rho(\zeta) := \sum_{i=0}^{k} a_i \zeta^{k-i}, \qquad \sigma(\zeta) := \sum_{i=0}^{k} b_i \zeta^{k-i}.$$

This interesting class of (ρ,σ)*-reducible quadrature rules is the leading thread running through this thesis.*

In their general form, (ρ,σ)-reducible quadrature rules were introduced by MATTHYS [16] with the principal aim of proving A-stability results of numerical methods for Volterra integro-differential equations. However, a detailed study of the properties of these quadrature rules was not undertaken, nor was their suitability to other types of Volterra equations investigated.

In paper [D] we discuss the construction of (ρ,σ)-reducible quadrature rules and derive an asymptotic expression for the quadrature error. We also describe a technique for generating the quadrature weights in an efficient and stable manner. Particular attention is paid to the quadrature rules which are reducible to the backward differentiation methods. Furthermore, we give a concise treatment of convergence and stability results of these methods for the solution of (2.1) and (2.3).

In paper [C] we investigate the applicability of (ρ,σ)-reducible quadrature rules for the solution of Volterra integral equations of the first kind. A theorem establishing the order of convergence, is given which unifies and extends partial results previously derived by various authors. Its proof is rather involved and relies heavily upon the reducibility of the quadrature rules. An important condition for convergence is that also the second characteristic polynomial σ must have its zeros inside or on the unit circle, those on the unit circle being required to be simple.

Paper [F] was motivated by the rather awkward and inefficient implementation of some (ρ,σ)-reducible quadrature rules. In order to offset this disadvantage, we constructed the class of so-called multilag methods. Unfortunately, the price to be paid for this gain in efficiency is the loss of (ρ,σ)-reducibility. It turns out, however, that this property can be restored by changing the multilag methods in a suitable way and this led us to the class of so-called modified multilag methods. In this paper, we establish for the solution of (2.1) and (2.3) the order of convergence of the multilag methods as well as their modification, whereas for the solution of (2.2) a special class of modified multilag methods is analyzed.

In addition to the theoretical results, we also report in the papers [C], [D] and [F] on several numerical experiments with quadrature rules which are reducible to the well-known backward differentiation methods.

4. STABILITY

In the discussion of stability we shall restrict our considerations to the linear version of (2.1):

$$f(x) = g(x) + \int_0^x L(x,y)f(y)dy. \tag{4.1}$$

Before focussing our attention to the stability analysis of numerical methods, we shall first make some remarks on the stability of the continuous problem.

4.1. Stability of the continuous problem

The study of stability of (4.1) is concerned with the sensitivity of $f(x)$ to perturbations in the equation (4.1). Particular attention has been paid to the effect of a perturbation $\varepsilon(x)$ in $g(x)$ on $f(x)$, and various stability definitions arise on restricting the class of perturbations $\varepsilon(x)$ to various normed linear spaces (see e.g. BOWNDS & CUSHING [6]).

The perturbation $\delta(x)$ in $f(x)$ due to the perturbation $\varepsilon(x)$ in $g(x)$ can be expressed in terms of the resolvent kernel $R(x,y)$ by

$$\delta(x) = \varepsilon(x) + \int_0^x R(x,y)\varepsilon(y)dy, \tag{4.2}$$

where $R(x,y)$ is the solution of the equation

$$R(x,y) = L(x,y) + \int_y^x L(x,z)R(z,y)dz.$$

Therefore, in this case the study of stability reduces essentially to the study of the resolvent kernel (cf. BOWNDS & CUSHING [7], see also GROSSMAN [12]).

The general problem of deriving properties of the resolvent kernel for an arbitrary kernel function $L(x,y)$ is difficult to solve. Insight into this problem, however, can be obtained under simplifying assumptions on the nature of the kernel. Partial results exist and in [7], for example, the kernel is assumed to be *separable* or *degenerate*, i.e. of the form

$$L(x,y) = \sum_{i=0}^{r} A_i(x)B_i(y). \tag{4.3}$$

This assumption permits a reduction of (4.1) to a system of ordinary differential equations, and stability results for differential equations (cf. COPPEL [10]) can be utilized to establish results for (4.1).

4.2. Stability of the numerical method

In the stability analysis of numerical methods for (2.1) or (4.1) similar difficulties and approaches occur. For the direct quadrature method (3.2) applied to (4.1), the stability analysis involves the study of the effect of perturbations ε_n in $g(x_n)$ $(n=0,1,\ldots)$ on the resulting changes δ_n in f_n, where

$$\delta_n = \varepsilon_n + h \sum_{j=0}^{n} w_{nj} L(x_n,x_j)\delta_j . \tag{4.4}$$

Equation (4.4), frequently called a discrete Volterra equation, reflects the structure of the Volterra operator: the perturbation δ_n depends directly on *all previous perturbations* δ_j, $j = 0(1)n-1$. This is caused not only by the kernel L but also by the quadrature weights w_{nj}, and therefore the main difficulties in the stability analysis arise from these two sources. Also, the derivation of stability results for (4.4) is impeded by the lack of a general theory of discrete Volterra equations. The theory of difference equations, in which a perturbation δ_n depends on a fixed (finite) number of perturbations $\delta_{n-1},\ldots,\delta_{n-k}$, say, is well developed (MILLER [18]) and insight into the general problem (4.4) can be obtained by establishing a link with this theory under suitable assumptions on the nature of the kernel and the quadrature weights.

In the next sections we shall distinguish two approaches followed in the literature, namely the stability analysis for h sufficiently small and the analysis for fixed positive h; both approaches have their advantages and disadvantages.

4.2.1. Numerical stability for small h

This type of numerical stability, used for example by LINZ [14] and NOBLE [21], requires the perturbation sensitivity of the numerical method to be "roughly equivalent" to the perturbation sensitivity of the original continuous problem, and bears a resemblance to the stability concept used by Henrici in connection with linear multistep methods for ODEs. The analysis is based on the asymptotic expansion of the global discretization

error and has the advantage that it is applicable to general equations (2.1), i.e. without any restrictions on the kernel and the forcing function. Essential in the analysis is the structure of the quadrature weights, that is, the existence of a repetition factor. In this connection, LINZ [14] conjectured that "methods with a repetition factor greater than one tend to be numerically stable, those with a repetition factor greater than one numerically unstable".

Motivated by this conjecture, we investigate in paper [E] the relation between the repetition factor and numerical stability for small h for the class of (ρ,σ)-reducible quadrature methods. We derive a simple characterization of both numerical stability for small h and the repetition factor, and with this characterization results with regard to the conjecture of Linz can be derived in a straightforward manner. In particular, we show that methods with a repetition factor greater than one are not necessarily numerically unstable.

A disadvantage of the stability analysis discussed above is its asymptotic nature (as $h \to 0$) and therefore it may fail to give a good model for practical purposes when the stepsize h is large.

4.2.2. Numerical stability for fixed h

In order to obtain insight into the general stability problem (4.4), special cases of (4.1) have been considered in the literature. The most simple case arises on choosing in (4.1) $L(x,y) = \lambda$ ($\lambda \in \mathbb{C}$), yielding the test equation (cf. MAYERS [17])

$$\delta(x) = \varepsilon(x) + \lambda \int_0^x \delta(y)dy. \tag{4.5}$$

Since the kernel in this test equation is independent of x, equation (4.5) is equivalent to an ordinary differential equation. Therefore, in view of the discussion in §3.1, only the structure of the quadrature weights plays a role in reducing the discrete Volterra equation to a finite-term recurrence relation. Stability conditions can then be derived by a root condition on the associated characteristic (or stability) polynomial. BAKER & KEECH [5] give a systematic study along these lines for a large class of numerical methods including block-by-block methods and certain Runge-Kutta methods. Since (4.5) with $\varepsilon(x)$ constant is equivalent to the ODE test equation $\delta' = \lambda\delta$, the stability analysis based on (4.5) is reminiscent of

the study of absolute and relative stability for fixed h in the numerical treatment of ordinary differential equations.

Since the essential features of a general Volterra integral operator are not reflected in (4.5), the use of (4.5) as a test equation is disputable. In order to give a firmer foundation to the stability analysis based on (4.5), we consider in paper [A] test equations with kernels of the form (compare with (4.3))

$$(4.6) \qquad K(x,y,f) = \sum_{i=0}^{r} A_i(x)B_i(y,f).$$

In this paper, we show that, without any additional assumptions, (ρ,σ)-reducible quadrature methods applied to such test equations can be reduced to a system of finite-term recurrence relations from which (local) stability conditions can be derived. An important result we obtain is that the stability condition can be expressed completely in terms of the Jacobian matrix $\partial K/\partial f$. Therefore, the existence of some decomposition (4.6) is essential only for the analysis, but irrelevant for the final stability result. It should be remarked, however, that the conditions are rather complicated and cannot be characterized by a problem-independent region of stability. Only by first specifying the kernel function, the stability condition can be converted into conditions which are feasible from a practical point of view.

More contributions to the stability theory for fixed h exist, which vary in the class of methods considered and in the special case of (4.1) adopted as a test equation (see [1] for a brief survey). In all these contributions, however, a restricted class of kernel functions is considered having the property that the associated test equation can be reduced to a system of ordinary differential equations.

In paper [B] the analysis of numerical methods for (2.1) is treated *without restricting the class of kernel functions*. The main tool 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 this differential equation and this connection suggests a technique for deriving numerical methods for (2.1). To be specific, we apply well-known ODE methods, including Runge-Kutta methods and (cyclic) linear multistep methods, and identify the resulting scheme with a method for solving (2.1) directly. By carrying out a stability analysis of the ODE method it is possible to derive the characteristic equation associated

with the integral equation method for general kernel functions. As in paper [A], the stability conditions are rather complicated, in general.

To conclude this section, it can be stated that the contributions to stability theory, published so far, may be regarded as attempts to gain insight into the general stability problem. Much work remains to be done in this area, and it is hoped that the contributions mentioned or referred to above will prove to be useful in reaching the eventual goal of producing a general stability analysis for discrete Volterra equations.

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On the stability of multistep formulas for Volterra integral equations of the second kind

by

P.J. van der Houwen and P.H.M. Wolkenfelt

ABSTRACT

The purpose of this paper is to analyse the stability properties of a class of multistep methods for second kind Volterra integral equations. Our approach follows the usual analysis in which the kernel function is a priori restricted to a special class of test functions. In most stability investigations these test functions only depend linearly on the unknown function. Since such simple test equations are in fact equivalent to ordinary differential equations, one may dispute its relevance for the integral equation situation. Our aim is to give the use of this simple test equation a firmer foundation. To this end, we consider the large class of finitely decomposable kernels. Stability conditions will be derived and compared with those obtained with the simple test equation. As an example, it is shown that the trapezoidal rule may become unstable whereas application of the usual stability conditions would predict a stable behaviour.

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

1. INTRODUCTION

Suppose we are given the system of non-linear Volterra integral equations

$$f(x) = g(x) + \int_{x_0}^{x} K(x,y,f(y))dy, \qquad x_0 \le x \le X \tag{1.1}$$

where g and K are given vector functions and f is the unknown vector function.

Several numerical methods have been proposed to solve this equation, the most familiar ones of which are based on a direct quadrature rule. These methods have the form

$$f_{n+1} = g(x_{n+1}) + \sum_{j=0}^{n+1} w_{n+1,j} K(x_{n+1},x_j,f_j), \qquad n \ge k-1, \tag{1.2}$$

where $f_0,f_1,\ldots$ are approximations to $f(x_0),f(x_1),\ldots$ and $w_{n,j}$ are given weight parameters. In this paper we assume that the weights $w_{n,j}$ are such that for $K = af$ and $g(x) \equiv 1$ scheme (1.2) reduces to a linear multistep method (with constant coefficients) for the solution of (1.4). Further we assume that the vectors $f_0,\ldots,f_{k-1}$ have been computed by some adequate starting procedure.

In the literature, the stability analysis of this and other methods is carried out either for $h_n \to 0$ ($h_n = x_{n+1}-x_n$), where general kernel functions K are admitted (cf. KOBAYASI [9] and NOBLE [11]), or for fixed $h \neq 0$, where the kernel is of the form $K = af$, yielding the test equation

$$f(x) = g(x) + a\int_{0}^{x} f(y)dy, \qquad a \in \mathbb{C}. \tag{1.3}$$

(cf. MAYERS [10], BAKER and KEECH [1]). The main idea behind this last approach is that the kernel function is chosen in such a way that the numerical scheme can be rewritten as a recurrence relation with a *fixed* number of terms. In this connection, a remark of KERSHAW [3, p.159] about the use of this kernel function may be quoted: "... it is obviously convenient, however its true relevance to the integral equation situation does not appear

to have been thoroughly examined". Indeed, the use of (1.3) makes the stability analysis straightforward which is due to the fact that it is equivalent to the ordinary differential equation

$$f'(x) = g'(x) + af(x), \quad f(0) = g(0). \tag{1.4}$$

However, the use of (1.3) is also disputable, because the kernel does not depend on x and therefore may be considered as an equation without a "past", which does not reflect the genuine character of a Volterra integral equation.

In order to give a firmer foundation to the stability analysis based on (1.3) we have considered more general kernel functions. The present paper is based on two earlier institute reports [6] and [7]. In [6] the kernel functions K(x,y,f) were allowed to be of the form

$$K(x,y,f) = (a+bx)f, \tag{1.5}$$

where a and b are constants, and in [7] we considered the class of *finitely decomposable kernels* (cf. [2]), i.e. kernels of the form

$$K(x,y,f) = \sum_{i=0}^{r} A_i(x)B_i(y,f), \tag{1.6}$$

where the A_i are matrices only depending on x and where the B_i are vectors which only depend on (y,f) and which are differentiable with respect to f.

Like (1.3) one may dispute the relevance of equations with kernel functions (1.5) because they can be reduced to a second order differential equation. Nevertheless, the stability analysis for kernels of the form (1.5) was of some value because it indicated how to generalize the analysis for kernel functions of the form (1.6). This generalization is presented in [7] and, in a slightly modified version, reproduced in this paper.

In section 2.1 we discuss the extension of the space of perturbations of f_j with additional perturbations which makes it possible to convert the variational equation of the scheme (1.2) into a system of fixed-term recurrence relations. In theorem 2.1 our main stability result is stated, holding for kernel functions of the form (1.6). In order to see the effect of the

additional perturbations on the stability conditions we tried in section 2.2 to avoid the introduction of such perturbations. By sufficiently restricting the class of kernels it is possible to obtain stability conditions which are very similar to those given by theorem 2.1.

In section 2.3, examples are given of the trapezoidal rule when applied to a scalar integral equation and when applied to a special class of convolution kernels. In section 3, the stability conditions are tested by solving a few test problems. In all cases the theoretical results are confirmed by the numerical examples.

As to the generality of the stability analysis presented in this paper, it is subject to two assumptions: finitely decomposable kernel functions and "linear multistep" weights (i.e. the equivalence of (1.2) and a linear multistep method). The restriction of the kernels is rather mild and is only a restriction to *continuous* kernel functions. In fact, by the well-known theorem of Stone-Weierstrass, the class of continuous functions of the form (1.6) is dense in the class of all continuous functions. Hence, if K is *not* of the form (1.6) but *continuous* in x,y and f, it can be approximated by a function K^* of the form (1.6) within any degree of accuracy (for an interesting discussion on this subject we refer to [2]). Furthermore, it can be proved that if (1.2) yields the numerical solutions f_n and f_n^* corresponding to K and K^*, respectively, then $f_n - f_n^*$ is of the order $K - K^*$ as $K^* \to K$. Therefore, the behaviour of the numerical solution corresponding to any continuous kernel function K can be investigated by considering the numerical solution corresponding to a finitely decomposable approximation K^* to K. The assumption on the weights in (1.2) is more restrictive in the sense that it does not include all direct quadrature formulas. For instance, it *excludes* the formulas which are based on repeated Newton-Cotes rules combined with a different end formula (see e.g. [1]). However, it *includes* both some well-known formulas such as the Gregory rules, and unconventional quadrature formulas such as those based on the famous Curtiss-Hirschfelder formulas [4]. The generalization of the stability analysis to arbitrary quadrature rules is subject to further research.

Finally, with respect to the stability conditions derived in theorem 2.1, we remark that this condition is rather complicated and, unlike the situation in the stability analysis of ordinary differential equations, it

cannot be characterized by a problem-independent region of stability for the eigenvalues of the Jacobian matrix of K. Only by first specifying the kernel function, the stability condition can be converted into conditions which are feasible from a practical point of view.

Comparing the stability conditions derived for kernels of the form $K = af$ and derived for (1.6), we conclude that the first class of kernel functions gives a rough indication of the stability behaviour of the numerical scheme. Hence, the test equation (1.3) may be considered as a first sieve for the selection of an appropriate scheme for the solution of Volterra integral equations of the second kind. A result of our analysis is that the stability conditions derived with the simple test equation can be used for more general equations provided that the Jacobian matrix $\partial K(x,y,f)/\partial f$ is "slowly varying" in x,y and f. Since our analysis is able to quantify this "slow variation" and hence leads to more rigorous stability conditions, it may serve as a second sieve to choose a suitable scheme for the particular problem at hand.

2. DERIVATION OF RECURRENCE RELATIONS

For sufficiently small perturbations Δf_j, the variational equation of (1.2) is of the form

$$\Delta f_{n+1} = \sum_{j=0}^{n+1} w_{n+1,j} \frac{\partial K}{\partial f}(x_{n+1},x_j,f_j)\Delta f_j, \qquad n \geq k-1. \tag{2.1}$$

In order to obtain a fixed-term recurrence relation for the perturbations Δf_j we impose two conditions. Firstly, the arguments x, y and f in the Jacobian matrix are assumed to be separable according to the formula

$$\frac{\partial K}{\partial f}(x,y,f) = P(y,f) + \sum_{i=1}^{r} Q_i(x)R_i(y,f), \tag{2.2}$$

where P and R_i are arbitrary matrices only depending on y and f, and Q_i is an arbitrary matrix only depending on x. It is easily verified that all kernel functions of the form (1.6) have a Jacobian matrix of the form (2.2). Secondly, the weights $w_{n,j}$ are assumed to satisfy the relation

$$\text{(2.3)}\qquad \begin{aligned} &\sum_{\ell=0}^{k} a_\ell w_{n+1-\ell,j} = 0 \qquad j = 0,1,\ldots,n-k;\ n \geq 2k-1. \\ &\sum_{\ell=0}^{k} a_\ell = 0 \end{aligned}$$

where the parameters a_ℓ are independent of j, and k is a positive integer.

From condition (2.2) it follows that

$$\text{(2.4)}\qquad \Delta f_{n+1-\ell} = \sum_{j=0}^{n+1} w_{n+1-\ell,j}\Big[P(x_j,f_j) + \sum_{i=1}^{r} Q_i(x_{n+1-\ell})R_i(x_j,f_j)\Big]\Delta f_j$$

$$n+1-\ell \geq k;\ \ell = 0,1,\ldots,k,$$

where $w_{n,j} = 0$ for $j > n$. By virtue of (2.3) Δf_n satisfies the relation

$$\text{(2.5)}\qquad \begin{aligned} &\sum_{\ell=0}^{k} [a_\ell I + b_\ell h_n P(x_{n+1-\ell},f_{n+1-\ell})]\Delta f_{n+1-\ell} = \\ &= \sum_{i=1}^{r}\sum_{\ell=0}^{k}\sum_{j=0}^{n+1} a_\ell w_{n+1-\ell,j} Q_i(x_{n+1-\ell})R_i(x_j,f_j)\Delta f_j \end{aligned}$$

where we have written

$$\text{(2.6)}\qquad \sum_{\ell=0}^{k} a_\ell w_{n+1-\ell,j} = -h_n b_{n+1-j}, \qquad j = n-k+1,\ldots,n+1.$$

It should be remarked that the coefficients a_ℓ and b_ℓ are related to the coefficients of a linear multistep method for ordinary differential equations. To see this, let scheme (1.2) be applied to an integral equation of the form $f(x) = 1 + \int_{x_0}^{x} K^*(y,f(y))dy$. Using (2.3) and (2.6) it is easily verified that (1.2) can be written as

$$\sum_{\ell=0}^{k} a_\ell f_{n+1-\ell} + h_n \sum_{\ell=0}^{k} b_\ell K^*(x_{n+1-\ell},f_{n+1-\ell}) = 0.$$

Exactly the same formula is obtained by first writing the integral equation as the initial value problem

$$f'(x) = K^*(x,f(x)), \quad f(x_0) = 1,$$

and applying a linear k-step method with coefficients a_ℓ and b_ℓ. Note that the choice $a_0 = -1$, $a_1 = 1$ lead to quadrature formulas having repetition factor 1 (cf. NOBLE [11]). For example the Adams-Moulton formulas generate the weights of Gregory's rule. In this paper it will be assumed that $\{a_\ell, b_\ell\}$ correspond to a convergent k-step method.

In the next section relation (2.5) will be converted into a system of fixed-term recurrence relations by introducing additional perturbations which are expressed in all preceding perturbations Δf_j. In section 2.2 it will be shown that the introduction of such additional perturbations can be avoided for special classes of kernel functions, e.g. when in (1.6) the matrices $A_i(x)$ are of the form $x^i I$, I being the unit matrix.

2.1. Introduction of additional perturbations

Let us define the additional perturbations

$$\Delta G_n^{(i)} = \sum_{j=0}^{n} w_{n,j} R_i(x_j, f_j)\Delta f_j, \qquad n = 0,1,\ldots, \quad i = 1,2,\ldots,r. \tag{2.7}$$

Substitution into (2.5) leads to the (r+1)(k+1)-terms relation

$$\sum_{\ell=0}^{k} [a_\ell I + b_\ell h_n P(x_{n+1-\ell}, f_{n+1-\ell})]\Delta f_{n+1-\ell} = \tag{2.5'}$$
$$= \sum_{i=1}^{r} \sum_{\ell=0}^{k} a_\ell Q_i(x_{n+1-\ell})\Delta G_{n+1-\ell}^{(i)}.$$

In addition, we have from (2.3) for the perturbations $\Delta G_n^{(i)}$ the recurrence relations

$$\sum_{\ell=0}^{k} a_\ell \Delta G_{n+1-\ell}^{(i)} + h_n \sum_{\ell=0}^{k} b_\ell R_i(x_{n+1-\ell}, f_{n+1-\ell})\Delta f_{n+1-\ell} = 0 \tag{2.8}$$
$$i = 1,2,\ldots,r.$$

By introducing the abbreviations

$$L_\ell = a_\ell I + h_n b_\ell P(x_{n+1-\ell}, f_{n+1-\ell}),$$

$$M_\ell^{(i)} = -a_\ell Q_i(x_{n+1-\ell}), \tag{2.9}$$

$$N_\ell^{(i)} = b_\ell h_n R_i(x_{n+1-\ell}, f_{n+1-\ell}),$$

and writing

$$\Delta G_n^{(0)} = \Delta f_n,$$

the relations (2.5') and (2.8) assume the form

$$\sum_{\ell=0}^{k} [L_\ell \Delta G_{n+1-\ell}^{(0)} + \sum_{i=1}^{r} M_\ell^{(i)} \Delta G_{n+1-\ell}^{(i)}] = 0,$$

$$\sum_{\ell=0}^{k} [N_\ell^{(i)} \Delta G_{n+1-\ell}^{(0)} + a_\ell \Delta G_{n+1-\ell}^{(i)}] = 0, \qquad i = 1,2,\ldots,r. \tag{2.10}$$

or more compactly

$$\sum_{\ell=0}^{k} \mathcal{B}_\ell \Delta \vec{G}_{n+1-\ell} = 0, \tag{2.11}$$

where

$$\Delta \vec{G}_{n+1-\ell} = (\Delta G_{n+1-\ell}^{(0)}, \ldots, \Delta G_{n+1-\ell}^{(r)})^T,$$

and

$$\mathcal{B}_\ell = \begin{bmatrix} L_\ell & M_\ell^{(1)} & \cdots & M_\ell^{(r)} \\ N_\ell^{(1)} & a_\ell I & & \\ \vdots & & \ddots & \\ N_\ell^{(r)} & & & a_\ell I \end{bmatrix}. \tag{2.12}$$

Assuming that $\mathcal{B}_0^{-1}$ exists, we write (2.11) as

(2.14) $DC_m = C_m D$ *for* $m = 1,\ldots,r,$

then

$$(2.15)\quad \det\begin{pmatrix} A & B_1 & \cdots & B_r \\ C_1 & D & & \\ \vdots & & \ddots & \\ C_r & & & D \end{pmatrix} = \det(AD - \sum_{m=1}^{r} B_m C_m)(\det D)^{r-1}.$$

The proof of this lemma may be found in [8].

THEOREM 2.1.

(i) *The eigenvalues of the matrix* (2.13) *satisfy*

$$(2.16a)\quad \sum_{\ell=0}^{k} a_\ell \zeta^{k-\ell} = 0$$

or

$$(2.16b)\quad \det\left\{ \sum_{\ell=0}^{k} \sum_{i=0}^{k} \left[a_\ell L_i - \sum_{m=1}^{r} M_i^{(m)} N_\ell^{(m)} \right] \zeta^{2k-\ell-i} \right\} = 0.$$

(ii) *Let the polynomial* $\sum_{\ell=0}^{k} a_\ell \zeta^{k-\ell}$ *satisfy the root condition. The scheme* (1.2) *is locally stable in the sense of definition* 2.2 *when the eigenvalues satisfying* (2.16b) *are strongly stable. In the special case where* $\partial K/\partial f$ *does not depend on* x, *the scheme* (1.2) *is locally stable when the eigenvalues satisfying*

$$(2.16c)\quad \det\left\{ \sum_{\ell=0}^{k} L_\ell \zeta^{k-\ell} \right\} = 0,$$

are strongly stable.

PROOF. Consider the matrix A_n given by (2.13). It is easily verified that the characteristic equation of A_n can be written in the form

$$(2.17)\quad \det(A_n - \zeta I) = \det(B_0^{-1})\det\left(\sum_{\ell=0}^{k} B_\ell \zeta^{k-\ell} \right)[\det(-I)]^k.$$

Definition For kernel functions of the class (2.2) scheme (1.2) satisfying (2.3) will be called *locally stable* at the point x_n with respect to the perturbations $\Delta g_n^{(1)}$ when all roots of (2.18) are within or on the unit circle, those on the unit circle having Jordan blocks of order 1.

Substitution of (2.12) into (2.17) gives the characteristic equation

$$(2.18)\quad \det \begin{pmatrix} \sum_0^k L_\ell \zeta^{k-\ell} & \sum_0^k M_\ell^{(1)} \zeta^{k-\ell} & \cdots & \sum_0^k M_\ell^{(r)} \zeta^{k-\ell} \\ \sum_0^k N_\ell^{(1)} \zeta^{k-\ell} & \sum_0^k a_{\ell I} \zeta^{k-\ell} & & \\ \vdots & & \ddots & \\ \sum_0^k N_\ell^{(r)} \zeta^{k-\ell} & & & \sum_0^k a_{\ell I} \zeta^{k-\ell} \end{pmatrix} = 0.$$

By observing that the matrix $\Sigma_0^k a_\ell \zeta^{k-\ell} I$ in (2.18) is a multiple of the unit matrix, and therefore commutes with all matrices of the same order, we obtain by virtue of lemma 2.1 that (2.18) may be reduced to

$$(2.19)\quad \det\left\{ \sum_{\ell=0}^{k} \sum_{i=0}^{k} \left[a_\ell L_i - \sum_{m=1}^{r} M_i^{(m)} N_\ell^{(m)} \right] \zeta^{2k-\ell-i} \right\} \cdot \left(\det\left\{ \sum_{\ell=0}^{k} a_{\ell I} \zeta^{k-\ell} \right\} \right)^{r-1} = 0,$$

from which (2.16a) and (2.16b) immediately follow.

In order to prove the second part of the theorem, we have to prove that the eigenvalues which satisfy (2.16a) are strongly or weakly stable. From the root condition it follows that all eigenvalues which satisfy (2.16a) are within or on the unit circle. Hence, it remains to show that the eigenvalues on the unit circle are weakly stable. Let $\tilde{\zeta}$ be a root of $\sum_{\ell=0}^{k} a_\ell \zeta^{k-\ell}$ with $|\tilde{\zeta}| = 1$. From the root condition it follows that $\tilde{\zeta}$ is simple. If the matrices in (2.12) have order s then $\tilde{\zeta}$ is a root of (2.19) with multiplicity s(r-1). The next step is to prove that there exist s(r-1) independent eigenvectors of A_n corresponding to the eigenvalue $\tilde{\zeta}$. Let $\vec{e}(\tilde{\zeta})$ be such an eigenvector with component vectors $(\vec{e}_1, \ldots, \vec{e}_k)$. Solving

$$A_n \vec{e}(\tilde{\zeta}) = \tilde{\zeta}\, \vec{e}(\tilde{\zeta})$$

we find

$$\vec{e}_1 = \tilde{\zeta}^{k-1}\vec{e}_k, \ldots, \vec{e}_{k-1} = \tilde{\zeta}\,\vec{e}_k$$

and

$$\left(\sum_{\ell=0}^{k} B_\ell \tilde{\zeta}^{k-\ell}\right)\vec{e}_k = \vec{0}. \tag{2.20}$$

Thus, the number of independent eigenvectors $\vec{e}(\tilde{\zeta})$ equals the number of independent vectors $\vec{e}_k$ which satisfy (2.20). Denoting the components of $\vec{e}_k$ by $(\vec{e}_k^{(0)}, \ldots, \vec{e}_k^{(r)})$ and solving (2.20) we find the system of equations

$$\left(\sum_{0}^{k} L_\ell \tilde{\zeta}^{k-\ell}\right)\vec{e}_k^{(0)} + \left(\sum_{0}^{k} M_\ell^{(1)} \tilde{\zeta}^{k-\ell}\right)\vec{e}_k^{(1)} + \ldots + \left(\sum_{0}^{k} M_\ell^{(r)} \tilde{\zeta}^{k-\ell}\right)\vec{e}_k^{(r)} = \vec{0}, \tag{2.21a}$$

$$\left(\sum_{0}^{k} N_\ell^{(m)} \tilde{\zeta}^{k-\ell}\right)\vec{e}_k^{(0)} = \vec{0}, \qquad m = 1, \ldots, r. \tag{2.21b}$$

Since each vector $\vec{e}_k^{(i)}$ has s components, i = 0,...,r, we have at most s(r+1) unknowns which must satisfy (2.21a)-(2.21b). Recall that we have to prove that s(r-1) unknowns can be chosen independently. This is achieved by choosing the components of $\vec{e}_k^{(0)}$ equal to zero, i.e. $\vec{e}_k^{(0)} = \vec{0}$, in which case (2.21b) is satisfied. The number unknowns is then reduced to sr, and we are left with the s equations

$$\left(\sum_{0}^{k} M_\ell^{(1)} \tilde{\zeta}^{k-\ell}\right)\vec{e}_k^{(1)} + \ldots + \left(\sum_{0}^{k} M_\ell^{(r)} \tilde{\zeta}^{k-\ell}\right)\vec{e}_k^{(r)} = \vec{0}. \tag{2.22}$$

From (2.22) it is immediate that s(r-1) components can be chosen arbitrarily, and therefore one can find s(r-1) independent vectors $\vec{e}_k$.

When $\partial K/\partial f$ does not depend on x, i.e. when $\partial K/\partial f$ in (2.2) is of the form P(y,f), we have $M_i^{(m)} = 0$. It is readily seen that in this case the eigenvalues satisfy (2.16a) or (2.16c), and one can prove along similar lines as above that the scheme is locally stable when the eigenvalues ζ satisfying (2.16c) are strongly stable. □

Using (2.9) we see that (2.16c) is identical with

$$\det\left\{\sum_{\ell=0}^{k}(a_\ell I+b_\ell h_n \frac{\partial K}{\partial f}(x_{n+1-\ell},x_{n+1-\ell},f_{n+1-\ell}))\zeta^{k-\ell}\right\} = 0. \tag{2.23}$$

Likewise, equation (2.16b) can completely be expressed in terms of the Jacobian matrix $\partial K/\partial f$ in a number of points close to (x_n,x_n,f_n). A straightforward calculation yields by substitution of L_i, $M_i^{(m)}$ and $N_\ell^{(m)}$

$$\det\left\{\sum_{i=0}^{k} a_i\zeta^{k-i}\left[\sum_{\ell=0}^{k}(a_\ell I+b_\ell h_n \frac{\partial K}{\partial f}(x_{n+1-i},x_{n+1-\ell},f_{n+1-\ell}))\zeta^{k-\ell}\right]\right\} = 0. \tag{2.16b'}$$

The problem now is how to derive practical criteria from theorem 2.1. When we proceed as in the stability analysis of integration methods for ordinary differential equations, the Jacobian matrices $K_f(x_{n+1-i},x_{n+1-\ell},f_{n+1-\ell})$, in the characteristic equation (2.23) are replaced by a locally constant matrix J (the "slowly varying Jacobian" approach), which leads to the characteristic equation

$$\sum_{\ell=0}^{k}(a_\ell + b_\ell z)\zeta^{k-\ell} = 0, \tag{2.24}$$

where z denotes an eigenvalue of $h_n J$. Since this equation is just the characteristic equation of the linear multistep method with coefficients a_ℓ and b_ℓ when it is applied to the differential equation $df/dx = Jf$, stability criteria can directly be derived from the stability theory for ordinary differential equations. This immediately suggests to choose scheme (1.2) such that it corresponds to a multistep method with good stability properties. Such methods are the Curtiss-Hirschfelder or backward differentiation formulas [4] defined by

$$a_0 = -1, \quad \sum_{\ell=1}^{k}(1-\ell)^j a_\ell + jb_0 = 1, \qquad j = 0,1,\ldots,k,$$

$$b_\ell = 0, \qquad \ell = 1,2,\ldots,k.$$

The stability regions of these formulas contain the whole left half plane for $k \leq 2$ and almost the whole left half plane (except for a small region near the imaginary axis) for $k = 3,4,5$ and 6. In order to make use of these

excellent stability properties one should find the corresponding weights $w_{n,j}$ by solving the relations (2.3) and (2.6). In [13] solutions are given and the resulting quadrature formulas are investigated.

We should bear in mind, however, that the replacement of $K_f(x_{n+1-i}, x_{n+1-\ell}, f_{n+1-\ell})$ by a constant matrix J is dubious when the Jacobian matrix is a rapidly changing function of x, y and f. In order to obtain more rigorous stability criteria additional information about the integral equation should be provided.

In section 2.3, stability results will be derived in terms of the eigenvalues of the Jacobian matrices $K_f(x_{n+1-i}, x_{n+1-\ell}, f_{n+1-\ell})$ for two specific classes of kernel functions and a specific integration scheme. Firstly, however, we describe in the next section an approach to generate recurrence relations with a fixed number of terms only containing perturbations Δf_j.

2.2. Recurrence relations without additional perturbations

When the Jacobian matrix of the kernel function has the form

$$\frac{\partial K}{\partial f}(x,y,f) = P(y,f) + xR(y,f) \tag{2.25}$$

it is possible to obtain a recurrence relation only containing a fixed number of perturbations Δf_j. This will be shown as follows. For kernel functions satisfying (2.25) relation (2.4) can be written in the form

$$\begin{aligned} \Delta f_{n+1-\ell} = & \sum_{j=0}^{n+1} w_{n+1-\ell,j}\{P(x_j,f_j) + x_{n+1}R(x_j,f_j)\}\Delta f_j \\ & - \ell h \sum_{j=0}^{n+1} w_{n+1-\ell,j}R(x_j,f_j)\Delta f_j, \qquad n+1-\ell \geq k,\ 0 \leq \ell \leq k, \end{aligned} \tag{2.26}$$

where we have assumed $h_n = h$, i.e. a constant step size. Taking suitable linear combinations of (2.26) and using (2.3) and (2.6) we obtain the relations

$$\sum_{\ell=0}^{k} a_\ell \Delta f_{n+1-\ell} +$$

$$+ h \sum_{\ell=0}^{k} b_\ell \{P(x_{n+1-\ell}, f_{n+1-\ell}) + x_{n+1} R(x_{n+1-\ell}, f_{n+1-\ell})\} \Delta f_{n+1-\ell} \tag{2.27}$$

$$+ h \sum_{\ell=0}^{k} \ell a_\ell \sum_{j=0}^{n+1} w_{n+1-\ell,j} R(x_j, f_j) \Delta f_j = 0, \qquad n \geq 2k-1.$$

Since (2.27) holds for all $n \geq 2k-1$ we may write down $k+1$ consecutive relations as follows

$$\sum_{\ell=0}^{k} a_\ell \Delta f_{n+1-i-\ell} + h \sum_{\ell=0}^{k} b_\ell \{P(x_{n+1-i-\ell}, f_{n+1-i-\ell}) +$$

$$+ x_{n+1-i} R(x_{n+1-i-\ell}, f_{n+1-i-\ell})\} \Delta f_{n+1-i-\ell} +$$

(2.28)

$$+ h \sum_{\ell=0}^{k} \ell a_\ell \sum_{j=0}^{n+1-i} w_{n+1-i-\ell,j} R(x_j, f_j) \Delta f_j = 0,$$

$$n+1-i \geq 2k, \quad 0 \leq i \leq k.$$

Again taking linear combinations of (2.28) yields the relations

$$\sum_{i=0}^{k} a_i \sum_{\ell=0}^{k} [a_\ell + h b_\ell \{P(x_{n+1-i-\ell}, f_{n+1-i-\ell}) +$$

$$+ x_{n+1-i} R(x_{n+1-i-\ell}, f_{n+1-i-\ell})\}] \Delta f_{n+1-i-\ell} +$$

(2.29)

$$+ h \sum_{i=0}^{k} a_i \sum_{\ell=0}^{k} \ell a_\ell \sum_{j=0}^{n+1-i} w_{n+1-i-\ell,j} R(x_j, f_j) \Delta f_j = 0,$$

$$n \geq 3k-1.$$

By interchanging the summations of the last term of the left-hand side of (2.29) this term reduces to

$$h \sum_{j=0}^{n+1} \sum_{\ell=0}^{k} \ell a_\ell \Big(\sum_{i=0}^{k} a_i w_{n+1-i-\ell,j} \Big) R(x_j, f_j) \Delta f_j =$$

$$h \sum_{\ell=0}^{k} \ell a_\ell \sum_{j=0}^{n+1-\ell} \Big(\sum_{i=0}^{k} a_i w_{n+1-i-\ell,j} \Big) R(x_j, f_j) \Delta f_j =$$

$$- h^2 \sum_{\ell=0}^{k} \ell a_\ell \sum_{i=0}^{k} b_i R(x_{n+1-i-\ell}, f_{n+1-i-\ell}) \Delta f_{n+1-i-\ell},$$

where we have used (2.3) and (2.6). Substitution into (2.29) yields the recurrence relation

$$\sum_{i=0}^{k} a_i \sum_{\ell=0}^{k} \Big[a_\ell I + h b_\ell \{ P(x_{n+1-i-\ell}, f_{n+1-i-\ell}) + (x_{n+1-i} - ih) R(x_{n+1-i-\ell}, f_{n+1-i-\ell}) \} \Big] \Delta f_{n+1-i-\ell} = 0, \tag{2.30}$$

$$n \geq 3k-1.$$

Note that Δf_{n+1} only depends on Δf_j for $n+1-2k \leq j \leq n$. As in section 2.1 we write this recurrence relation in the form

$$(\Delta f_{n+1}, \ldots, \Delta f_{n+2-2k})^T = A_n^* (\Delta f_n, \ldots, \Delta f_{n+1-2k})^T, \tag{2.30'}$$

where A_n^* is completely determined by (2.30). The definition of local stability, given in section 2.1, is now restricted to kernel functions satisfying (2.25) and to matrices of the form A_n^*. From (2.30) we finally have the following analogue of theorem 2.1.

THEOREM 2.2.

(i) *The eigenvalues of the matrix* A_n^* *(in (2.30')) satisfy*

$$\det\Big\{ \sum_{i=0}^{k} a_i \zeta^{k-i} * \sum_{\ell=0}^{k} \Big(a_\ell I + b_\ell h \frac{\partial K}{\partial f}(x_{n+1-2i}, x_{n+1-i-\ell}, f_{n+1-i-\ell}) \Big) \zeta^{k-\ell} \Big] \Big\} = 0 \tag{2.31}$$

(ii) *Let the polynomial* $\sum_{\ell=0}^{k} a_\ell \zeta^{k-\ell}$ *satisfy the root condition, then the scheme* (1.2) *is locally stable in the sense of definition* (2.2) *when the eigenvalues satisfying* (2.31) *are strongly stable.*

Comparing (2.31) and (2.16b') we see that in (2.31) more of the "history" of $\frac{\partial K}{\partial f}$ is taken into account. However, when the Jacobian matrix $\frac{\partial K}{\partial f}$ is locally approximated by a constant matrix J it is easily seen that (2.31) reduces to (2.24).

We remark that the analysis presented in this section can be generalized for the class of kernel functions satisfying

$$\frac{\partial K}{\partial f}(x,y,f) = P(y,f) + \sum_{i=1}^{r} x^i R_i(y,f),$$

by repeatly taking suitable linear combinations. The resulting recurrence relation for Δf_{n+1} contains $k(r+1) + 1$ terms Δf_j.

2.3. Derivation of stability conditions

In the derivation of stability conditions from the theorems 2.1 and 2.2 the following lemma is frequently used:

LEMMA 2.2. *Let* $F(\zeta)$ *be a matrix-valued function of the scalar* ζ *with eigenvalues* $\phi_j(\zeta)$, $j = 1,2,\ldots,s$. *Then the roots of the equation*

$$\det[F(\zeta)] = 0$$

are within (or on) the unit circle when the roots of the equations

$$\phi_j(\zeta) = 0, \qquad j = 1,2,\ldots,s$$

are within (or on) the unit circle.

PROOF. Let $\tilde{\zeta}$ be a root of $\det[F(\zeta)] = 0$ then the matrix $F(\tilde{\zeta})$ necessarily has a zero eigenvalue. Since the eigenvalues of $F(\tilde{\zeta})$ are of the form $\phi_j(\tilde{\zeta})$ we have $\phi_j(\tilde{\zeta}) = 0$ for some j. Thus, by requiring that all roots ζ of $\phi_j(\zeta) = 0$ satisfy $|\zeta| \le 1$ for all j, the roots of $\det[F(\zeta)] = 0$ certainly are within (or on) the unit circle. □

2.3.1. Jacobian matrices with locally constant eigensystems

When the eigensystems of the matrices $K_f(x_{n+1-i}, x_{n+1-\ell}, f_{n+1-\ell})$ coincide for $i,\ell = 0,1,\ldots,k$ (e.g. in case of *scalar* integral equations), it is immediate from theorem 2.1 and lemma 2.2 that we have local stability if the roots ζ of the equation

$$\sum_{i,\ell=0}^{k} a_i[a_\ell + b_\ell z_{n+1-i,n+1-\ell}]\zeta^{2k-i-\ell} = 0, \tag{2.32}$$

satisfy $|\zeta| < 1$ for all eigenvalues $z_{n+1-i,n+1-\ell}$ of $h_n K_f(x_{n+1-i}, x_{n+1-\ell}, f_{n+1-\ell})$.

For small values of k this equation easily gives the stability region in the eigenvalue space $\{z_{n+1-i,n+1-\ell}\}_{i,\ell=0}^{k}$. We shall illustrate this by analyzing the trapezoidal rule defined by

$$2w_{n,0} = w_{n,1} = w_{n,2} = \ldots = w_{n,n-1} = 2w_{n,n} = h. \tag{2.33}$$

This quadrature rule satisfies (2.3) with $k = 1$, $a_0 = -a_1 = -1$. From this it follows that $b_0 = b_1 = \frac{1}{2}$, so that equation (2.32) assumes the form

$$(1 - \tfrac{1}{2} z_{n+1,n+1})\zeta^2 - (2 + \tfrac{1}{2} z_{n+1,n} - \tfrac{1}{2} z_{n,n+1})\zeta + (1 + \tfrac{1}{2} z_{n,n}) = 0. \tag{2.34}$$

Let the eigenvalues z be real then by the Hurwitz criterion we arrive at the stability region

$$\begin{aligned} &z_{n+1,n+1} < 0, \\ &z_{n+1,n+1} + z_{n,n} < 0, \\ &z_{n+1,n+1} - z_{n,n} + z_{n+1,n} - z_{n,n+1} < 0, \\ &z_{n+1,n+1} - z_{n,n} + z_{n,n+1} - z_{n+1,n} < 8, \end{aligned} \tag{2.35}$$

Next we consider the stability conditions resulting from the analysis presented in section 2.2. From theorem 2.2 and lemma 2.2 it follows that we

have local stability if the roots of the equation

$$(2.36)\qquad \sum_{i,\ell=0}^{k} a_i[a_\ell + b_\ell z_{n+1-2i,n+1-i-\ell}]\zeta^{2k-i-\ell} = 0,$$

satisfy $|\zeta| < 1$ for all eigenvalues $z_{n+1-2i,n+1-i-\ell}$. In the case of the trapezoidal rule we arrive at the stability region

$$(2.37)\qquad \begin{aligned} &z_{n+1,n+1} < 0,\\ &z_{n+1,n+1} + z_{n-1,n-1} < 0,\\ &z_{n+1,n+1} - z_{n-1,n-1} + z_{n+1,n} - z_{n-1,n} < 0,\\ &z_{n+1,n+1} - z_{n-1,n-1} - z_{n+1,n} + z_{n-1,n} < 8. \end{aligned}$$

It is not surprising that the regions defined by (2.35) and (2.37) are different because the spaces of perturbations are different.

The preceding derivations become increasingly difficult for larger values of k. In such cases one may get a rough impression of the stability region by applying the "slowly varying Jacobian" approach mentioned above. In case of the trapezoidal rule this would give the familiar condition (for complex eigenvalues)

$$(2.35')\qquad \operatorname{Re} z_{n+1,n+1} < 0.$$

Although the conditions resulting from (2.32) and (2.36) depend on n, i.e. only have a local meaning, there is an important class of kernel functions for which the analysis of section 2.1 and 2.2 may give conditions independent of n. This is investigated in the next section.

2.3.2. Convolution kernels

An important class of integral equations has kernels of the form

(2.38) $\quad K(x,y,f) = k^*(x-y)Af,$

where k^* is a polynomial in $(x-y)$ and A is a matrix with constant elements. Evidently the Jacobian of (2.38) can be presented in the finitely decomposable form (2.2). Furthermore, the eigensystem of $\partial K/\partial f$ does not depend on x, y and f so that we arrive at the characteristic equation (2.32) with

$$z_{n+1-i,n+1-\ell} = h_n k^*(x_{n+1-i} - x_{n+1-\ell})\alpha$$

where α runs through the eigenvalues of A. In the case where constant integration steps h are used equation (2.32) reduces to

$$(2.39) \qquad \sum_{i,\ell=0}^{k} a_i[a_\ell + b_\ell hk^*((\ell-i)h)\alpha]\zeta^{2k-i-\ell} = 0.$$

Note that the characteristic equation (2.39) is independent of n and hence the conditions for local stability will not depend on n. Secondly, we note that the analysis of section 2.2 can be applied only when $k^*(x-y) = \gamma_1+\gamma_2(x-y)$. Therefore, in order to compare the results of section 2.1 and 2.2, we will derive stability conditions when the scheme is applied to such kernel functions. It is easily verified that for such kernel functions (2.31) is identical to (2.39) and has the form

$$(2.39') \qquad \sum_{i=0}^{k} a_i\zeta^{k-i} \sum_{\ell=0}^{k} [a_\ell + b_\ell h\alpha\gamma_1]\zeta^{k-\ell} + h^2\alpha\gamma_2 \sum_{i,\ell=0}^{k} a_i b_\ell(\ell-i)\zeta^{2k-i-\ell} = 0.$$

The second double sum in this equation is due to taking into account the variation of the Jacobian matrix with x and y. Especially, when γ_1 is small, i.e. $\gamma_1 = O(h)$, these terms cannot be neglected so that equation (2.39') may differ considerably from the "multistep equation" (2.24).

Finally, we give the conditions for local stability of the trapezoidal rule in the case of a convolution kernel (compare (2.37)).

$$(2.37') \qquad h\alpha\gamma_1 < 0, \quad h^2\alpha\gamma_2 < 0, \quad h^2\alpha\gamma_2 > -4.$$

From the last condition we conclude that the stepsize h is *restricted* by $h^2 < \frac{4}{|\alpha\gamma_2|}$, α being an eigenvalue of A. Numerical experiments, reported in the next section, confirm this result.

3. NUMERICAL ILLUSTRATION

In this section we will verify the stability analysis when applied to the trapezoidal rule. In particular we are interested in the difference between conditions (2.35) and (2.37) resulting from a different analysis. It should be noted however that (2.37) is applicable only if $K_{xxf} = 0$.

In order to illustrate the analysis we specify a number of scalar integral equations. For each problem we will check the conditions for stability yielding a prediction for stable or unstable computation. A final numerical experiment will verify this prediction. All problems were solved using a constant stepsize h, the range of integration was 100h.

Problem 1:

$$K(x,y,f) = (-a + bx + cy)f;$$

$$g(x) = (1-c)\sin x + a - bx + ((b+c)x - a)\cos x$$

solution $f(x) = \sin x$.

For this set of problems the (local) stability conditions (2.35) and (2.37) are

$$(3.1) \qquad (b+c)(x_n+h) < a;\ (b+c)(x_n+\tfrac{1}{2}h) < a;\ bh^2 < 0;\ ch^2 < 4,$$

and

$$(3.2) \qquad (b+c)(x_n+h) < a;\ (b+c)x_n < a;\ 2bh^2+ch^2 < 0;\ ch^2 < 4.$$

Note that (3.1) is more stringent that (3.2) as it allows the parameter b only to be negative. We have chosen the following values of the parameters:

1a) $a = 1001, \quad b = -900, \quad c = 1000, \quad h = 0.1$

The conditions (3.1) and (3.2) predict instability. The numerical solution was indeed unstable. The true error was amplified by a factor of approximately -4.

1b) $a = 1501, \quad b = -50, \quad c = 200, \quad h = 0.1.$

Condition (3.1) predicts stability, whereas (3.2) predicts an unstable behaviour. No severe instabilities were developed during the computation, only a small increase in the absolute error was detected. Hence, the numerical solution did not give a decisive answer to the question whether it was stable or not. In fact, it was difficult to find an example for which the numerical solution was strongly unstable.

1c) $a = 1, \quad b = -400, \quad c = 400, \quad h = 0.1.$

Conditions (3.1) and (3.2) reveal that for this choice of the parameters we have a point on the boundary of the stability region. Indeed, inspection of the true error confirmed that the amplification factor was approximately -1.

1d) convolution kernel. $a > 0 \quad b < a \quad h < \frac{2}{|b|}$

$a = 1/4, \quad b = -320, \quad c = 320, \quad h = 1/8.$

For convolution kernels conditions (3.1) and (3.2) coincide and predict instability. In every step, the absolute error was amplified by a factor $\simeq -2.8$, indicating a severe instability.

1e) convolution kernel

$a = 1/4, \quad b = -128, \quad c = 128, \quad h = 1/8.$

Both conditions predict stability. The numerical results confirmed this behaviour.

Problem 2. (nonlinear)

$$K(x,y,f) = -x^2 f^3; \quad g(x) = x^2 + \frac{1}{7} x^9$$

solution: $f(x) = x^2$, $h = 0.1$.

It is easily seen that (2.37) gives no decisive answer, since it is not applicable, (2.35) predicts stability. No instabilities were developed during the computation.

From these experiments we conclude that the stability conditions (2.35) and (2.37) give a good prediction for the global numerical behaviour, although they result from a local analysis.

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Analysis of Numerical Methods for Second Kind Volterra Equations by Imbedding Techniques

P. H. M. Wolkenfelt and P. J. van der Houwen

Numerical Mathematics Department, Mathematisch Centrum, Amsterdam, The Netherlands

Chr. T. H. Baker

Department of Mathematics, University of Manchester, Manchester, England

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 (nonlinear) 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 can exploit by pursuing the stability approach for numerical methods applied to differential equations.

1. Introduction

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

$$f(x)=g(x)+\int_0^x K(x, y, f(y))\,dy, \qquad 0\leqslant x\leqslant X, \tag{1.1}$$

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

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

(cf. Baker and Keech [4], van der Houwen [7]) to rather general kernel functions of the form (cf. van der Houwen and Wolkenfelt [8], Baker [3])

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

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 and Wolkenfelt [9] this approach is described for a class of direct quadrature methods. [Quadrature methods that may be obtained by applying quadrature rules of the form

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

to discretize (1.1) yield equations of the form

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

for values $\tilde{f}_n$ approximating $f(nh)$, $n=1,2,\ldots$, with given $\tilde{f}_0=f(0)=g(0)$.] In the present paper the analysis outlined in Ref. [9] is developed and extended to a larger class of methods using the insight obtained 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 relation 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

$$\Psi(t, x)=g(x)+\int_0^t K(x, y, f(y))\, dy, \qquad 0 \leqslant t,\ x \leqslant X, \tag{1.4}$$

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

$$f(x)=\Psi(x,x), \tag{1.5}$$

we may write (1.4) as

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

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, Sec. V])

$$\left.\begin{aligned}\frac{d}{dt}\Psi(t,x)&=K(x,t,\Psi(t,t))\\ \Psi(0,x)&=g(x)\end{aligned}\right\},\qquad 0\leqslant x,\ t\leqslant X. \tag{1.7}$$

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 Sec. 2.1.2 and 2.2.2). When such an identification is not possible (see, e.g. Sec. 2.3) then convergence must be established by other means. In Ref. [14] this is done by constructing quadrature rules from convergent linear multistep methods and by verifying the conditions of a general convergence theorem for second kind Volterra integral equations (see Ref. [1, Chap. 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 $a_0=1$) adapted to (1.7). Then we construct a scheme of the form

$$\sum_{j=0}^{k}\left[a_j\tilde{\psi}_{n+1-j}(x)+b_j hK\big(x,\eta_{n+1-j},\tilde{\psi}_{n+1-j}(\eta_{n+1-j})\big)\right]=0,$$
$$n=k-1,k,\ldots,N-1, \tag{2.1}$$

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

$$\tilde{\psi}_{n+1}(\eta_{n+1}) + b_0 hK\big(\eta_{n+1}, \eta_{n+1}, \tilde{\psi}_{n+1}(\eta_{n+1})\big)$$

$$= -\sum_{j=1}^{k} \Big[a_j \tilde{\psi}_{n+1-j}(\eta_{n+1}) + b_j hK\big(\eta_{n+1}, \eta_{n+1-j}, \tilde{\psi}_{n+1-j}(\eta_{n+1-j})\big)\Big], \tag{2.2}$$

and then writing

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

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 $x = \eta_{n+1}, \eta_{n+2}, \ldots, \eta_N$. 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, formulas of the form

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

where ω_{nj} $(j = 0, 1, \ldots, n,\ n = 1, 2, \ldots, N)$ are given weight parameters and 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* $n \geqslant k-1$)

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

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

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*

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

PROOF. The proof is straightforward on verifying by substitution that

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

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 $\tilde{\psi}_{n+1}(\eta_{n+1})$.[1] □

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

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

Evidently, conditions (2.5) are satisfied when we choose $k=2$, $a_0=-1$, $a_1=1$, $a_2=0$, $b_0=\frac{5}{12}$, $b_1=\frac{8}{12}$, and $b_2=-\frac{1}{12}$. 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 kth order Gregory scheme for the integral equation (1.1) may be identified with a kth order Adams–Moulton method for Eq. (1.7), provided that the required starting functions are properly chosen. Of course, this correspondence is a consequence of the

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

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].

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

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

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

2.2.1. Integration by Runge–Kutta Methods

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

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

(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 that may be written in the form

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

for each x, where the parameters θ_s, β_{rs}, and c_s specify the Runge–Kutta method (a survey of all kinds of formulas can be found in Lambert [10] and Lapidus and Seinfeld [11]).

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

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

$$r=0,1,\ldots,p-1, \quad (2.12a)$$

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

$$n=0,1,\ldots,N-1. \quad (2.12b)$$

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

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

then (2.12a, b) can be written

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

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 motivation). Therefore, we shall 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 Sec. 2.1.1.

2.2.2. Equivalence with Runge–Kutta Type Quadrature Methods

From (2.14) one derives that

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

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

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

yields the scheme

$$\tilde{f}_{n(p+1)+r}=g(\eta_{n(p+1)+r})+h\sum_{j=0}^{n-1}\sum_{s=0}^{p}\beta_{ps}K\left(\eta_{n(p+1)+r},\eta_{j(p+1)+s},\tilde{f}_{j(p+1)+s}\right)$$

$$+h\sum_{s=0}^{p}\beta_{rs}K\left(\eta_{n(p+1)+r},\eta_{n(p+1)+s},\tilde{f}_{n(p+1)+s}\right), \tag{2.16}$$

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 (Ref. [1]) do not fall within the class considered in Sec. 2.2.1, but they are included in the general setting presented in Sec. 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 differential equations. Therefore, the imbedding technique (which produces an ordinary differential equation) does not generate any new methods of this kind. However, in the 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 that are based on backward differentiation formulas (also known as Curtiss–Hirschfelder formulas). These formulas are among those recommended[2] 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 formulas for the integration of (1.1). The coefficients of these formulas are defined by

$$a_0=1,\qquad \sum_{r=1}^{q}(1-r)^j a_r+jb_0=-1,\qquad j=0(1)q.$$

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).

[2] However, one should bear in mind the possibility of "over-stability."

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 Sec. 2.1 and 2.2. Such extensions yield equations of the form

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

where $\tilde{f}_n\simeq f(\eta_n)$ and, for example, $\eta_0=0$, $\tilde{f}_0=g(0)$, $\eta_j=ih+\theta_r h$ $(i=0,1,\ldots,N-1, r=0,1,\ldots,p)$, with $i=[(j-1)/(p+1)]$, $r\equiv(j-1) \bmod(p+1)$ ($[z]$ denotes the integer part of z). For (semi-) explicit methods $m\{n+1\}=n+1$, while for block-by-block methods typified by those of Linz and those of de Hoog and Weiss (Baker [1, Sec. 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 (to yield, for example, 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 abscissas), 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 Eq. (1.1) reduces to an initial value problem of the form

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

In this case the quadrature methods considered in Sec. 2.1.2 reduce to linear multistep methods for solving (3.2). Hence, it is not surprising that Eqs. (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 form

$$\sum_{j=0}^{k}\left\{\mathbf{A}_j\tilde{\boldsymbol{\phi}}_{n+1-j}+h\mathbf{B}_j\tilde{\boldsymbol{\kappa}}_{n+1-j}\right\}=\mathbf{0},\qquad (3.3)$$

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

$$\tilde{\phi}_j = \left[\tilde{f}_m, \ldots, \tilde{f}_{m+p} \right]^T, \qquad m = j(p+1), \tag{3.4}$$

and

$$\tilde{\kappa}_j = \left[F(\eta_m, \tilde{f}_m), \ldots, F(\eta_{m+p}, \tilde{f}_{m+p}) \right]^T, \qquad m = j(p+1), \tag{3.5}$$

and the matrices $\{\mathbf{A}_j, \mathbf{B}_j\}_{j=0}^k$ 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

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

(compare, for example, the cyclic linear multistep methods of Donelson and Hansen [5, p. 138]; see also Stetter [13, Sec. 4.3]).

Let us now apply the method associated with (3.3) to Eq. (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

$$\sum_{j=0}^{k} \left\{ \mathbf{A}_j \tilde{\phi}_{n+1-j}(x) + h \mathbf{B}_j \tilde{\kappa}_{n+1-j}(x) \right\} = \mathbf{0}, \qquad (n \geqslant k-1), \tag{3.6}$$

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

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

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

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

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

$$\tilde{\phi}_{n+1}(x)=g(x)\mathbf{e}+h\sum_{j=0}^{n+1}\mathbf{V}_{n+1,j}\tilde{\kappa}_j(x) \tag{3.9}$$

where $\mathbf{e}=[1,1,\ldots,1]^{\mathrm{T}}$. We have the following result.

Theorem 3.1. *If there exist fixed matrices* $\{\mathbf{A}_j,\mathbf{B}_j\}_{j=0}^{k}$ *such that (for* $n \geqslant k-1$)

$$\begin{aligned}
&\sum_{i=0}^{k}\mathbf{A}_i\mathbf{V}_{n+1-i,j}=\mathbf{0} && (j=0,1,\ldots,n-k),\\
&\sum_{i=0}^{k}\mathbf{A}_i\mathbf{V}_{n+1-i,j}=-\mathbf{B}_{n+1-j} && (j=n-k+1,\ldots,n+1),\\
&\sum_{i=0}^{k}\mathbf{A}_i\mathbf{e}=\mathbf{0}, &&
\end{aligned} \tag{3.10}$$

then (3.6) *follows from* (3.9).

To illustrate, it frequently occurs, in practice, that

$$[\Omega_{nj}]=\begin{bmatrix}
\vdots & \vdots & \vdots & & & & & & & \\
\mathbf{W} & \mathbf{W}_0 & \mathbf{W}_1 & & \cdots & \mathbf{W}_{k-1} & \mathbf{W}_k & & & \\
\mathbf{W} & \mathbf{W}_0 & \mathbf{W}_0 & \mathbf{W}_1 & \cdots & \mathbf{W}_{k-2} & \mathbf{W}_{k-1} & \mathbf{W}_k & & \\
\mathbf{W} & \mathbf{W}_0 & \mathbf{W}_0 & \mathbf{W}_0 & \cdots & \mathbf{W}_{k-3} & \mathbf{W}_{k-2} & \mathbf{W}_{k-1} & \mathbf{W}_k & \\
\vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots &
\end{bmatrix},$$

where $\mathbf{W},\mathbf{W}_0,\mathbf{W}_1,\ldots,\mathbf{W}_k$ are fixed matrices, so that for $n=k,k+1,\ldots$

$$\mathbf{V}_{n+1,r}=\begin{cases}
\mathbf{W}_{k+r-n-1} & \text{if } n+1-k\leqslant r\leqslant n+1\\
\mathbf{W}_0 & \text{if } 1\leqslant r\leqslant n-k\\
\mathbf{W} & \text{if } r=0.
\end{cases}$$

Then appropriate matrices $\{\mathbf{A}_j,\mathbf{B}_j\}_{j=0}^{k}$ 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 Sec. 3.1, Eq. (3.6) results from discretizing Eq. (1.7) with an appropriate method, and Eq. (1.7) results from imbedding (1.1) in

(1.6). We may instead take as our starting point Eq. (3.1) in the form

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

and imbed this equation in

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

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

Since $\tilde{\psi}_{n+1}(x)=\tilde{\Psi}(\eta_{n+1},x)$, Eq. (3.12) defines a function $\tilde{\Psi}(t,x)$ for $t=\eta_0,\eta_1,\ldots$; instead of differentiating $\tilde{\Psi}(t,x)$ with respect to t [as was undertaken for $\Psi(t,x)$ in Section 1.1] we can apply a differencing technique (in the variable t) associated with the matrices $\mathbf{A}_j$ to form $\Sigma_{j=0}^{k}\mathbf{A}_j\tilde{\boldsymbol{\phi}}_{n+1-j}(x)$ 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 Sec. 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 Sec. 4.2 the ideas are extended to the more general class of methods of Sec. 3.

4.1.1. Linear Multistep Methods

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

$$\sum_{j=0}^{k}\left[a_j\Delta\tilde{\psi}_{n+1-j}(x)+hb_jJ_{n+1-j}(x)\Delta\tilde{\psi}_{n+1-j}(\eta_{n+1-j})\right]=0, \tag{4.1}$$

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

$$C_j\colon \phi(x)\to a_j\phi(x)+b_jhJ_{n+1-j}(x)\phi(\eta_{n+1-j}). \tag{4.2}$$

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

$$a_0\phi(x)+b_0hJ_{n+1}(x)\phi(\eta_{n+1})=\chi(x). \tag{4.3}$$

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

$$\phi(\eta_{n+1})=\left[a_0+hb_0J_{n+1}(\eta_{n+1})\right]^{-1}\chi(\eta_{n+1}), \tag{4.4}$$

unless $[a_0+hb_0J_{n+1}(\eta_{n+1})]=0$ (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

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

or equivalently,

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

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

$$\Delta\mathbf{v}_{n+1}(x)=\left[\Delta\tilde{\psi}_{n+1}(x),\ldots,\Delta\tilde{\psi}_{n+2-k}(x)\right]^{\mathrm{T}}$$

and the *amplification* operator M_n is given by

$$M_n=\begin{bmatrix} -C_0^{-1}C_1 & -C_0^{-1}C_2 & \cdots & -C_0^{-1}C_{k-1} & -C_0^{-1}C_k \\ 1 & & & & \\ & 1 & & 0 & \\ & & \ddots & & \\ 0 & & & 1 & 0 \end{bmatrix}. \tag{4.7}$$

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

$$\Delta\boldsymbol{\nu}_{n+1}^{\#}=\mathbf{M}_n^{\#}\Delta\boldsymbol{\nu}_n^{\#},$$

where

$$\Delta\boldsymbol{\nu}_n^{\#}=\left[\Delta\tilde{\psi}_n,\ldots,\Delta\tilde{\psi}_{n+1-k}\right]^{\mathrm{T}}$$

and

$$\Delta\tilde{\psi}_n=\left[\Delta\tilde{\psi}_n(\eta_0),\ldots,\Delta\tilde{\psi}_n(\eta_N)\right]^{\mathrm{T}}.$$

The operator $\mathbf{M}_n^{\#}$ 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 $\mathbf{C}_j^{\#}$, where

$$\mathbf{C}_j^{\#}=\left[a_j\delta_{is}+hb_jJ_{n+1-j}(\eta_i)\delta_{i,i+s-(n+1-j)}\right]_{i,s=0}^{N};$$

here, δ_{is} denotes the Kronecker symbol. For such a matrix operator, the location of the eigenvalues of $\mathbf{M}_n^{\#}$ gives an indication of the stability

behavior 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 $\mathbf{R}(\zeta)$ be the matrix with elements

$$r_{ij}=\rho(\zeta)\delta_{ij}+b_j hJ_{n+1-j}(\eta_{n+1-i})\zeta^{k-j}, \qquad i,j=0,1,\ldots,k,$$

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*

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

PROOF. Let $\mathbf{e}(x)=[e_1(x),\ldots,e_k(x)]^{\mathrm{T}}$ be an eigenfunction of M_n with eigenvalue ζ. We first construct the function $\mathbf{e}$, and ζ. The equation $M_n\mathbf{e}=\zeta\mathbf{e}$ for $\mathbf{e}=\mathbf{e}(x)$ leads to the expression

$$\mathbf{e}(x)=e(x)\left[\zeta^{k-1},\zeta^{k-2},\ldots,\zeta,1\right]^{\mathrm{T}}, \tag{4.9}$$

where $e(x)$ satisfies

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

Substitution of (4.2) yields

$$\sum_{j=0}^{k}\left[a_j e(x)+hb_j J_{n+1-j}(x)e(\eta_{n+1-j})\right]\zeta^{k-j}=0. \tag{4.11}$$

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

$$\sum_{j=0}^{k}\left[a_j e(\eta_{n+1-i})+hb_j J_{n+1-j}(\eta_{n+1-i})e(\eta_{n+1-j})\right]\zeta^{k-j}=0,$$

$$i=0,1,\ldots,k, \tag{4.12}$$

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 nontrivial solution is obtained if the matrix of coefficients has a zero-determinant, i.e., if the eigenvalue ζ satisfies the

"auxiliary" or characteristic equation

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

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 $\mathbf{e}(x)$ can be derived by virtue of (4.9). □

REMARKS.

(i) Recall that Eq. (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 $\Delta\tilde{\psi}_{n+1-j}(x)$ in (4.1) by $\zeta^{n+1-j}e(x)$, then we obtain Eq. (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 Sec. 4.1.2 and 4.2 this approach will be followed.

(ii) Let $\tilde{\mathbf{R}}(\zeta)$ be the $(k+1-\mu)*(k+1-\mu)$ matrix obtained from $\mathbf{R}(\zeta)$ by omitting the jth row and the jth 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

$$\{\rho(\zeta)\}^{\mu}\det\{\tilde{\mathbf{R}}(\zeta)\}=0. \tag{4.8′}$$

(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 and 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 and 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 $(0\leqslant i\leqslant k)$ and $b_j=0$ for $j\neq i$ (cf. the midpoint rule, backward differentiation

methods), then we obtain from (4.8′) the equation

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

(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 that is similar to (4.8) with J_n replaced by Jacobian matrices $\mathbf{J}_n$. Only by assuming that these Jacobians can be diagonalized by the same set of eigenvectors is a reduction to (4.8) possible with $\mathbf{J}_n$ replaced by an eigenvalue that 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 $j=1,2,\ldots,k$. However, in actual computations we only calculate $\tilde{\psi}_n(x_i)$, $i=n, n+1,\ldots,N$, $n=k, k+1,\ldots, N$, so that one is inclined to put $\Delta\tilde{\psi}_{n+1-j}(x)=0$ for $x<x_{n+1-j}, j=1,2,\ldots,k$. 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

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

where $\xi_{n+1}^s=nh+\theta_s$ 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) we substitute a trial solution of the form $\zeta^{n+1}[e_0(x),\ldots,e_p(x)]^{\mathrm{T}}$ and arrive at the equations

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

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

$$\boldsymbol{\varepsilon}_p-\zeta\left\{\boldsymbol{\varepsilon}_r-h\sum_{s=0}^{p}\beta_{rs}\mathbf{P}_s\boldsymbol{\varepsilon}_s\right\}=\mathbf{0}\qquad(r=0,1,\ldots,p),$$

where $\boldsymbol{\varepsilon}_r=[e_r(\xi_{n+1}^0),\ldots,e_r(\xi_{n+1}^p)]^{\mathrm{T}}$ and where $\mathbf{P}_s$ denotes the matrix defined by

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

This system of $p+1$ vector equations for the $p+1$ vectors ε_r has a nontrival solution if ζ satisfies the equation

$$\det\{\zeta[\beta_{ij}h\mathbf{P}_j-\delta_{ij}\mathbf{I}_{p+1}]+[\delta_{i,i+j-p}\mathbf{I}_{p+1}]\}=0, \tag{4.15}$$

where $\mathbf{I}_{p+1}$ 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 Eq. (3.6), in which (we recall) the components of $\tilde{\kappa}_j(x)$ are values $K(x,\eta_i,\tilde{\psi}_i(\eta_i))$ may be written

$$\sum_{j=0}^{k}\left\{\mathbf{A}_j\Delta\tilde{\phi}_{n+1-j}(x)+h\mathbf{B}_j\mathbf{J}_{n+1-j}(x)R_{n+1-j}\left(\Delta\tilde{\phi}_{n+1-j}(x)\right)\right\}=\mathbf{0}, \tag{4.16}$$

where $\mathbf{J}_j(x)$ is a diagonal matrix whose diagonal elements are values $(\partial/\partial f)K(x,\eta_i,\tilde{\psi}_i(\eta_i))$ $[i=m,m+1,\ldots,m+p$, where $m=j(p+1)]$, while

$$\Delta\tilde{\phi}_j(x)=\left[\Delta\tilde{\psi}_m(x),\ldots,\Delta\tilde{\psi}_{m+p}(x)\right]^{\mathrm{T}} \tag{4.17}$$

and

$$R_j\left(\Delta\tilde{\phi}_j(x)\right)=\left[\Delta\tilde{\psi}_m(\eta_m),\ldots,\Delta\tilde{\psi}_{m+p}(\eta_{m+p})\right]^{\mathrm{T}}. \tag{4.18}$$

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

$$R_j\left(\Delta\tilde{\phi}_j(x)\right)=\sum_{i=1}^{p+1}\mathbf{E}_i\Delta\tilde{\phi}_j(\eta_{m+i-1}),\qquad m=j(p+1), \tag{4.19}$$

where $\mathbf{E}_i=\mathbf{e}_i\mathbf{e}_i^{\mathrm{T}}$ and $\mathbf{e}_i$ is the ith column of the identity matrix of order $p+1$.

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

$$\sum_{j=0}^{k}\zeta^{k-j}\left\{\mathbf{A}_j\mathbf{e}(x)+h\mathbf{B}_j\mathbf{J}_{n+1-j}(x)\sum_{i=1}^{p+1}\mathbf{E}_i\mathbf{e}\left(\xi_{n+1-j}^{i-1}\right)\right\}=\mathbf{0}, \tag{4.20}$$

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

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

and

$$\sum_{j=0}^{k} \zeta^{k-j}\left\{ \mathbf{A}_j \mathbf{e}(\xi_{n+1-s}^{r}) + h\mathbf{B}_j \mathbf{J}_{n+1-j}(\xi_{n+1-s}^{r}) \sum_{i=1}^{p+1} \mathbf{E}_i \mathbf{e}\left(\xi_{n+1-j}^{i-1}\right) \right\} = \mathbf{0}$$

$$r = 0, 1, \ldots, p, \qquad s = 0, 1, \ldots, k. \tag{4.21}$$

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 that 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 $\Delta\tilde{\phi}_j(x)$ in (4.16).

The required polynomial may be written

$$\det\left\{ \sum_{j=0}^{k} \zeta^{k-j}\left(\mathbf{A}_j^{\#} + h\mathbf{B}_j^{\#}\right) \right\} = 0, \tag{4.22}$$

where $\mathbf{A}_j^{\#}$ and $\mathbf{B}_j^{\#}$ are matrices of order $(p+1)^2(k+1)$. If we partition $\mathbf{A}_j^{\#}$ and $\mathbf{B}_j^{\#}$ into blocks of order $p+1$ and treat each block as a single matrix element, we may write

$$\mathbf{A}_j^{\#} = \operatorname{diag}(\mathbf{A}_j, \ldots, \mathbf{A}_j),$$

and

$$\mathbf{B}_j^{\#} = \operatorname{diag}\left(\mathbf{B}_j \mathbf{J}_{n+1-j}(\xi_{n+1-k}^{0}), \ldots, \mathbf{B}_j \mathbf{J}_{n+1-j}(\xi_{n+1-k}^{p}), \ldots,\right.$$
$$\left.\mathbf{B}_j \mathbf{J}_{n+1-j}(\xi_{n+1}^{0}), \ldots, \mathbf{B}_j \mathbf{J}_{n+1-j}(\xi_{n+1}^{p})\right) \times \mathbf{G}_j,$$

where $\mathbf{G}_j$ is the matrix in which the $[(k-j)(p+1)+i]$th column $(i = 1, \ldots, p+1)$ has entries $\mathbf{E}_i$ and zeros elsewhere. As an example, the matrix $\mathbf{G}_k$ has the form

$$\mathbf{G}_k = \begin{bmatrix} \mathbf{E}_1 & \mathbf{E}_2 & \cdots & \mathbf{E}_{p+1} & & & \\ \vdots & \vdots & & \vdots & 0 & \cdots & 0 \\ \mathbf{E}_1 & \mathbf{E}_2 & \cdots & \mathbf{E}_{p+1} & & & \end{bmatrix}.$$

4.3. Examples

In order to illustrate the application of 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, nonlinear kernel. For the

trapezoidal rule that is generated by the multistep coefficients

$$k=1, \qquad a_0=-a_1=1, \qquad b_0=b_1=-\tfrac{1}{2},$$

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

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

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. Ref. [8]).

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

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

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

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

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

where

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

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

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

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

$$\det\begin{bmatrix} \rho & -\rho & & & & \\ & \rho & & -\rho & & 0 \\ & 0 & \ddots & & \ddots & \\ & & & \rho & & -\rho \\ S_0 & S_1 & \cdots & & \rho+S_{k-1} & S_k \\ s_0 & s_1 & \cdots & & s_{k-1} & \rho+s_k \end{bmatrix}=0,$$

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

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

where $S_j^{*}=\Sigma_{i=0}^{j}S_i$ and $s_j^{*}=\Sigma_{i=0}^{j}s_i$. 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

$$\begin{aligned} S_{k-1}^{*}(\zeta)&=\mu h^2\zeta\sigma'(\zeta), \qquad S_k(\zeta)=\mu h^2\sigma(\zeta),\\ s_{k-1}^{*}(\zeta)&=(\lambda-\mu h)h\zeta\sigma'(\zeta)-\mu h^2\zeta^2\sigma''(\zeta),\\ s_k(\zeta)&=\lambda h\sigma(\zeta)-\mu h^2\zeta\sigma'(\zeta). \end{aligned}$$

Substitution into (4.25) yields the characteristic equation

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

Finally, we consider the characteristic equation of the family of extended 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

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

where z_{ij} here denotes the value[3] of $hJ^{(i)}_{n+1}(nh+\theta_j h)$. A straightforward calculation leads to the characteristic equation

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

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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Reducible quadrature methods for Volterra integral equations of the first kind

by

P.H.M. Wolkenfelt

ABSTRACT

Quadrature rules, generated by linear multistep methods for ordinary differential equations, are employed to construct a wide class of direct quadrature methods for the numerical solution of first kind Volterra integral equations. Our class covers several methods previously considered in the literature. The methods are shown to be convergent provided that both the first and the second characteristic polynomial of the linear multistep method satisfy the root condition. Furthermore, the stability behaviour for fixed positive values of the stepsize h is analyzed, and it turns out that convergence implies (fixed h) stability. The subclass formed by the backward differentiation methods upto order six is discussed and illustrated with numerical examples.

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KEY WORDS & PHRASES: *Numerical analysis, Volterra integral equations of the first kind, convergence.*

1. INTRODUCTION

We shall consider the numerical solution of the (linear) Volterra integral equation of the first kind

$$(1.1) \qquad \int_{x_0}^{x} K(x,y)f(y)dy = g(x), \quad x_0 \le x \le X,$$

where the forcing function g, defined on $[x_0,X]$, and the kernel K defined on $\{(x,y) \mid x_0 \le y \le x \le X\}$ are known, and where f is the unknown function. We assume that the following conditions are satisfied:

(C.1) the functions g and K are sufficiently smooth on their domain of definition,

(C.2) $g(x_0) = 0$,

(C.3) $K(x,x) \neq 0$ on $x_0 \le x \le X$.

These conditions ensure the existence of a (sufficiently smooth) unique solution f to (1.1).

Direct quadrature methods for the numerical solution of (1.1) are obtained by discretizing the integral term by suitable quadrature rules with weights w_{nj} and abscissae $x_j = x_0+jh$. Such quadrature methods yield equations of the form

$$(1.2) \qquad h \sum_{j=0}^{n} w_{nj} K(x_n,x_j)f_j = g(x_n),$$

for values f_n approximating $f(x_n)$. Methods of the form (1.2) have been studied by many authors (see e.g. ANDRADE & McKEE [1] and the references therein).

In this paper we shall consider the class of direct quadrature methods employing quadrature rules which are *reducible* (see §2) to linear multistep (LM) methods for ordinary differential equations (ODEs). In its general form, this class has not been treated before, although specific members occur in the literature. Examples are the midpoint and trapezoidal rule [12], the modified Adams-Moulton methods [5,6], and the backward differentiation methods [15]. An essential part in each of the papers referred to above is the convergence proof, which (in contrast to the proofs of corresponding methods for second kind Volterra integral equations) is rather complicated.

The main purpose of this paper is to discuss in a uniform way the convergence and stability behaviour of reducible quadrature methods for first kind Volterra integral equations. As a consequence, it unifies and extends the various convergence theorems of the papers mentioned above.

In §2 we derive quadrature rules from LM methods and indicate an important structure of the quadrature weights w_{nj}. In addition, the quadrature error is given. Reducible quadrature methods for (1.1) and their implementation are discussed in §3. The convergence theorem is stated in §4. An important condition for convergence is that both the first and the second characteristic polynomial of the associated LM method are simple von Neumann polynomials (see §2 for a definition). Furthermore we give the convergence proof which is rather involved and relies heavily upon the structure of the quadrature weights. In §5 we discuss the stability behaviour of the methods and show that convergence implies stability in the sense of BAKER & KEECH [3]. Moreover, we show that the methods yield "local differentiation formulae" if and only if the second characteristic polynomial has its roots clustered at the origin. In §6 the backward differentiation methods are illustrated with numerical examples and compared with a method of GLADWIN [5]. We conclude in §7 with some additional remarks.

2. REDUCIBLE QUADRATURE RULES

Consider the quadrature problem

$$I'(x) = \phi(x), \quad I(x_0) = 0, \tag{2.1}$$

where ϕ is a sufficiently smooth function. The solution of (2.1) at $x = x_n$ is

$$I(x_n) = \int_{x_0}^{x_n} \phi(y)\,dy. \tag{2.2}$$

In order to find numerical approximations I_n to $I(x_n)$ we apply a LM method with real coefficients a_i and b_i (see e.g. [11, p.11]) to obtain the relations

$$\sum_{i=0}^{k} a_i I_{n-i} = h \sum_{i=0}^{k} b_i \phi(x_{n-i}), \quad n \geq k, \tag{2.3}$$

where $h > 0$ denotes the stepsize and where $x_j = x_0+jh$ are the equidistant gridpoints. We assume that the starting values $I_0,\ldots,I_{k-1}$ are given by the *starting quadrature rules*

$$(2.4) \qquad I_n = h \sum_{j=0}^{k-1} w_{nj}^{(s)} \phi(x_j), \quad n = 0(1)k-1,$$

where $w_{0j}^{(s)} = 0$ for all j. From (2.3) and (2.4) one can easily verify that I_n depends linearly on $\phi(x_0),\ldots,\phi(x_n)$, that is I_n can be written as

$$(2.5) \qquad I_n = h \sum_{j=0}^{n} w_{nj}\phi(x_j), \quad n \geq k.$$

In this form, (2.5) is recognized as a quadrature rule with abscissae x_j $(j = 0(1)n)$ for the approximation of (2.2). In order to determine the weights w_{nj} in (2.5) we identify (2.3) and (2.5) to obtain the relations

$$(2.6) \qquad \sum_{i=0}^{k} a_i w_{n-i,j} = \begin{cases} 0 & \text{for} \quad 0 \leq j \leq n-k-1, \\ b_{n-j} & \text{for} \quad n-k \leq j \leq n, \end{cases} \qquad n \geq k$$

where we have defined $w_{nj} = 0$ for $j \geq n \geq k$. By means of the relations (2.6) the weights w_{nj} can be generated provided that the weights of the starting quadrature rules and the coefficients a_i and b_i are given.

With regard to the LM method we assume that $a_0 \neq 0$ and that the characteristic polynomials ρ and σ, defined by

$$(2.7) \qquad \rho(\zeta) := \sum_{i=0}^{k} a_i \zeta^{k-i}, \quad \sigma(\zeta) := \sum_{i=0}^{k} b_i \zeta^{k-i},$$

have no common zeros. Furthermore, we assume that the LM method, from now on denoted by (ρ,σ), is convergent, that is

(i) $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$ (consistency),

(ii) ρ is a simple von Neumann polynomial (zero-stability).

DEFINITION 1 (from [14, p.398]). A polynomial P of degree ≥ 1 is said to be *a simple von Neumann polynomial* if

(i) $P(\zeta) = 0$ implies $|\zeta| \leq 1$, and

(ii) $P(\zeta) = P'(\zeta) = 0$ implies $|\zeta| < 1$.

Note that definition 1 is only given for polynomials of degree ≥ 1. For the sake of uniformity however, it is convenient to define that a non-vanishing constant polynomial is also a simple von Neumann polynomial.

The quadrature rules (2.5) generated by (2.6) are called (ρ,σ)-*reducible* (cf. [13,16]). The following properties of the weights (which we need in the convergence proof) can be derived (see [16]):

(i) the weights w_{nj} are uniformly bounded (which follows from (2.6) and the fact that ρ is a simple von Neumann polynomial);

(ii) only the weights w_{nj} for $0 \leq j \leq k-1$, $n \geq k$ depend upon the choice of the starting quadrature rules;

(iii) the weights w_{nj} for $k \leq j \leq n$ $(n \geq k)$ depend only on the coefficients a_i and b_i; moreover, it holds that

$$w_{nj} = w_{n+\ell,j+\ell} \quad \text{for } k \leq j \leq n \ (n \geq k) \text{ and all } \ell > 0. \tag{2.8}$$

For the quadrature error Q_n defined by

$$Q_n[\phi] := I_n - I(x_n) = h \sum_{j=0}^{n} w_{nj}\phi(x_j) - \int_{x_0}^{x_n} \phi(y)dy, \tag{2.9}$$

we have the following results:

THEOREM 1 (from [16]). *Let* (ρ,σ) *be a convergent* LM *method of order* p *with error constant* C_{p+1}. *Then*

$$\sum_{i=0}^{k} a_i Q_{n-i} = -C_{p+1}h^{p+1}\phi^{(p)}(x_n) + \mathcal{O}(h^{p+2}) \text{ as } h \to 0. \tag{2.10}$$

Furthermore, let the starting quadrature rules be of order p+1, *that is* $Q_n = \mathcal{O}(h^{p+1})$ *as* $h \to 0$ *for* $n = 0(1)k-1$. *Then*

$$Q_n[\phi] = -h^p\{\phi^{(p-1)}(x_n) - \phi^{(p-1)}(x_0)\}C_{p+1}/\sigma(1) + \mathcal{O}(h^{p+1}), \tag{2.11}$$

as $h \to 0$, $n \to \infty$ *while* $nh = x_n - x_0$ *remains fixed.* □

Reducible quadrature rules generated by a LM method (ρ,σ) of order p and starting quadrature rules of order p+1 are called *convergent of order* p.

3. REDUCIBLE QUADRATURE METHODS

In §2 we have discussed the construction of the quadrature weights w_{nj} for $n \geq k$. These weights are now used for the discretization of the integral term in (1.1) to obtain the equations

$$h \sum_{j=0}^{n} w_{nj} K(x_n, x_j) f_j = g(x_n), \quad n \geq k, \tag{3.1}$$

where f_n denotes the numerical approximation of $f(x_n)$. The method (3.1) which employs (ρ,σ)-reducible quadrature rules is called a (ρ,σ)-*reducible quadrature method*. Recall that $w_{nj} = 0$ for $j \geq n \geq k$, and, therefore, the values $f_k, f_{k+1}, \ldots$, can be computed in a step-by-step fashion, provided that the required starting values are known. Such starting values can be obtained by one-step Runge-Kutta methods [9,10] or by collocation methods [4]. In contrast to certain block-by-block and implicit Runge-Kutta methods where the kernel is evaluated outside its domain of definition, the step-by-step method (3.1) requires only kernel values $K(x,y)$ for $y \leq x$. With respect to the computational effort of (3.1) we remark that the number of kernel evaluations necessary to reach the endpoint $X = x_0+Nh$ is $\frac{1}{2}N^2+O(N)$. Furthermore the methods can easily be adapted to deal with non-linear integral equations.

If $b_0 = 0$ and $b_1 \neq 0$ (compare the midpoint rule) then $w_{nn} = 0$ and $w_{n,n-1} \neq 0$, and (3.1) cannot be solved for f_n. In such a case the equation (3.1) is used to compute f_{n-1} $(n \geq k+1)$. Similarly, if b_μ is the first non-zero coefficient of σ, then (3.1) with $n = m+\mu$ yields the value f_m $(m \geq k)$.

The form (3.1) is convenient for theoretical purposes (such as convergence). From a computational point of view it is a disadvantage to calculate the weights from the recurrence relation (2.6) (see a remark in [15]). We shall indicate, however, that the explicit calculation of the quadrature weights (and hence their storage) can be avoided by implementing the methods in a way which parallels (2.2-4). Let $\Psi_n(x) = \int_{x_0}^{x} K(x_n,y) f(y)\,dy$, then we want an approximation Ψ_{nn} of $\Psi_n(x_n)$ and solve $\Psi_{nn} = g(x_n)$ for f_n. Using (2.4) and (2.3) we then obtain the following numerical scheme for finding f_n (assuming that $f_0, \ldots, f_{n-1}$ are known).

Compute Ψ_{nm} *for* m = 0(1)k-1, *using the starting quadrature rules* (2.4), *that is*

$$\Psi_{nm} := h \sum_{j=0}^{k-1} w_{mj}^{(s)} K(x_n,x_j) f_j; \tag{3.2a}$$

compute Ψ_{nm} *for* m = k(1)n-1, *using* (2.3), *that is*

$$\Psi_{nm} := - \sum_{i=1}^{k} a_i \Psi_{n,m-i} + h \sum_{i=0}^{k} b_i K(x_n,x_{m-i}) f_{m-i}; \tag{3.2b}$$

set up the equation $\Psi_{nn} = g(x_n)$ *and solve for* f_n, *that is find* f_n *from*

$$h \sum_{i=0}^{k} b_i K(x_n,x_{n-i}) f_{n-i} = \sum_{i=1}^{k} a_i \Psi_{n,n-i} + g(x_n). \tag{3.2c}$$

Note that we have applied the normalization $a_0 = 1$. It is easily shown using (2.6) that the scheme (3.2a-c) is equivalent to (3.1).

4. CONVERGENCE

In this section we establish the order of convergence of the methods (3.1) under suitable conditions. First we derive a necessary condition for convergence. Assume that the quadrature method (3.1) is convergent. Then application of (3.1) to the equation $\int_0^x f(y)dy = 0$ (whose exact solution is $f(x) \equiv 0$) yields the equations $h \sum_{j=0}^{n} w_{nj} f_j = 0$. Multiply the (n-i)-th equation by a_i (i = 0,1,...,k) and sum over i to obtain

$$h \sum_{i=0}^{k} a_i \sum_{j=0}^{n-i} w_{n-i,j} f_j = h \sum_{i=0}^{k} b_i f_{n-i} = 0,$$

by virtue of (2.6). Since the method is convergent, f_n must tend to zero as $n \to \infty$, $h \to 0$, $nh = x_n$ fixed. Therefore a *necessary* condition for convergence is that σ is a simple von Neumann polynomial. In the following Theorem we shall see that this condition is also one of the sufficient conditions.

THEOREM 2. *In addition to the conditions* (C.1-3) *for the existence and uniqueness of a smooth solution* f(x) *of* (1.1), *assume that*

(i) *the quadrature method* (3.1) *employs the weights* w_{nj} *of* (ρ,σ)*-reducible*

quadrature rules of order $p \geq 1$,

(ii) σ *is a simple von Neumann polynomial,*

(iii) *the errors in the starting values* $f_0,\ldots,f_{k-1}$ *are of order* s, *i.e.* $|f_i - f(x_i)| = O(h^s)$ *as* $h \to 0$.

Then, the method (3.1) *is convergent of order* r, *where* $r = \min(p,s)$, *that is*

$$|f_n - f(x_n)| \leq C h^r \quad \text{as } h \to 0,\ n \to \infty,\ nh \text{ fixed}, \tag{4.1}$$

where C *is a constant independent of* n *and* h.

REMARK 1. If ρ is not a simple von Neumann polynomial, then condition (i) of Theorem 2 cannot be satisfied. Therefore, in view of (ii), both ρ and σ must be simple von Neumann polynomials.

REMARK 2. Theorem 2 generalizes the results derived in [5,6,12,15]. LINZ [12] considers the midpoint rule ($\rho = \zeta^2-1$, $\sigma = \zeta$) and the trapezoidal rule ($\rho = \zeta-1$, $\sigma = (\zeta+1)/2$). TAYLOR [15] "inverts" the backward differentiation methods ($\rho = \sum a_i\zeta^{k-i}$, $\sigma = b_0\zeta^k$). GLADWIN & JELTSCH [6] prove that (in our notation) the polynomial σ of a k-step p-th order *implicit* LM method derived from interpolatory quadrature (i.e. $\rho = \zeta^k-\zeta^{k-r}$) cannot be a simple von Neumann polynomial if $p > k$, and therefore the associated direct quadrature method for (1.1) is divergent. (The classical Adams-Moulton methods, which generate the Newton-Gregory rules, are examples of such divergent methods). GLADWIN [5] constructs methods of Adams-type ($\rho = \zeta^k-\zeta^{k-1}$) of a given order (upto six) containing some free parameters b_i. These parameters are then chosen such that σ is a simple von Neumann polynomial.

REMARK 3. Due to the general form of the polynomials ρ and σ the proof of the convergence theorem is rather involved and lengthy, and requires careful attention to details. For special choices of the polynomials ρ and σ such as those considered in the papers mentioned in Remark 2, the proof can be simplified.

In the proof we shall need a few lemmas listed below. In these lemmas α and β denote non-negative integers, ζ and ξ are complex numbers, and ρ and σ are the characteristic polynomials (with real coefficients) associated

with a difference equation.

LEMMA 1.a. *Let* $c_n = n^{\alpha}\zeta^n$ *where* $\alpha = 0$ *if* $|\zeta| = 1$. *If* $|\zeta| \leq 1$ *and* $\zeta \neq 1$, *then* $|\sum_{n=m}^{N} c_{N-n}|$ *is bounded uniformly in* m *and* N.

PROOF. Observe that $\sum_{n=m}^{N} c_{N-n} = \sum_{n=0}^{N-m} c_n$. The proof that $|\sum_{n=0}^{N} n^{\alpha}\zeta^n|$ is uniformly bounded, is elementary. □

Since c_n in Lemma 1.a can be regarded as an element from the fundamental system of solutions of a difference equation, we have the following Corollary.

COROLLARY 1.a. *Let* γ_n *satisfy the difference equation* $\sum_{i=0}^{k} b_i \gamma_{n-i} = 0$. *If the characteristic polynomial* $\sigma(\zeta)$ *is simple von Neumann and* $\sigma(1) \neq 0$, *then* $|\sum_{n=m}^{N} \gamma_{N-n}|$ *is bounded uniformly in* m *and* N.

Next we give a "two-dimensional" analogue of the above results.

LEMMA 1.b. *Let* $c_n = n^{\alpha}\zeta^n$ *where* $\alpha = 0$ *if* $|\zeta| = 1$, *and let* $d_n = n^{\beta}\xi^n$ *where* $\beta = 0$ *if* $|\xi| = 1$. *If* $|\zeta| \leq 1$, $|\xi| \leq 1$ *and* $\zeta \neq \xi$, *then* $|\sum_{n=m}^{N} c_{N-n}d_n|$ *is bounded uniformly in* m *and* N.

PROOF. We consider only the case that $|\zeta| \leq |\xi|$. (The case $|\zeta| \geq |\xi|$ is treated along similar lines.) Defining $w = \zeta/\xi$ we may write

$$\sum_{n=m}^{N} c_{N-n}d_n = \xi^N \sum_{n=m}^{N} (N-n)^{\alpha} n^{\beta} w^{N-n}.$$

Note that $|w| \leq 1$ and $w \neq 1$ since $\zeta \neq \xi$. Next we distinguish between the cases $|\xi| = 1$ and $|\xi| < 1$.

(i) $|\xi| = 1$. In this case $\beta = 0$ and thus

$$|\sum_{n=m}^{N} c_{N-n}d_n| = |\sum_{n=m}^{N} (N-n)^{\alpha} w^{N-n}|,$$

which is uniformly bounded in view of Lemma 1.a.

(ii) $|\xi| < 1$. In this case we write

$$|\sum_{n=m}^{N} c_{N-n}d_n| = |\xi^N N^{\alpha+\beta}||\sum_{n=m}^{N} (\frac{N-n}{N})^{\alpha} (\frac{n}{N})^{\beta} w^{N-n}| \leq |\xi^N N^{\alpha+\beta+1}|,$$

which is readily seen to be uniformly bounded. □

COROLLARY 1.b. *Let* γ_n *and* δ_n *satisfy the difference equations* $\sum_{i=0}^{k} b_i \gamma_{n-i} = 0$ *and* $\sum_{i=0}^{k} a_i \delta_{n-i} = 0$, *respectively. Suppose that the characteristic polynomials* ρ and σ *have no common zeros. If* ρ *and* σ *are simple von Neumann polynomials, then* $|\sum_{n=m}^{N} \gamma_{N-n} \delta_n|$ *is bounded uniformly in* m *and* N.

We shall also need the following lemmas.

LEMMA 2.a. *Let the function* ϕ, *defined on* $[x_0,X]$, *be continuously differentiable; let* $x_n = x_0+nh$ *and* $Nh \le X-x_0$ *and let* $\{\gamma_n\}_{n=0}^{\infty}$ *be a sequence of complex numbers. Then* $|\sum_{n=n_0}^{N} \gamma_{N-n}\phi(x_n)|$ *is bounded uniformly in* N *if* $|\sum_{n=m}^{N} \gamma_{N-n}|$ *is bounded uniformly in* m *and* N ($n_0 \le m \le N$).

PROOF. Let $\Gamma_{N-n} := \sum_{j=n}^{N} \gamma_{N-j}$, $\Gamma_0 := \gamma_0$, $\Gamma_{-1} := 0$. Then

$$\sum_{n=n_0}^{N} \gamma_{N-n}\,\phi(x_n) = \sum_{n=n_0}^{N} (\Gamma_{N-n} - \Gamma_{N-n-1})\phi(x_n)$$

$$= \Gamma_{N-n_0}\,\phi(x_{n_0}) + \sum_{n=n_0+1}^{N} \Gamma_{N-n}\,(\phi(x_n) - \phi(x_{n-1}))$$

$$= \Gamma_{N-n_0}\,\phi(x_{n_0}) + \sum_{n=n_0+1}^{N} \Gamma_{N-n}h\,\phi'(\xi_n),\ \xi_n \in [x_{n-1},x_n]$$

Therefore $|\sum_{n=n_0}^{N} \gamma_{N-n}\,\phi(x_n)| \le \Gamma^*\{\max|\phi| + (X-x_0)\max|\phi'|\}$, where Γ^* is the uniform bound of $|\sum_{n=m}^{N} \gamma_{N-n}|$. □

The "two dimensional" analogue of Lemma 2.a reads:

LEMMA 2.b. *In addition to Lemma* 2.a, *let* $\{\delta_n\}_{n=0}^{\infty}$ *be a sequence of complex numbers. Then* $|\sum_{n=n_0}^{N} \gamma_{N-n}\,\delta_n\phi(x_n)|$ *is bounded uniformly in* N *if* $|\sum_{n=m}^{N} \gamma_{N-n}\,\delta_n|$ *is bounded uniformly in* m *and* N ($n_0 \le m \le N$).

PROOF. Similar to the proof of Lemma 2.a. □

PROOF OF THEOREM 2. For a function F(x,y) in two variables we shall use the following abbreviations

$$F^{pq} = F^{pq}(x,y) := \frac{\partial^{p+q}}{\partial^p x \partial^q y} F(x,y);$$

$$F^{pq}_{nj} := F^{pq}(x_n,x_j);\quad F_{nj} := F(x_n,x_j).$$

For $n \geq k$ the equation for the global error $e_n := f_n - f(x_n)$ reads

$$h\sum_{j=0}^{n} w_{nj}K_{nj}e_j + T_n = 0, \quad n \geq k \tag{4.2}$$

where the truncation error T_n at $x = x_n$ is given by

$$T_n = h\sum_{j=0}^{n} w_{nj}K_{nj}f(x_j) - \int_{x_0}^{x_n} K(x_n,y)f(y)dy. \tag{4.3}$$

For $n \geq 2k$ and $i = 0(1)k$ multiply the $(n-i)$-th equation in (4.2) by a_i and sum over i to obtain

$$\sum_{i=0}^{k} a_i \sum_{j=0}^{n-i} w_{n-i,j}\, K_{n-i,j}\, e_j + (1/h)\sum_{i=0}^{k} a_i\, T_{n-i} = 0, \quad n \geq 2k.$$

Expanding $K_{n-i,j}$ in a Taylor series about $x = x_n$, $y = x_j$ and using the relations (2.6) for the weights w_{nj}, yields

$$\begin{aligned}\sum_{i=0}^{k} b_i\, K_{n,n-i}\, e_{n-i} = {} & h\sum_{i=1}^{k} ia_i\sum_{j=0}^{n-i} w_{n-i,j}\, K_{nj}^{1,0}\, e_j + \\ & - h^2 \sum_{i=1}^{k} i^2 a_i \sum_{j=0}^{n-i} w_{n-i,j}\, \theta_{nj}(i)e_j + \\ & - (1/h) \sum_{i=0}^{k} a_i T_{n-i}, \quad n \geq 2k,\end{aligned}$$

where, due to the smoothness of K, $|\theta_{nj}(i)| \leq \theta = \tfrac{1}{2} \max |K^{2,0}|$.

Next we expand $K_{n,n-i}$ in a Taylor series about $x = x_n$, $y = x_n$ and divide through by K_{nn} to obtain

$$\begin{aligned}\sum_{i=0}^{k} b_i\, e_{n-i} = {} & K_{nn}^{-1}\{h\sum_{i=1}^{k} ib_i\chi_{nn}(i)e_{n-i} - h^2\sum_{i=1}^{k} i^2 a_i \sum_{j=0}^{n-i} w_{n-i,j}\, \theta_{nj}(i)e_j\} \\ & + K_{nn}^{-1}\, h\sum_{i=1}^{k} ia_i \sum_{j=n-k}^{n-i} w_{n-i,j}\, K_{nj}^{1,0}\, e_j + h\sum_{i=1}^{k} ia_i\, G_n^{(i)} - T_n^*\end{aligned} \tag{4.4}$$

where $|\chi_{nn}(i)| \leq \chi = \max |K^{0,1}|$;

$$G_n^{(i)} = \sum_{j=0}^{n-k-1} w_{n-i,j}(K_{nj}^{1,0} / K_{nn})e_j;$$

$$T_n^* = \sum_{i=0}^{k} a_i\, T_{n-i}/(hK_{nn}).$$

Without loss of generality we assume that $b_0 \neq 0$. (If $b_0 = 0$ and b_μ is the first non-zero coefficient, then (4.4) actually defines the error equation for $e_{n-\mu}$. In such a case the proof of this theorem requires no essential modifications.) As in HENRICI [7, p.242] we define the coefficients γ_n as:

$$\begin{aligned} &\gamma_n = 0 \text{ for } n < 0,\ \gamma_0 = 1/b_0, \\ &\textstyle\sum_{i=0}^{k} b_i \gamma_{n-i} = 0 \text{ for } n \geq 1. \end{aligned} \tag{4.5}$$

Since by assumption, $\sigma(\zeta) = \sum_{i=0}^{k} b_i \zeta^{k-i}$ is a simple von Neumann polynomial, $|\gamma_n| \leq \Gamma$ uniformly in n.

Next we take a fixed N ($N \geq 2k$, $Nh \leq X-x_0$), multiply for each n ($2k \leq n \leq N$) equation (4.4) by γ_{N-n} and sum over n. For the left-hand side of (4.4) we then obtain, using (4.5)

$$e_N + (\gamma_{N-2k} b_k) e_k + (\gamma_{N-2k} b_{k-1} + \gamma_{N-2k-1}\, b_k) e_{k-1} + \ldots +$$

$$(\gamma_{N-2k} b_1 + \ldots + \gamma_{N-2k-k} b_k) e_{2k-1}.$$

Consider now the right-hand side of (4.4). For the first, second and third term we obtain expressions which can be bounded by $kB\chi\kappa^{-1}\Gamma\, h \sum_{j=0}^{N-1} |e_j|$, $k^2 AW\Theta\kappa^{-1}\Gamma(X-x_0)\, h \sum_{j=0}^{N-1} |e_j|$ and $kAW \max |K^{1,0}|\kappa^{-1}\Gamma\, h \sum_{j=0}^{N-1} |e_j|$, respectively, where A, B and W are the uniform bounds of $|a_i|$, $|b_i|$ and $|w_{nj}|$. Note that we have used here that $|K_{nn}| \geq \kappa = \min |K(x,x)| > 0$. Hence the first three terms can be bounded by $A_1 h \sum_{j=0}^{N-1} |e_j|$ where A_1 is independent of N and h. For the fourth and fifth term we obtain

$$h \sum_{i=1}^{k} i a_i \sum_{n=2k}^{N} \gamma_{N-n} G_n^{(i)} \tag{4.6}$$

and

$$\sum_{n=2k}^{N} \gamma_{N-n}\, T_n^{*}. \tag{4.7}$$

For a fixed i ($1 \leq i \leq k$) in (4.6) we derive that

$$(4.8)\qquad \sum_{n=2k}^{N} \gamma_{N-n}\, G_n^{(i)} = \sum_{j=0}^{k-1} \{\sum_{n=2k}^{N} \gamma_{N-n}\, w_{n-i,j}\, K_{nj}^{1,0} / K_{nn}\} e_j$$

$$+ \sum_{j=k}^{N-k-1} \{\sum_{n=j+k+1}^{N} \gamma_{N-n}\, w_{n-i,j}\, K_{nj}^{1,0} / K_{nn}\} e_j .$$

We have to show that the two expressions between brackets in (4.8) are uniformly bounded. Consider the first expression. Since, by assumption $K^{(1,0)}(x,x_j)/K(x,x)$ is continuously differentiable, if follows from application of Lemma 2.b, that it is sufficient to prove that for each i ($1 \le i \le k$) and each j ($0 \le j \le k-1$)

$$(4.9)\qquad \left|\sum_{n=m}^{N} \gamma_{N-n}\, w_{n-i,j}\right| \le D_j^{(i)}$$

uniformly in m and N ($2k \le m \le N$). If we define $\delta_n := w_{n-i,j}$ for fixed i and j, then δ_n satisfies $\sum_{i=0}^{k} a_i \delta_{n-i} = 0$. Moreover γ_n satisfies (4.5), and, hence, application of Corollary 1.b establishes that (4.9) is true. Next we consider the second expression between brackets in (4.8). Similar reasoning as above (using Lemma 2.b) yields that we have to prove that for each i ($1 \le i \le k$) and each j ($k \le j \le N-k-1$)

$$\left|\sum_{n=m}^{N} \gamma_{N-n}\, w_{n-i,j}\right| \le D_j^{(i)}$$

is bounded uniformly in m and N ($j+k+1 \le m \le N$). Moreover, we have to show that $\max\{D_j^{(i)};\ j = k,k+1,\ldots,N-k-1\}$ is independent of N. This we prove as follows.

For j = k, one proves, as we did above, that

$$(4.10)\qquad \left|\sum_{n=m}^{N} \gamma_{N-n}\, w_{n-i,k}\right| \le D_k^{(i)}, \qquad 2k+1 \le m \le N.$$

For $j > k$, one has to find a uniform bound for

$$\left|\sum_{n=m^*}^{N} \gamma_{N-n}\, w_{n-i,j}\right|$$

independent of m^* and N with $j+k+1 \le m^* \le N$. Recall from (2.8) that $w_{n-i,j} = w_{n-i-j+k,k}$. Therefore,

$$(4.11)\qquad \left|\sum_{n=m^*}^{N} \gamma_{N-n}\, w_{n-i,j}\right| = \left|\sum_{n=m}^{N^*} \gamma_{N^*-n}\, w_{n-i,k}\right|,$$

where $N^* = N-j+k$ and $2k+1 \le m \le N^*$. The last expression in (4.11), however, is bounded by $D_k^{(i)}$ in view of (4.10). Hence we have shown that the terms between brackets in (4.8) are uniformly bounded, and therefore (4.6) can be bounded by $A_2 h \sum_{j=0}^{N-1} |e_j|$, where A_2 is independent of N and h.

Finally, we investigate the term (4.7). If we define $\psi(x,y) := K(x,y)f(y)$, then the truncation error T_{n-i} defined in (4.3) is given by the quadrature error in the approximation of the integral of the function $\psi(x_{n-i},\cdot)$ on the interval $[x_0,x_{n-i}]$ (see (2.9)); that is

$$T_{n-i} = Q_{n-i}[\psi(x_{n-i},\cdot)].$$

Expanding the function $\psi(x_{n-i},y)$ in a Taylor series about $x = x_n$ the truncation error can be split into

$$T_{n-i} = Q_{n-i}[\psi(x_n,\cdot)] - ihQ_{n-i}[\psi^{1,0}(x_n,\cdot)]$$

$$+ \tfrac{1}{2}i^2h^2Q_{n-i}[\psi^{2,0}(\xi_{n-i},\cdot)], \quad \xi_{n-i} \in [x_{n-i},x_n].$$

Next we form $\sum_{i=0}^{k} a_i T_{n-i}$ and obtain the following terms:

$$\sum_{i=0}^{k} a_i Q_{n-i}[\psi(x_n,\cdot)] = -C_{p+1}h^{p+1}\psi^{0,p}(x_n,x_n) + O(h^{p+2}),$$

by virtue of (2.10);

$$h\sum_{i=0}^{k} ia_i Q_{n-i}[\psi^{1,0}(x_n,\cdot)] =$$

$$-\sum_{i=0}^{k} ia_i C_{p+1}/\sigma(1)h^{p+1}\{\psi^{1,p-1}(x_n,x_{n-i}) - \psi^{1,p-1}(x_n,x_0)\} + O(h^{p+2}) =$$

$$-C_{p+1}h^{p+1}\{\psi^{1,p-1}(x_n,x_n) - \psi^{1,p-1}(x_n,x_0)\} + O(h^{p+2}),$$

by virtue of (2.11), and

$$\tfrac{1}{2}h^2 \sum_{i=0}^{k} i^2 a_i Q_{n-i}[\psi^{2,0}(\xi_{n-i},\cdot)] = O(h^{p+2}).$$

Hence T_n^* defined by $\sum_{i=0}^{k} a_i T_{n-i}/(hK_{nn})$ has the form

$$T_n^* = -(1/K_{nn})h^p C_{p+1}\{\psi^{0,p}(x_n,x_n) - \psi^{1,p-1}(x_n,x_n) + \psi^{1,p-1}(x_n,x_0)\} + O(h^{p+1}). \tag{4.12}$$

Note that we have to prove that (4.7) is uniformly bounded. It is easily seen that the terms of $O(h^{p+1})$ in (4.12) yield, due to the boundedness of γ_n, a term of $O(h^p)$ in (4.7). Omitting, therefore, the $O(h^{p+1})$-terms in (4.12) and observing that the functions $\psi^{(0,p)}(x,x)/K(x,x)$, $\psi^{(1,p-1)}(x,x)/K(x,x)$ and $\psi^{(1,p-1)}(x,x_0)/K(x,x)$ are continuously differentiable on $[x_0,X]$, application of Lemma 2.a yields that the expression (4.7) is uniformly bounded if $|\sum_{n=m}^{N} \gamma_{N-n}|$ is uniformly bounded for all m and N, $(2k \le m \le N)$. This, however, follows directly from Corollary 1.a. Hence we have shown that

$$|\sum_{n=2k}^{N} \gamma_{N-n} T_n^*| \le A_3 h^p.$$

Piecing the bits together, we have shown that

$$|e_N| \le A_3 h^p + A_4 \sum_{j=0}^{2k-1} |e_j| + hA_5 \sum_{j=2k}^{N-1} |e_j|,$$

where A_3, A_4 and A_5 are independent of h and N. The solution of this inequality is well-known to be (see e.g. [7, p.244] or [2, p.925])

$$|e_N| \le \{A_3 h^p + A_4 \sum_{j=0}^{2k-1} |e_j|\} \exp(A_5(X-x_0)). \tag{4.13}$$

The errors $e_0,\ldots,e_{k-1}$ are $O(h^s)$. The error e_k is defined in (4.2) and is readily seen to be $O(h^s) + O(h^{-1}T_k)$. From (2.11) we derive that

$$\begin{aligned} T_k &= -C_{p+1}/\sigma(1)h^p\{\psi^{1,p-1}(x_k,x_k) - \psi^{1,p-1}(x_k,x_0)\} + O(h^{p+1}) \\ &= -C_{p+1}/\sigma(1)kh^{p+1}\psi^{1,p}(x_k,\xi_k) + O(h^{p+1}) \\ &= O(h^{p+1}), \end{aligned}$$

and, therefore, $e_k = O(h^s) + O(h^p)$. Similarly one shows that the errors $e_{k+1},\ldots,e_{2k-1}$ are $O(h^s) + O(h^p)$, and together with (4.13) this establishes that $|e_N| = O(h^s) + O(h^p)$. This completes the proof. □

5. STABILITY

The stability behaviour of a numerical method for (1.1) is frequently analyzed (compare [3], [10], [15]) by applying that method with a fixed positive step size h to the equation

$$(5.1) \qquad \int_0^x f(y)dy = g(x),\ g(0) = 0,$$

whose solution is $f(x) = g'(x)$. For the class of reducible quadrature methods (3.1) we obtain the equations

$$(5.2) \qquad h \sum_{j=0}^{n} w_{nj} f_j = g(x_n),$$

which, in view of (2.6), can be reduced to the difference equation

$$(5.3) \qquad \sum_{i=0}^{k} b_i f_{n-i} = (1/h) \sum_{i=0}^{k} a_i g(x_{n-i}).$$

From (5.3) it is obvious that (3.1) is stable in the sense of BAKER & KEECH [3] if and only if σ is a simple von Neumann polynomial. Since this condition is also necessary for convergence (see §4), we have the following Corollary.

COROLLARY 2. *Let the* (ρ,σ)*-reducible quadrature method* (3.1) *be convergent. Then the method is stable in the sense of* BAKER & KEECH.

From (5.3) we observe that the (in modulus) largest zero of σ is of practical importance, and gives an indication of the damping properties of the method. If this value exceeds unity then the method is unstable and therefore divergent.

Some methods applied to (5.1) yield "local differentiation formulae" (see e.g. [10, p.317] for a definition). A precise characterization is given by the following Theorem.

THEOREM 3. *A convergent* (ρ,σ)*-reducible quadrature method applied to* (5.1) *yields a local differentiation formula if and only if*

$$\sigma(\zeta) = b_j\zeta^{k-j} \quad \textit{for some } j,\ 0 \le j \le k. \tag{5.4}$$

PROOF. Note that (3.1) applied to (5.1) yields (5.3). Suppose that at least two coefficients b_i are different from zero. Then (5.3) does not define a differentiation formula. Hence (5.4) is necessary. Next we prove that (5.4) is also sufficient. Let b_j be the only non-zero coefficient of σ. From (5.3) we then derive that $b_j f_{n-j} = (1/h)\sum a_i g(x_{n-i}) = \rho'(1)g'(x_{n-j}) + O(h)$. Therefore $f_{n-j} = \rho'(1)/\sigma(1)g'(x_{n-j}) + O(h) = g'(x_{n-j}) + O(h)$. □

Examples of methods which satisfy (5.4) (i.e. methods for which the polynomial σ has only zeros at the origin) are the backward differentiation methods and the mid-point rule.

6. NUMERICAL EXAMPLES

In this section we consider quadrature methods which are reducible to the k-step backward differentiation methods for $k = 2,3,\ldots,6$. The coefficients of the polynomials $\rho(\zeta) = \sum_{i=0}^{k} a_i\zeta^{k-i}$ and $\sigma(\zeta) = b_0\zeta^k$ can be found for example in [11, p.242]. The methods were implemented as described in (3.2a-c). Interpolatory quadrature rules of maximal precision were employed for the starting quadrature formulae (2.4). Furthermore exact starting values $f_0,\ldots,f_{k-1}$ were used. In view of Theorem 2 the resulting quadrature method is of order k. All computations were performed on a CDC 73/173 Computer System using single precision (60 bit wordlength with a 48 bit mantissa).

The methods were applied to the following problems (taken from [5]):

I. $\int_0^x (a^2+1)\cos(x-y)f(y)dy = a\cdot\exp(ax) + \sin x - a\cdot\cos x,\quad f(x) = \exp(ax),$

II. $a\int_0^x \exp a(x-y)f(y)dy = \sinh(ax),\quad f(x) = \exp(-ax),$

with $a = 1$ and -1, and $0 \le x \le 4$. Our numerical results can be compared with those obtained by GLADWIN [5].

No difficulties were experienced. The true error was a smooth function and, in most cases, of constant sign. In the Tables 1 and 2 we list the number of correct digits (defined by $-{}^{10}\log(\text{absolute error})$) at $x = 2$ and $x = 4$, respectively, for $h = 0.1$ and, in brackets, for $h = 0.05$. Furthermore, we give the results obtained by a fourth order method of GLADWIN (method D in [5, p.714]).

	PROBLEM			
method	I(a=1)	I(a=-1)	II(a=1)	II(a=-1)
BD2	1.38(1.98)	2.26(2.85)	2.68(3.31)	1.07(1.64)
BD3	3.83(4.74)	3.39(4.25)	3.46(4.42)	1.93(2.79)
BD4	3.37(4.50)	5.53(6.40)	4.22(5.49)	2.77(3.90)
BD5	4.15(5.59)	5.37(6.84)	4.95(6.55)	3.59(5.00)
BD6	5.18(6.96)	6.13(7.88)	5.68(7.60)	4.39(6.09)
GLADWIN	3.09(4.21)	5.59(6.22)	3.96(5.21)	2.48(3.62)

Table 1. Number of correct digits at $x = 2$, $h = 0.1$ ($h = 0.05$)

	PROBLEM			
method	I(a=1)	I(a=-1)	II(a=1)	II(a=-1)
BD2	0.46(1.05)	2.21(2.80)	3.55(4.18)	0.20(0.77)
BD3	2.30(3.51)	3.41(4.26)	4.33(5.29)	1.06(1.92)
BD4	2.51(3.64)	5.01(6.54)	5.08(6.36)	1.90(3.03)
BD5	3.25(4.70)	5.21(6.70)	5.82(7.42)	2.72(4.13)
BD6	4.24(6.03)	6.07(7.81)	6.54(8.72)	3.53(5.22)
GLADWIN	2.22(3.35)	4.57(6.15)	4.80(6.10)	1.60(2.74)

Table 2. Number of correct digits at $x = 4$, $h = 0.1$ ($h = 0.05$)

From these tables the correct order of convergence is obvious (note that for a method of order p, halving the stepsize yields an increase of $0.3*p$ in the number of correct digits). Since all methods above require the same number ($\simeq N^2/2$) of kernel evaluations, it is obvious that the sixth-order backward

differentiation method is the most efficient one. Moreover, we observe that the fourth order method BD4 is more accurate than Gladwin's method D (of the same order) at the same computational costs.

7. CONCLUDING REMARKS

We have discussed direct quadrature methods which are reducible to linear multistep methods for ordinary differential equations, and established high order convergence under suitable conditions. Furthermore, we have indicated that several methods previously considered in the literature are special cases of the class presented in this paper. However, not all direct quadrature methods are covered by our theory. In order to include most (if not all) of the direct quadrature methods for (1.1), it seems a natural step to construct quadrature rules by means of more general methods for ODEs such as the cyclic linear multistep methods. We feel that such a general treatment is possible and some partial results are already known in this direction (see HOLYHEAD et al. [8], ANDRADE & McKEE [1], who essentially employ the class of cyclic LM methods derived from interpolatory quadrature).

The backward differentiation methods considered in §6 turned out to perform well, but their order cannot exceed 6 (see [7, p.207] stating that the polynomial ρ is no longer simple von Neumann for $k > 6$). It is well-known, however, that the use of cyclic LM methods may improve the stability behaviour while retaining high accuracy. This suggests considering backward differentiation type methods employed in a cyclic fashion for the solution of (1.1). We intend to investigate such methods in the near future.

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The construction of reducible quadrature rules for Volterra integral and integro-differential equations

by

P.H.M. Wolkenfelt

ABSTRACT

A formal relationship between quadrature rules and linear multistep methods for ordinary differential equations is exploited for the generation of quadrature weights. Employing the quadrature rules constructed in this way, step-by-step methods for second kind Volterra integral equations and integro-differential equations are defined and convergence and stability results are presented.

The construction of the quadrature rules generated by the backward differentiation formulae is discussed in detail. The use of these rules for the solution of Volterra type equations is proposed and their good performance is demonstrated by numerical experiments.

KEY WORDS & PHRASES: *Numerical analysis, Volterra integral and integro-differential equations, reducible quadrature rules, convergence and stability.*

1. INTRODUCTION

Consider the second kind Volterra integral equation

$$(1.1) \qquad f(x) = g(x) + \int_{x_0}^{x} K(x,y,f(y))dy, \quad x_0 \le x \le X,$$

and the Volterra integro-differential equation

$$(1.2) \qquad f'(x) = F(x,f(x), \int_{x_0}^{x} K(x,y,f(y))dy), \quad x_0 \le x \le X$$

with initial condition $f(x_0) = f_0$. We assume that the functions g, F and K (the kernel) are continuously differentiable to sufficiently high order, so that the existence of a sufficiently smooth solution f is ensured. A wide variety of methods for (1.1) is discussed in [2], whereas a survey of methods for (1.2) can be found in e.g. [1].

An essential part in the derivation of numerical methods is the discretization of the integrals occurring in (1.1) and (1.2) by numerical quadrature, that is we write

$$(1.3) \qquad \int_{x_0}^{x_n} K(x_n,y,f(y))dy \simeq h \sum_{j=0}^{n} w_{nj} K(x_n,x_j,f_j), \quad n \ge k,$$

where h denotes the stepsize, $x_j = x_0+jh$ are equidistant gridpoints and where f_j denotes a numerical approximation to $f(x_j)$. The values w_{nj} are the weights associated with a family of quadrature rules.

In this paper we consider the use of (ρ,σ)-*reducible* quadrature rules, that is rules which are constructed by means of linear multistep (LM) methods for ordinary differential equations. It is well known that certain LM methods, such as the Adams-Bashforth-Moulton or the Nyström-Milne-Simpson formulae are derived from interpolatory quadrature (see e.g. [7]), so that the relationship between such LM methods and quadrature rules is quite natural. However, within the general class of LM methods there exist methods which are *not* derived from quadrature (e.g. the backward differentiation formulae) and therefore, their connection with quadrature rules is less transparent.

Some specific examples which fall within the class of (ρ,σ)-reducible quadrature rules have been investigated before in the literature. Among them we mention the Gregory quadrature rules for the solution of second kind Volterra equations (STEINBERG [14]), and the use of "inverted differentiation formulae" for first kind equations (TAYLOR [15]).

In their general form, reducible quadrature rules were introduced by MATTHYS [13] with the aim of proving A-stability results of numerical methods for (1.2). However, a study of the *explicit construction* of such general quadrature rules and a *unifying analysis* of the associated methods for (1.1) and (1.2) has not yet been undertaken.

A result of our analysis is that, for the construction of highly stable methods for (1.1) and (1.2), one should choose quadrature rules generated by highly stable LM methods for ordinary differential equations. Motivated by this result, we propose in this paper the use of the backward differentiation (BD) formulae.

In §2 we discuss the construction of (ρ,σ)-reducible quadrature rules, and derive an asymptotic expression for the quadrature error. Furthermore, we describe a technique for generating the quadrature weights in an efficient and stable manner. Particular attention is paid to the construction of the quadrature rules generated by the BD formulae.

In §3 we give a concise treatment of convergence and stability results of numerical methods for (1.1) and (1.2) employing (ρ,σ)-reducible quadrature rules. In addition, we present the stability regions of two classes of methods for (1.2) employing the BD formulae.

Numerical experiments with methods for (1.1) and (1.2) based on the BD formulae are reported in §4. For the solution of (1.1) our methods are compared with those employing the Gregory quadrature rules and with the highly stable, fifth order, block-implicit Runge-Kutta method proposed by DE HOOG & WEISS [8].

We remark that the main part of this paper is based on the institute report [17], and the reader interested in the technical details of some of the proofs omitted here is referred to that report.

2. REDUCIBLE QUADRATURE RULES

2.1. Derivation

The application of an LM method with real coefficients a_i and b_i (see e.g. LAMBERT [10, p.11]) to the quadrature problem

$$I'(x) = \phi(x), \qquad I(x_0) = 0, \tag{2.1}$$

yields the relations

$$\sum_{i=0}^{k} a_i I_{n-i} = h \sum_{i=0}^{k} b_i \, \phi(x_{n-i}), \qquad n \geq k, \tag{2.2}$$

for values I_n approximating $I(x_n) = \int_{x_0}^{x_n} \phi(y)dy$. If we assume that the starting values $I_0,\ldots,I_{k-1}$ are defined by

$$I_n = h \sum_{j=0}^{k-1} w_{nj}^{(s)} \, \phi(x_j), \qquad n = 0(1)k-1, \tag{2.3}$$

then I_n defined in (2.2) depends linearly on $\phi(x_0),\ldots,\phi(x_n)$. To be specific,

$$I_n = h \sum_{j=0}^{n} w_{nj} \, \phi(x_j), \qquad n \geq k, \tag{2.4}$$

where the weights w_{nj} satisfy the relations

$$\sum_{i=0}^{k} a_i \, w_{n-i,j} = \begin{cases} 0 & \text{for } j = 0(1)n-k-1, \\ & \qquad n \geq k, \\ b_{n-j} & \text{for } j = n-k(1)n. \end{cases} \tag{2.5}$$

In (2.5) we have defined $w_{nj} = w_{nj}^{(s)}$ for $n,j = 0(1)k-1$ and $w_{n,j} = 0$ for $j > \max\{n,k-1\}$. The rules (2.3) employing the weights $\{w_{nj}^{(s)}\}_{n,j=0}^{k-1}$ are called the *starting quadrature rules*, and denoted by S_k. Specific examples of starting rules are given in Appendix I.

By means of the relations (2.5) the weights w_{nj} can be generated provided that the starting quadrature rules S_k and the LM coefficients a_i and b_i are

given. The quadrature rules (2.4) constructed in this way are called (cf. [13]) (ρ,σ)-*reducible*, and denoted by $[S_k;(\rho,\sigma)]$. Here, ρ and σ are the first and second characteristic polynomial of the LM method defined by

$$\rho(\zeta) := \sum_{i=0}^{k} a_i \zeta^{k-i}, \quad \sigma(\zeta) := \sum_{i=0}^{k} b_i \zeta^{k-i}.$$

For subsequent use we recall from the theory of LM methods (see e.g. HENRICI [7], LAMBERT [10]) the following definitions.

DEFINITION 2.1. (1) A polynomial is said to *satisfy the root condition* if it has no zeros outside the closed unit disk and only simple zeros on the unit circle;
(2) it is said to *satisfy the strong root condition* if it satisfies the root condition and 1 is its only zero on the unit circle;
(3) an LM method (ρ,σ) is called *consistent of order p* if for all $y \in C^{p+1}[x_0,X]$:

$$\sum_{i=0}^{k} a_i y(x_{n-i}) - h \sum_{i=0}^{k} b_i y'(x_{n-i}) = C_{p+1} h^{p+1} y^{(p+1)}(x_n) + O(h^{p+2}) \text{ as } h \to 0$$

where $C_{p+1} \neq 0$;
(4) the constant $C^*_{p+1} = C_{p+1}/\sigma(1)$ is called the *normalized error constant*;
(5) an LM method (ρ,σ) is convergent (of order 1) if (i) $\rho(1) = 0$, $\rho'(1) = \sigma(1)$ and (ii) ρ satisfies the root condition.

2.2. Explicit construction of the quadrature weights

Arranging the weights w_{nj} in a matrix of the form

$$(2.6)\quad W = \left[\begin{array}{ccc|ccc} w_{00} & \cdots & w_{0,k-1} & & & \\ \vdots & & & & & \\ w_{k-1,0} & \cdots & w_{k-1,k-1} & & & \\ \hline w_{k0} & \cdots & w_{k,k-1} & w_{kk} & & \\ \vdots & & \vdots & \vdots & \ddots & \\ w_{n0} & \cdots & w_{n,k-1} & w_{nk} & \cdots & w_{nn} \\ \vdots & & \vdots & \vdots & & \vdots \end{array}\right] = \left[\begin{array}{c|c} S_k & O \\ \hline W_k & \Omega \end{array}\right]$$

we observe from (2.5) that the entry w_{nj} in the j-th column of W depends only on $w_{n-k,j},\ldots,w_{n-1,j}$. As a consequence, only the weights in the matrix W_k in (2.6) depend on the entries of S_k. The remaining weights (i.e. the entries of Ω) are independent of the starting quadrature rules. Moreover, due to the zero entries in the upper-triangular part of W, one can easily derive from (2.5) (with $j \geq k$) that Ω is a semi-circulant matrix, viz.

$$(2.7)\quad \Omega = \begin{bmatrix} \omega_0 & & & \\ \omega_1 & \omega_0 & & \\ \omega_2 & \omega_1 & \omega_0 & \\ \cdot & \omega_2 & \omega_1 & \omega_0 \\ \cdot & & \ddots & \ddots \\ \cdot & & & \ddots \end{bmatrix},$$

where the sequence $\{\omega_n\}_{n=0}^{\infty}$ satisfies

$$(2.8a)\quad \begin{cases} a_0\omega_0 = b_0 \\ a_0\omega_1 + a_1\omega_0 = b_1 \\ \quad\cdots \qquad\qquad \cdots \\ a_0\omega_k + a_1\omega_{k-1} + \ldots + a_k\omega_0 = b_k \end{cases}$$

$$(2.8b)\quad a_0\omega_n + a_1\omega_{n-1} + \ldots + a_k\omega_{n-k} = 0, \quad n \geq k+1.$$

From (2.6) and (2.7) it is obvious that $w_{nj} = \omega_{n-j}$ for $n-j \geq 0$, $j \geq k$.

Thus, for the construction of the quadrature weights W it is sufficient to generate the first k columns by means of (2.5) (yielding W_k) and to generate the sequence $\{\omega_n\}$ by means of (2.8).

2.3. Asymptotic expression for the quadrature error

In [13, Lemma 2] MATTHYS proved that the order of a (ρ,σ)-reducible quadrature formula is at most the order of the underlying LM method (ρ,σ). In this section we shall derive a precise expression for the quadrature error Q_n defined by

$$Q_n[\phi] := I_n - I(x_n) = h \sum_{j=0}^{n} w_{nj}\, \phi(x_j) - \int_{x_0}^{x_n} \phi(y)dy.$$

Since, by construction, the value I_n obtained with (2.4) is identical to the value I_n resulting from the application of the LM method (ρ,σ) to the differential equation (2.1) with starting values $I_0,\ldots,I_{k-1}$ defined in (2.3), we can apply the convergence theorem of LM methods for ordinary differential equations. The following result holds.

THEOREM 2.1. *Let (ρ,σ) be a convergent LM method of order p with normalized error constant C^*_{p+1}. Assume that the quadrature errors in the starting rules S_k have the asymptotic expansion*

$$Q_i[\phi] = d_i h^{s_i} \phi^{(s_i-1)}(x_0) + O(h^{s_i+1}) \quad \text{as } h \to 0,\ i = 0(1)k-1.$$

Let $s = \min\{s_0,\ldots,s_{k-1}\}$ and define, for $i = 0(1)k-1$, $d_i^* = d_i$ if $s_i = s$ and $d_i^* = 0$ if $s_i > s$. Then the quadrature error $Q_n[\phi]$ associated with the quadrature rules $[S_k;(\rho,\sigma)]$ assumes the form

$$(2.9) \qquad Q_n[\phi] = -C^*_{p+1} h^p \{\phi^{(p-1)}(x_n) - \phi^{(p-1)}(x_0)\} + O(h^{p+1})$$

$$+ d_n^* h^s + O(h^{s+1}) \quad \text{as } h \to 0,\ n \to \infty \text{ with } nh \text{ fixed},$$

where d_n^* is the solution of $\sum_{i=0}^{k} a_i d^*_{n-i} = 0$ $(n \geq k)$ with starting values

$d_0^*,\ldots,d_{k-1}^*$.

PROOF. p-th order consistency implies that $Q_n = Q_n[\phi]$ satisfies the error equation

$$(2.10) \qquad \sum_{i=0}^{k} a_i Q_{n-i} = - C_{p+1} h^{p+1} \phi^{(p)}(x_n) + O(h^{p+2}) \text{ as } h \to 0,$$

where C_{p+1} denotes the error constant of (ρ,σ). On writing $Q_n = Q_n^{(1)} + Q_n^{(2)}$, where $Q_n^{(1)}$ represents the solution of (2.10) with zero starting values and where $Q_n^{(2)}$ represents the solution of the homogeneous version of (2.10) with starting values $Q_0,\ldots,Q_{k-1}$, it is readily seen that

$$Q_n^{(2)} = d_n^* h^s + O(h^{s+1}).$$

The expression for $Q_n^{(1)}$ follows by applying techniques described in HENRICI [7, p.250]. □

Since the polynomial ρ satisfies the root condition, the sequence $\{d_n^*\}$ is uniformly bounded. This observation together with (2.9) yields

COROLLARY 2.1. *If the starting rules* S_k *are of order at least* p, *and if the* LM *method* (ρ,σ) *is convergent of order* p, *then the quadrature rules* $[S_k;(\rho,\sigma)]$ *are convergent of order* p. *To be specific*

$$|Q_n[\phi]| \leq A h^p \text{ as } h \to 0,\ n \to \infty,\ nh \text{ fixed}$$

where A *is a constant independent of* n *and* h. □

2.4. Asymptotic behaviour of the quadrature weights

From (2.5) it is immediate that for j = 0(1)k-1 and n sufficiently large

$$(2.11) \qquad \sum_{i=0}^{k} a_i w_{n-i,j} = 0.$$

Since (2.11) and also (2.8b) are homogeneous difference equations with constant coefficients, it will be clear that the asymptotic behaviour of the quadrature weights is determined by the location of the zeros of the polynomial ρ. The following theorem holds.

THEOREM 2.2. *Let* (ρ,σ) *be a convergent* LM *method. Then*

(i) *the weights* w_{nj} *generated by* (ρ,σ) *are uniformly bounded.*

If, in addition, ρ *satisfies the strong root condition, then*

$$\text{(ii)} \qquad \lim_{n\to\infty} w_{nj} = \bar{w}_j = \frac{1}{\rho'(1)} \sum_{i=0}^{k-1} \alpha_i w_{n_j-1-i} \quad \text{for } j = 0(1)k-1.$$

where n_j *denotes the smallest integer such that* (2.11) *holds, and where* α_i *are the coefficients of the deflated polynomial*

$$\text{(2.12)} \qquad \sum_{i=0}^{k-1} \alpha_i \zeta^{k-1-i} := \rho(\zeta)/(\zeta-1).$$

Furthermore

$$\text{(iii)} \qquad \lim_{n\to\infty} w_{nj} = \lim_{n\to\infty} \omega_n = \bar{\omega} = 1 \quad \text{for } j \geq k,$$

PROOF. See WOLKENFELT [17]. □

In order to verify the results of theorem 2.2, we computed the sequences $\{w_{nj}\}$, $n \geq k$, $j = 0(1)k-1$, and $\{\omega_n\}$ for the backward differentiation formulae. We observed however a *linear growth of rounding errors* which eventually destroyed the convergence to the limits expected from theorem 2.2. An explanation for this divergent behaviour is given by the fact that the homogeneous difference equations (2.8b) and (2.11) are marginally unstable due to the zero $\zeta = 1$ of ρ.

In order to construct numerically convergent sequences we have transformed the recurrence relations (2.8b) and (2.11) into strongly stable recurrence relations. This procedure is described in the following lemma.

LEMMA 2.1. *Let the sequence* $\{y_n\}_0^\infty$ *satisfy the difference equation*

$$\sum_{i=0}^{k} a_i y_{n-i} = 0, \qquad n \geq k, \tag{2.13}$$

with starting values $y_0,\ldots,y_{k-1}$, *and let the associated characteristic polynomial* ρ *satisfy the strong root condition. Then*

$$y_n = \bar{y}/\rho'(1) + v_n \quad \textit{for all } n \geq 0 \tag{2.14}$$

where

$$\bar{y} = \sum_{i=0}^{k-1} \alpha_i y_{k-1-i} \tag{2.15}$$

and where v_n *is the solution of*

$$\sum_{i=0}^{k-1} \alpha_i v_{n-i} = 0, \qquad n \geq k \tag{2.16}$$

with starting values $v_n = y_n - \bar{y}/\rho'(1)$, $n = 0(1)k-1$. *Here, the coefficients* α_i *are defined in* (2.12).

PROOF. In order to simplify the notation, we give the proof only for the case that all zeros of ρ are simple. Since y_n satisfies (2.13) the solution can be written in the form $y_n = c_1\zeta_1^n + c_2\zeta_2^n + \ldots + c_k\zeta_k^n$, where $\zeta_1 = 1$ and $|\zeta_i| < 1$, $i = 2(1)k$. Therefore, $y_n = c_1 + v_n$, where $c_1 = \bar{y}/\rho'(1)$ (see HENRICI [7, p.239]) and $v_n = c_2\zeta_2^n + \ldots + c_k\zeta_k^n$. Obviously, v_n is the solution of a homogeneous difference equation with characteristic polynomial $\rho(\zeta)/(\zeta-1)$. This yields (2.16). Finally, equality (2.14) is obtained by taking the correct starting values for v_n, that is $v_n := y_n - \bar{y}/\rho'(1)$ for $n = 0(1)k-1$. □

The above lemma states that instead of computing the sequence $\{y_n\}$ one may also compute the sequence $\{v_n\}$ and the limit $\bar{y}/\rho'(1)$. Since the characteristic polynomial associated with (2.16) has its roots strictly inside the unit circle, the sequence $\{v_n\}$ converges to zero, and therefore

$y_n \to \bar{y}/\rho'(1)$, *even in the presence of rounding errors*. We have followed this procedure for computing the weights of the quadrature rules which are reducible to the backward differentiation formulae (see §2.5).

An important consequence of Theorem 2.2 combined with the construction described in lemma 2.1 is that the computation of the quadrature weights can be stopped as soon as the limits $\bar{w}_j$ and $\bar{\omega} = 1$ are reached within machine precision. This implies that only a restricted number of quadrature weights need to be generated (and stored).

2.5. The quadrature rules generated by the backward differentiation formulae

Using the theory given in the previous sections, it is possible to construct rather unconventional quadrature rules $[S_k;(\rho,\sigma)]$. In this section we focus our attention on the class of quadrature rules which originate by choosing for (ρ,σ) the backward differentiation (BD) formulae. It turns out that with this class highly stable quadrature methods for the solution of (1.1) and (1.2) can be defined.

For k = 2(1)6 the coefficients $a_0,\ldots,a_k$ and b_0 ($b_1=\ldots=b_k = 0$) can be found in e.g. LAMBERT [10,p.242] and are reproduced here in Table 2.1 together with their order and normalized error constant.

k	b_0	a_0	a_1	a_2	a_3	a_4	a_5	a_6	p	C^*_{p+1}
2	2	3	-4	1					2	-1/3
3	6	11	-18	9	-2				3	-1/4
4	12	25	-48	36	-16	3			4	-1/5
5	60	137	-300	300	-200	75	-12		5	-1/6
6	60	147	-360	450	-400	225	-72	10	6	-1/7

Table 2.1. The coefficients, order and normalized error constant of the k-step BD formulae ($b_1=\ldots=b_k = 0$).

We shall now discuss the construction of the quadrature weights in more detail. Due to the vanishing of the coefficients $b_1,\ldots,b_k$ the recurrence relations (2.5) and (2.8) can be simplified. For j = 0(1)k-1, (2.5) reduces

to

$$(2.17)\qquad \sum_{i=0}^{k} a_i w_{n-i,j} = 0, \quad n \geq k$$

with starting values $w_{0j} = 0$, $w_{nj} = w_{nj}^{(s)}$, $n = 1(1)k-1$. For $j \geq k$, we set $w_{nj} = \omega_{n-j}$ $(n-j \geq 0)$ and determine ω_n from (compare (2.8))

$$(2.18)\qquad \sum_{i=0}^{k} a_i \omega_{n-i} = 0, \quad n \geq 1$$

with starting values $\omega_0 = b_0/a_0, \omega_{-1} = \ldots = \omega_{-k+1} = 0$.

For the starting rules S_k we have chosen quadrature rules of maximal precision (order k+1).

Only for $k = 2$ the zeros of ρ are known in explicit form ($\zeta_1 = 1, \zeta_2 = 1/3$), so that explicit expressions for the quadrature weights can be determined. Using the starting rules S_2 ($w_{0j}^{(s)} = 0$, $w_{10}^{(s)} = w_{11}^{(s)} = 1/2$) we derived in [17] the expressions

$$\begin{cases} w_{nj} = 3/4(1-(1/3)^n), & n \geq 1, \quad j = 0,1 \\ w_{nj} = \omega_{n-j} = 1-(1/3)^{n-j+1}, & n-j \geq 0, \quad j \geq 2. \end{cases}$$

For $k \geq 3$, the weights must be generated numerically, and for this purpose we followed the procedure described in lemma 2.1. Application of this lemma to (2.17) yields that for fixed j $(j = 0(1)k-1)$ $w_{nj} = \bar{w}_j + v_n^{(j)}$, where $v_n^{(j)}$ satisfies (2.16) with starting values $v_n^{(j)} = w_{nj}^{(s)} - \bar{w}_j$, $n = 0(1)k-1$, and where $\bar{w}_j$ is, in view of theorem 2.2, given by

$$\bar{w}_j = \frac{1}{b_0} \sum_{i=0}^{k-1} \alpha_i w_{k-1-i,j}^{(s)}, \qquad j = 0(1)k-1.$$

Here, we have used that $\rho'(1) = \sigma(1) = b_0$. The reader may verify that for $k = 4$ with the starting rules

$$S_4 = \frac{1}{24} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 9 & 19 & -5 & 1 \\ 8 & 32 & 8 & 0 \\ 9 & 27 & 27 & 9 \end{bmatrix}$$

the limits $\bar{w}_0 = 79/144$, $\bar{w}_1 = 93/144$, $\bar{w}_2 = 213/144$ and $\bar{w}_3 = 119/144$ are obtained. The sequence $\{\omega_n\}$ defined in (2.18) is computed by setting $\omega_n = 1+v_n$ and computing v_n from (2.16) with starting values $v_0 = 1-\omega_0$, $v_{-1} = \ldots = v_{-k+1} = 1$. In order to get an impression of the rate of convergence, we have determined the value $\bar{n}$ such that for $n \geq \bar{n}$ $|v_n| = |\omega_n - 1| \leq 10^{-15}$ (here, 10^{-15} is approximately the precision of our computer). These values are listed below.

k	2	3	4	5	6
$\bar{n}$	31	40	59	97	227

Thus, only a finite number ($\bar{n}$) of quadrature weights ω_n have to be generated.

Application of theorem 2.1 yields that the error in the quadrature rules generated by the BD formulae is given by

$$Q_n^{(BD)}[\phi] = \frac{1}{k+1} h^k \{\phi^{(k-1)}(x_n) - \phi^{(k-1)}(x_0)\} + O(h^{k+1}) \text{ as } h \to 0.$$

Since we have chosen starting rules S_k of order k+1, the principal term in the quadrature error is determined only by the BD formula.

3. DISCRETIZATION METHODS FOR FUNCTIONAL EQUATIONS OF THE VOLTERRA TYPE

We shall now employ the (ρ,σ)-reducible quadrature rules discussed in §2 for the discretization of Volterra functional equations. In this paper, we have restricted our considerations to Volterra integral equations of the second kind and to integro-differential equations given by (1.1) and (1.2), respectively. Results for reducible quadrature rules applied to first kind Volterra equations can be found in [18].

The methods we present below can be applied in a step-by-step fashion. The starting values, which are usually required, are assumed to result from some adequate starting procedure. If $w_{nn} \neq 0$ (i.e. $b_0 \neq 0$) then the methods are semi-explicit and, in case of a nonlinear continuous problem, the solution of a nonlinear equation is needed. The computational effort of the methods is approximately $\frac{1}{2}N^2$ kernel evaluations ($N = (X-x_0)/h$) increased

by N evaluations of g in case of (1.1) and N evaluations of F in case of (1.2). Further the methods are also applicable to systems of Volterra type equations.

In the following sections convergence of the methods is established and stability results are given. In the statement of the convergence theorems we assume that the quadrature rules $[S_k;(\rho,\sigma)]$ are convergent of order p (see corollary 2.1 for sufficient conditions).

3.1. Volterra integral equations of the second kind

Discretizations of (1.1) using (1.3) yields the so-called direct quadrature method

$$f_n = g(x_n) + h \sum_{j=0}^{n} w_{nj} K(x_n,x_j,f_j), \qquad n \geq k . \tag{3.1}$$

The required starting values are $f_0 = g(x_0)$, $f_1,\ldots,f_{k-1}$. Convergence of the method (3.1) is established in the following theorem.

THEOREM 3.1. *In addition to the conditions for existence and uniqueness of a sufficiently smooth solution* f *to* (1.1) *assume that*

(i) *the method* (3.1) *employs reducible quadrature rules* $[S_k;(\rho,\sigma)]$ *of order* p;

(ii) *the errors in the starting values* $f_0,\ldots,f_{k-1}$ *are of order* s, i.e. $|f_i - f(x_i)| = O(h^s)$ as $h \to 0$, $i = 0(1)k-1$.

Then the method (3.1) *is convergent of order* r, *where* $r = \min(p,s+1)$; *to be specific*

$$|f_n - f(x_n)| \leq Ah^r \text{ as } h \to 0,\ n \to \infty,\ nh \text{ fixed},$$

where A *is a constant independent of* n *and* h.

PROOF. In view of Theorem 2.2 the quadrature weights are uniformly bounded, and (i) states that the quadrature error is of order p. Application of a general convergence theorem for step-by-step quadrature methods (see BAKER [2, p.836]) yields the result. □

The stability behaviour of a numerical method for (1.1) is usually analyzed by applying the method with a fixed positive stepsize h to the test equation (see e.g. BAKER & KEECH [3])

$$f(x) = 1 + \lambda \int_0^x f(y)dy, \qquad \lambda \in \mathbb{C}.$$

This test equation is equivalent to the ODE test equation $f' = \lambda f$ and since by construction, the quadrature rules are equivalent to an LM method (ρ,σ), it is immediate that the stability results of LM methods for ordinary differential equations can be carried over directly to second kind Volterra equations. To be specific, the stability behaviour of the method (3.1) is determined by the stability polynomial $\rho(\zeta)-h\lambda\sigma(\zeta)$.

Thus, highly stable methods for solving ordinary differential equations can be used to generate highly stable methods for second kind Volterra equations. In particular, the use of the BD formulae is advocated when the kernel has a large Lipschitz constant.

3.2. Volterra integro-differential equations

The application of methods for ordinary differential equations in conjunction with numerical quadrature yields a rich source of numerical methods for (1.2). In this paper we consider the use of a linear $\tilde{k}$-step method $(\tilde{\rho},\tilde{\sigma})$ combined with (ρ,σ)-reducible quadrature rules (see also [9,13]) to obtain the methods

$$\begin{aligned} \sum_{i=0}^{\tilde{k}} \tilde{a}_i f_{n-i} &= h \sum_{i=0}^{\tilde{k}} \tilde{b}_i F(x_{n-i}, f_{n-i}, z_{n-i}), \qquad n \geq k+\tilde{k}, \\ z_n &= h \sum_{j=0}^{n} w_{nj} K(x_n, x_j, f_j), \qquad n \geq k. \end{aligned} \tag{3.2}$$

In general, the required starting values are $f_0,\ldots,f_{k+\tilde{k}-1}$. The methods (3.2) are denoted by $[(\tilde{\rho},\tilde{\sigma});W]$ where $W = [S_k;(\rho,\sigma)]$.

In the following Theorem convergence of the methods (3.2) is established.

THEOREM 3.2. *In addition to the conditions for existence and uniqueness of a smooth solution* f *to* (1.2) *assume that*

(i) *the LM method* $(\tilde{\rho},\tilde{\sigma})$ *is convergent of order* $\tilde{p}$;

(ii) *the quadrature rules* $W = [S_k;(\rho,\sigma)]$ *are of order* p;

(iii) *the errors in the starting values* $f_0,\ldots,f_{k+\tilde{k}-1}$ *are of order* s.
Then the method $[(\tilde{\rho},\tilde{\sigma});W]$ *is convergent of order* r, *where* $r = \min(\tilde{p},p,s)$; *to be specific*

$$|f_n - f(x_n)| \le Ah^r, \quad \text{as } h \to 0,\ n \to \infty,\ nh \text{ fixed},$$

where A *is a constant independent of* n *and* h.

PROOF. Along the lines indicated by LINZ [11]. □

The stability behaviour of a numerical method for (1.2) is usually analyzed by applying that method with a fixed positive stepsize h to the test equation (cf. [4,5,13])

$$f'(x) = \xi f(x) + \eta \int_0^x f(y)dy, \qquad \xi,\eta \in \mathbb{R}. \tag{3.3}$$

Following BRUNNER & LAMBERT [5] and MATTHYS [13] we come to the result that the method (3.2) is absolutely stable if the zeros of the stability polynomial

$$P(\zeta;h\xi,h^2\eta) := \rho(\zeta)[\tilde{\rho}(\zeta) - h\xi\tilde{\sigma}(\zeta)] - h^2\eta\sigma(\zeta)\tilde{\sigma}(\zeta) \tag{3.4}$$

lie inside the unit circle. Stability regions can be defined in the $(h\xi,h^2\eta)$-plane, and in [5] the regions of some first and second order methods were given. Below we give the stability regions of the k-step BD methods using BD-reducible quadrature rules and the Gregory quadrature rules, respectively. To be specific, we consider the methods

[BD;BD]: $(\tilde{\rho},\tilde{\sigma})$ is the k-step BD formula (k=2(1)6)
$W = [S_k;(\rho,\sigma)]$ where (ρ,σ) is also the k-step BD formula;

[BD;AM]: $(\tilde{\rho},\tilde{\sigma})$ is the k-step BD formula (k=2(1)6)
$W = [S_{k-1};(\rho,\sigma)]$ where (ρ,σ) is the (k-1)-step Adams-Moulton formula.

Note that the Gregory quadrature rules of order k are generated by the (k-1)-step Adams-Moulton formula with starting rules S_{k-1}. More details about these quadrature rules are given in Appendix II.

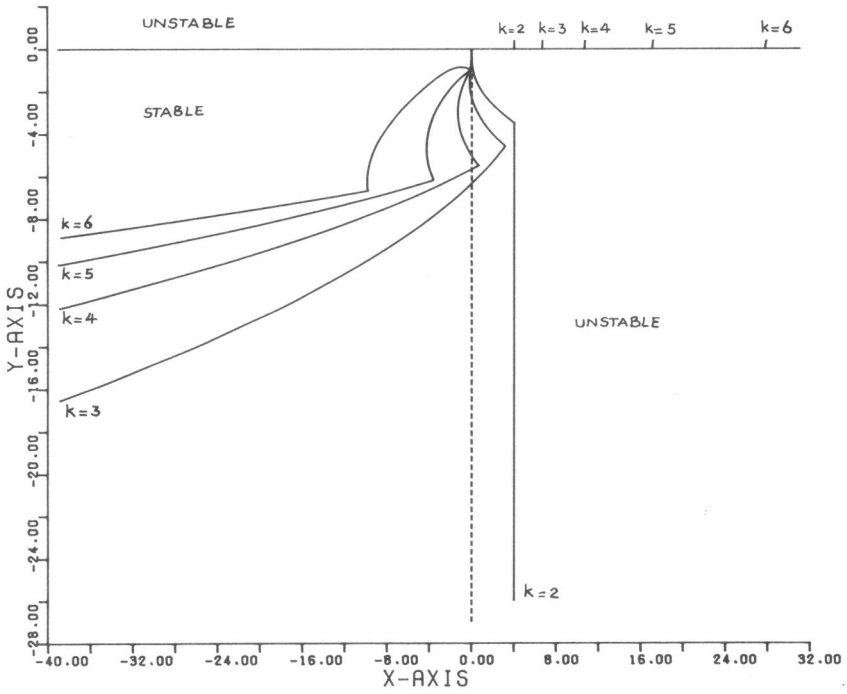

Figure 3.1. Stability regions of the [BD;AM] methods

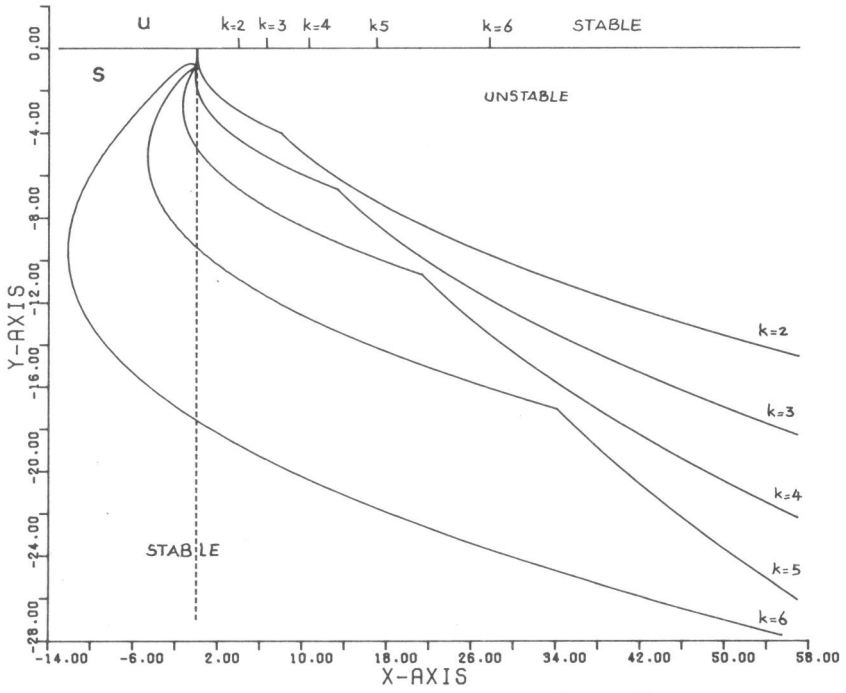

Figure 3.2. Stability regions of the [BD;BD] methods

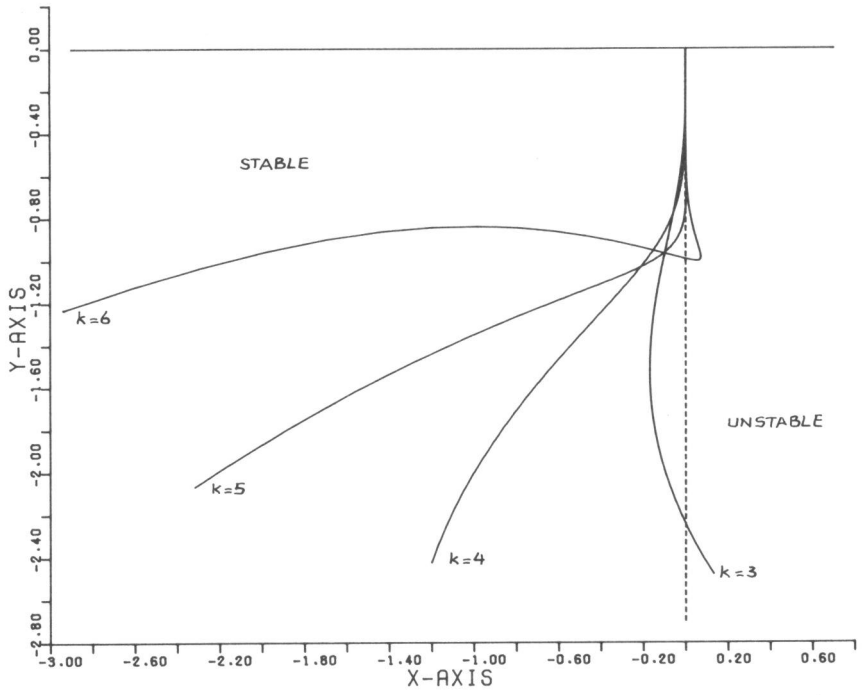

Figure 3.3. Close-up of Fig. 3.1 near the origin

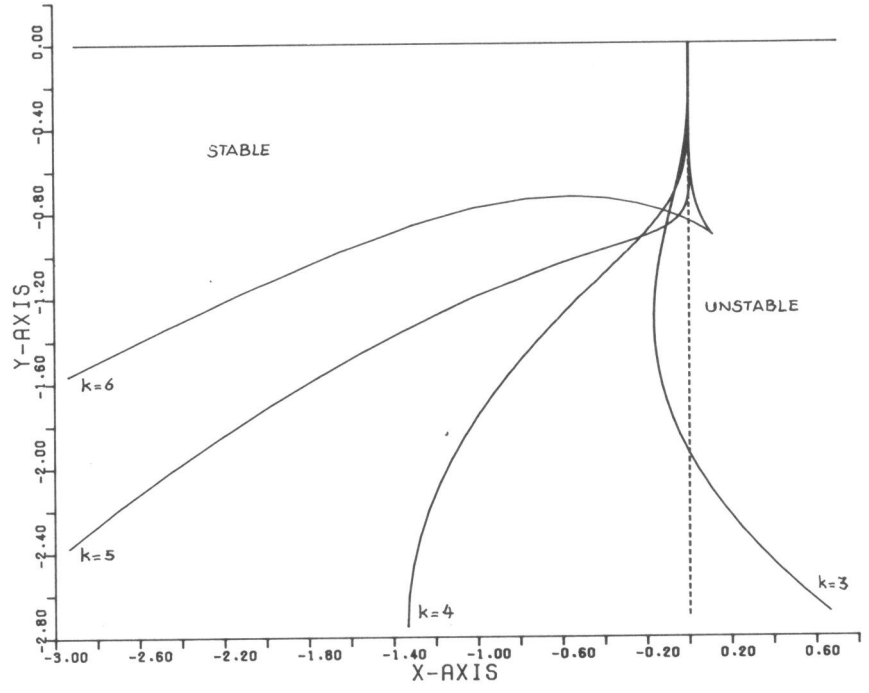

Figure 3.4. Close-up of Fig. 3.2 near the origin

The stability regions of the [BD;AM] and [BD;BD] methods were computed by means of a boundary locus method (see [10, p.82]). Taking $\zeta = e^{i\phi}$ in (3.4) and setting $P(e^{i\phi};h\xi,h^2\eta) = 0$ yields the equations

$$(3.5) \qquad h^2\eta = \frac{\rho(e^{i\phi})}{\sigma(e^{i\phi})}\left[\frac{\tilde{\rho}(e^{i\phi})}{\tilde{\sigma}(e^{i\phi})} - h\xi\right], \qquad \phi \in [0,\pi]$$

which has to be solved for real values of $h\xi$ and $h^2\eta$. In general, equation (3.5) yields a unique point $(h\xi,h^2\eta)$ of the boundary locus. For some values of ϕ, however, degenerate solutions of (3.5) may arise. As an example, we obtain for $\phi = \pi$ the set of points $\{(h\xi,h^2\eta) \mid h^2\eta = \beta(\tilde{\beta}-h\xi)\}$, where $\beta = \rho(-1)/\sigma(-1)$ and $\tilde{\beta} = \tilde{\rho}(-1)/\tilde{\sigma}(-1)$.

In Figure 3.1 and 3.2 plots of the stability regions are given. In order to display the regions corresponding to different orders in one diagram, we have used a square root scale in the vertical direction; to be specific, the plots are given in the (x,y)-plane, where $x = h\xi$ and $y = G(h^2\eta)$ with $G(v)$:= if $v \geq 0$ then $\sqrt{v}$ else $-\sqrt{|v|}$. An additional advantage of this scaling is that for fixed ξ and η, and decreasing h, the point (x,y) moves along a straight line towards the origin. Figure 3.3 and 3.4 display the shape of the stability region near the origin.

It is seen that the regions of the [BD;BD] methods are substantially larger than those of the [BD;AM] methods. Furthermore, it is observed that the regions of both the second order [BD;AM] and the second order [BD;BD] include the third quadrant $\{(h\xi,h^2\eta) \mid h\xi < 0,\ h^2\eta < 0\}$, which is the region where also the solution of the continuous problem (3.3) is stable.

4. NUMERICAL EXPERIMENTS

We have applied the methods (3.1) and (3.2) employing BD-reducible quadrature rules to a number of test problems with known exact solution, in order to obtain insight into their performance in actual computation. In our implementation the weights were generated explicitly as described in §2.5.

Our purpose was to test the convergence and stability properties of our methods, rather than design and implement an automatic integral (e.g. integro-

differential) equation solver. Therefore, no special strategies have been incorporated in our implementation. Integration was performed with a constant stepsize h. The necessary starting values were computed from the exact solution. The nonlinear equations arising in the case of test problems which are nonlinear in f, were solved by Newton-Raphson iteration. As initial guess for f_n the value f_{n-1} was used, and iteration was stopped as soon as the (relative) Newton-correction was below 10^{-12}. All calculations have been performed on a CDC CYBER 750 installation using 14 significant digits.

In the table of results we have tabulated for different orders and a sequence of stepsizes, the number of correct decimal digits (*cd*) at the endpoint of integration xe = x_0+Nh

$$cd := -{}^{10}\log|f_N - f(xe)|.$$

Note that for a method of order p and h sufficiently small one should expect theoretically that

$$cd(h/2) = cd(h) + 0.3.p \qquad (0.3 \simeq {}^{10}\log 2).$$

4.1. Second kind Volterra integral equations

The numerical methods (3.1) employing the BD-reducible quadrature rules are indicated by BDp where p denotes the order (p=2(1)6). For comparison, we have also listed the results obtained with the p-th order Gregory rules (which are reducible to the p-th order Adams-Moulton formula). We shall denote these methods by AMp. In addition, our methods are also compared with the fifth order, three-stage, block-implicit Runge-Kutta method of de Hoog and Weiss ([8, scheme (3.3)/(7.1)]. The computational effort of this method, which we shall denote by dHW5, is roughly $\frac{9}{2}N^2$ whereas the BD and AM methods need only $\frac{1}{2}N^2$ kernel evaluations. In order to compare the accuracies obtained by the different fifth order methods at the same computational costs, we have applied dHW5 with a stepsize $h^* = 3h$.

Problem 4.1.1. (renewal equation from FELLER [6])

$$f(x) = \tfrac{1}{2}x^2 \exp(-x) + \tfrac{1}{2}\int_0^x (x-y)^2 \exp(y-x) f(y)dy, \quad 0 \le x \le 6,$$

with exact solution $f(x) = \frac{1}{3} - \frac{1}{3}\exp(-3x/2)\{\cos(\tfrac{1}{2}x\sqrt{3}) + \sqrt{3}\sin(\tfrac{1}{2}x\sqrt{3})\}$. In Table 4.1.1. the results are tabulated for various choices of h (the results for the AM method are given in parentheses).

h^{-1}	BD2	(AM2)	BD3	(AM3)	BD4	(AM4)	BD5	(AM5)	BD6	(AM6)	dHW5
4	2.7	(4.7)	3.4	(3.3)	2.9	(3.6)	3.7	(4.2)	4.1	(4.9)	5.1
8	3.5	(5.9)	3.9	(4.1)	3.9	(4.7)	4.9	(5.5)	5.6	(6.5)	6.5
16	4.3	(7.1)	4.7	(5.0)	5.1	(5.9)	6.3	(6.9)	7.3	(8.3)	8.0
32	5.2	(8.3)	5.5	(5.9)	6.2	(7.1)	7.8	(8.4)	9.1	(10.0)	9.4
64	6.1	(9.5)	6.4	(6.8)	7.4	(8.3)	9.2	(9.9)	10.8	(11.9)	10.9

Table 4.1.1. Number of correct digits at x = 6 for problem 4.1.1.

From this table we observe that the methods BD2 and AM2 behave as a third and fourth order method, respectively. This higher order of convergence is explained by the fact that the coefficients of the h^2-term in the expression for the quadrature error vanish for this particular problem. This can be verified using (2.9).

For the remaining methods the correct order of convergence is obvious. Note that the AM methods are more accurate than the BD methods (approximately 0.5-1 decimal digit) which is probably due to the smaller error constant. The Runge-Kutta method dHW5 is more accurate than BD5 and AM5. We remark that the method dHW5 is fully implicit, which has the disadvantage that even in the case of a scalar linear problem the solution of a system of linear equations is needed.

Problem 4.1.2. (nonlinear)

$$f(x) = \cos x - \sin 2x - \sin x + 3\int_0^x \cos(x-y) f^2(y)dy, \quad 0 \le x \le 1.5$$

with exact solution $f(x) = \cos x$.

h^{-1}	BD2	(AM2)	BD3	(AM3)	BD4	(AM4)	BD5	(AM5)	BD6	(AM6)	dHW5
8	0.4	(0.5)	1.4	(1.0)	1.8	(2.3)	2.8	(2.9)	3.3	(3.9)	2.6
16	0.6	(0.9)	2.2	(1.6)	2.5	(3.2)	4.0	(3.8)	4.4	(5.2)	4.2
32	1.0	(1.5)	3.0	(2.3)	3.5	(4.3)	5.3	(5.0)	5.9	(6.7)	5.8
64	1.5	(2.1)	3.8	(3.2)	4.6	(5.4)	6.7	(6.4)	7.5	(8.4)	7.3
128	2.1	(2.7)	4.7	(4.0)	5.7	(6.6)	8.2	(7.8)	9.2	(10.1)	8.8

Table 4.1.2. Number of correct digits at x = 1.5 for problem 4.1.2.

Again the correct order of convergence is obvious. The AM methods of even order are more accurate than the BD methods, whereas for odd order the BD methods yield better results. Again the method dHW5 is more accurate than BD5 and AM5 (except for h = 1/8).

Problem 4.1.3. (nonlinear)

$$f(x) = g(x) - \lambda \int_0^x \frac{1+x}{1+y} f^2(y)dy, \qquad 0 \le x \le xe$$

with exact solution $f(x) = [1+(1+x)\exp(\mu x)]^{\frac{1}{2}}$ if we choose $g(x) = f(x) + \frac{\lambda}{\mu}(1+x)[\mu\, \ell n(1+x) + \exp(\mu x)-1]$. For $\mu = -10$, $\lambda = 10$ this problem was suggested by DE HOOG and WEISS [8]. In order that the stepsize is not restricted by accuracy, we considered a slowly varying exact solution and chose $\mu = -1$. This problem was chosen in order to illustrate the stability behaviour of our methods. We considered the values $\lambda = 1,10,100,1000$ and 10000, which makes the above problem increasingly "stiff". From ODE-theory we recall that the BD methods are stiffly stable (see [10,p.234] for a definition). Furthermore, the AM methods have finite stability regions (for $p \ge 3$) with a real stability boundary β, where $\beta = 6,3,1.8$ and 1.2 for $p = 3,4,5$ and 6 respectively. The method dHW5 is L-stable (see [8]). Thus, we expect unstable behaviour only for the AM methods if $|h\lambda| > \beta$. The endpoint of integration was xe = 192h. Table 4.1.3 gives the results (instability is indicated by an asterisk).

h^{-1}	λ	BD2	(AM2)	BD3	(AM3)	BD4	(AM4)	BD5	(AM5)	BD6	(AM6)	dHW5
	1	5.0	(5.7)	7.0	(7.8)	8.8	(9.7)	10.4	(11.1)	10.8	(11.9)	12.6
	10	5.1	(5.7)	7.0	(8.2)	8.8	(*)	10.7	(*)	11.1	(*)	11.0
4	100	5.1	(5.7)	7.0	(*)	8.8	(*)	10.4	(*)	10.3	(*)	10.7
	1000	5.1	(1.1)	7.0	(*)	8.8	(*)	10.1	(*)	10.3	(*)	10.7
	10000	5.1	(0.6)	7.0	(*)	8.8	(*)	10.0	(*)	10.6	(*)	11.4
	1	5.1	(5.7)	7.0	(7.8)	8.7	(9.6)	10.3	(11.1)	11.8	(12.1)	11.0
	10	5.1	(5.7)	7.1	(7.8)	8.8	(9.7)	10.4	(11.6)	11.2	(0.7)	9.4
16	100	5.1	(5.7)	7.1	(*)	8.8	(*)	10.5	(*)	10.9	(*)	8.6
	1000	5.1	(4.8)	7.1	(*)	8.8	(*)	10.5	(*)	10.8	(*)	8.6
	10000	5.1	(2.5)	7.1	(*)	8.8	(*)	11.2	(*)	10.3	(*)	8.6
	1	4.7	(5.3)	6.6	(7.5)	8.5	(9.4)	10.2	(11.2)	11.8	(12.5)	11.5
	10	4.9	(5.5)	6.9	(7.7)	8.8	(9.7)	10.6	(11.5)	12.2	(11.6)	9.5
64	100	4.9	(5.5)	6.9	(7.7)	8.8	(0.4)	10.5	(*)	11.0	(*)	8.1
	1000	4.9	(5.5)	6.9	(*)	8.8	(*)	11.2	(*)	10.7	(*)	7.8
	10000	4.9	(4.9)	6.9	(*)	8.8	(*)	11.0	(*)	10.6	(*)	7.7

Table 4.1.3. The number of correct digits at xe = 192h for problem 4.1.3.

For fixed h and increasing stiffness, the accuracy of the BD methods remains the same for p = 2,3 and 4, and roughly the same for BD5, whereas BD6 and dHW5 have a tendency towards a decreasing accuracy which is rather pronounced for dHW5 when h is small.

For non-stiff problems (λ = 1) the AM methods are more accurate than the BD methods. Further, dHW5 is more accurate than AM5 and BD5.

With increasing stiffness the AM methods become unstable depending on the value of h.

For h = 1/4, dHW5 performs better than BD5. For the mildly-stiff (λ = 10,100) and highly-stiff ($\lambda \geq 1000$) problems and h = 1/16 and 1/64 the superiority of BD5 over dHW5 is obvious.

4.2. Volterra integro-differential equations

In this section we report on some convergence and stability tests with the methods [BD;BD] and [BD;AM] specified in §3.2. Other experiments with the same methods can be found in the report [9].

Problem 4.2.1. (compare with LINZ [11], MAKROGLOU [12])

$$\begin{cases} f'(x) = 1 - x\exp(-x^2) + f(x) - 2\int_0^x xy\exp(-f^2(y))dy, & 0 \le x \le 2, \\ f(0) = 0 \end{cases}$$

with exact solution $f(x) = x$. In Table 4.2.1. the results are tabulated for different orders and stepsizes (the results for the [BD;AM] methods are given in parentheses).

h^{-1}	p = 2	p = 3	p = 4	p = 5	p = 6
10	1.3 (1.9)	3.0 (3.2)	2.8 (3.6)	3.9 (4.6)	4.1 (5.0)
20	1.9 (2.5)	3.6 (4.1)	3.9 (4.8)	6.2 (6.2)	5.7 (6.7)
40	2.5 (3.1)	4.4 (5.1)	5.1 (6.0)	7.4 (7.8)	7.5 (8.5)
80	3.1 (3.7)	5.3 (6.0)	6.3 (7.2)	8.6 (9.3)	9.3 (10.7)

Table 4.2.1. Number of correct digits at x = 2 for problem 4.2.1.

The correct order of convergence is obvious except for the 5th order [BD;BD]. The [BD;AM] methods are more accurate than the [BD;BD] methods.

Problem 4.2.2. (from BRUNNER & LAMBERT [5])

$$\begin{cases} f'(x) = -x - (1+x)^{-2} + \dfrac{1}{f(x)}\,\ell n\,\dfrac{2+2x}{2+x} + \displaystyle\int_0^x \frac{dy}{1+(1+x)f(y)}, & 0 \le x \le 10, \\ f(0) = 1, \end{cases}$$

with exact solution $f(x) = (1+x)^{-1}$. Within the precision given in Table 4.2.2. both methods give the same results, so that only one column per order is

given. From table 4.2.2. the correct order of convergence is obvious

h^{-1}	p=2	p=3	p=4	p=5	p=6
4	4.7	5.1	5.5	5.9	6.0
8	5.2	5.8	6.4	6.9	7.3
16	5.7	6.6	7.4	8.1	8.7
32	6.3	7.4	8.5	9.4	10.3
64	6.9	8.3	9.6	10.9	12.0

Table 4.2.2. Number of correct digits at x = 10 for problem 4.2.2.

The reader may verify that for this problem the integrand computed along the exact solution is a very smooth function of y. As a consequence, the quadrature error is negligible, which explains that both methods yield almost the same results.

Problem 4.2.3. (nonlinear, from [16])

$$f'(x) = [d(x) - \alpha f(x) - \beta z(x)]^3 - 1, \qquad f(0) = 1$$

$$z(x) = \int_0^x (x+\gamma y)^{\delta} f^3(y)dy.$$

Choosing $d(x) = 1+\alpha+\gamma^{-1}(1+\delta)^{-1}\beta x^{\delta+1}\{(1+\gamma)^{\delta+1}-1\}$ yields the exact solution $f(x) \equiv 1$. This problem was constructed in order to test whether the quantitative information of the stability regions, which are derived with the linear test equation (3.3), can also be used for nonlinear problems. We recall that the test equation (3.3) results from the variational equation of (1.2) on setting

$$(4.1) \qquad \xi(x) = \frac{\partial F}{\partial f}(x,f(x),z(x)), \quad \eta(x,y) = \frac{\partial F}{\partial z}(x,f(x),z(x)).\frac{\partial K}{\partial f}(x,y,f(y))$$

(where $z(x) = \int_0^x K(x,y,f(y))dy$) and assuming that ξ and η are constant (see [4,5,16]). Thus applying the linear stability theory of §3.2 in a local sense, and using (4.1) we obtain

$$\xi(x) = -3\alpha, \qquad \eta(x,x) = -9\beta x^{\delta}(1+\gamma)^{\delta}.$$

Hence, $|\eta(x,x)|$ increases monotonically, whereas $\xi(x)$ remains constant. We considered the case $\alpha = 40$, $\beta = 15$, $\gamma = 2$, $\delta = 3/2$ and $h = 1/8$. The values of α and h were chosen such that the vertical line $h\xi = -3h\alpha = -15$ is within the stability regions of the [BD;BD] methods. Therefore, it is expected that the [BD;BD] methods will integrate this problem in a stable manner. From the stability regions of the [BD;AM] methods one can predict, theoretically, the values of $h^2\eta$, and therefore the values of x for which the [BD;AM] method will be stable. The critical values of x are listed below

p	2	3	4	5	6
x_c	∞	5.20	3.67	3.07	2.77

Having stated our prediction, a final experiment must give a decisive answer. In table 4.2.3 we have listed the results of the [BD;AM] methods at some relevant meshpoints. The points were chosen as follows: for the p-th order [BD;AM] methods we have listed one point close to the x-value (x_c) at which instability is predicted by the theory, and another point at which the integration process was (mostly prematurely) terminated. In the table 4.2.3 the point x_c is marked with a dotted line. In table 4.2.4 we give the results of the [BD;BD] methods.

x	p=2	p=3	p=4	p=5	p=6
1.000	4.15	4.66	6.13	6.61	6.96
2.750	4.70	5.39	7.02	7.69	7.84
3.000	4.74	5.46	7.10	7.83	7.58
3.625	4.84	5.61	7.26	7.76	6.76
5.125	5.01	5.85	7.51	5.93	3.32
5.625	5.05	5.91	7.57	4.84	1.90
6.625	5.14	6.01	7.49	2.39	*
9.125	5.30	6.20	2.94	*	*
14.250	5.53	3.57	*	*	*
16.000	5.60	*	*	*	*

Table 4.2.3. The number of correct digits for problem 4.2.3 obtained with the [BD;AM] methods (h=1/8)

x	p=2	p=3	p=4	p=5	p=6
1.0	3.35	5.39	5.73	6.72	7.00
3.0	4.27	5.50	5.40	7.19	7.08
5.0	4.49	5.88	6.83	7.72	8.34
7.0	4.65	6.11	7.06	7.94	8.26
16.0	5.07	6.61	7.54	8.42	9.04

Table 4.2.4. The number of correct digits for problem 4.2.3 obtained with the [BD;BD] methods (h=1/8)

From these tables we conclude that for this problem:

(i) the [BD;BD] methods are stable; in fact, the accuracy increases;

(ii) the [BD;AM] methods become unstable for $p \geq 3$; however, for p=3,4 the (local) theory predicts instability for smaller values of x than shown in actual computation. For p=5 and 6 the prediction is rather precise.

5. CONCLUDING REMARKS

In this paper, we have employed linear multistep methods for ordinary differential equations to construct quadrature methods for solving functional equations with a Volterra integral operator. Of course, other methods for solving ordinary differential equations can be used: it is well known that the use of Runge-Kutta methods yields quadrature methods of extended Runge-Kutta type (see e.g. BAKER [2]). The question whether generalizations of our results are possible if we employ general cyclic linear multistep methods, multistep Runge-Kutta methods or other methods for solving ordinary differential equations is still open, and the answer to it will be the subject of further research. If such generalizations are possible, it is evident that we have a powerful tool for constructing and analysing, in a unified way, numerical methods for solving Volterra type equations.

Furthermore, we have emphasized the use of BD-reducible quadrature rules which are particularly suited for problems whose kernel function has a large Lipschitz constant.

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APPENDIX I: Examples of starting quadrature rules

Here, we give interpolatory quadrature rules of maximal precision for computing the starting values $I_0,\ldots,I_{k-1}$ defined in (2.3). Since $I_0 = 0$, the weights $w_{0j}^{(s)}$ are zero by definition (for all j). In the table below we have tabulated for k = 2(1)6 the weights w_{ij}^* for i = 1(1)k-1, j = 0(1)k-1, and the scaling factor D_k ($w_{ij}^{(s)} := w_{ij}^*/D_k$). In addition, we give the order s_i and error constant $c_i^{(k)}$ defined by

$$h \sum_{j=0}^{k-1} w_{ij}^{(s)} \phi(x_j) - \int_{x_0}^{x_i} \phi(y)dy = c_i^{(k)} h^{s_i} \phi^{(s_i-1)}(\xi).$$

where $\xi \in [x_0, x_{k-1}]$.

k	D_k	i	w_{i0}^*	w_{i1}^*	w_{i2}^*	w_{i3}^*	w_{i4}^*	w_{i5}^*	s_i	$c_i^{(k)}$
2	2	1	1	1					3	1/12
3	12	1	5	8	-1				4	-1/24
		2	4	16	4				5	1/90
4	24	1	9	19	-5	1			5	19/720
		2	8	32	8	0			5	1/90
		3	9	27	27	9			5	3/80
5	720	1	251	646	-264	106	-19		6	-3/160
		2	232	992	192	32	-8		6	-1/90
		3	243	918	648	378	-27		6	-3/160
		4	224	1024	384	1024	224		7	8/945
6	1440	1	475	1427	-798	482	-173	27	7	863/60480
		2	448	2064	224	224	-96	16	7	37/3780
		3	459	1971	1026	1026	-189	27	7	29/2240
		4	448	2048	768	2048	448	0	7	8/945
		5	475	1875	1250	1250	1875	475	7	275/12096

Table A.1. Starting quadrature rules S_k of maximal precision

APPENDIX II: the quadrature rules reducible to the Adams-Moulton formulae

The Adams-Moulton (AM) formulae are characterized by the polynomials $\rho(\zeta) = a_0(\zeta^k - \zeta^{k-1})$ and $\sigma(\zeta) = \Sigma_{i=0}^{k} b_i \zeta^{k-i}$. For k = 1(1)5 the coefficients a_0 and $b_0,\ldots,b_k$ can be found in e.g. HENRICI [7, p.194] and are reproduced in Table A.2, where we have also listed the order p(=k+1) and normalized error constant C_{p+1}^*.

k	a_0	b_0	b_1	b_2	b_3	b_4	b_5	p	C_{p+1}^*
1	2	1	1					2	-1/12
2	12	5	8	-1				3	-1/24
3	24	9	19	-5	1			4	-19/720
4	720	251	646	-264	106	-19		5	-3/160
5	1440	475	1427	-798	482	-173	27	6	-863/60480

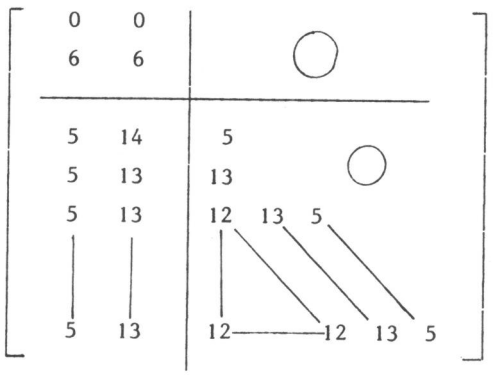
Table A.2. The coefficients, order and normalized error constant of the AM formulae ($a_1 = -a_0$, $a_2 = \ldots = a_k = 0$).

For this class of methods the recurrence relations (2.5) have the simple form

$$
\begin{aligned}
& w_{nj} = w_{n-1,j} && n \geq k,\ j = 0(1)n-k-1, \\
& w_{n,n-i} = w_{n-1,n-i} + b_i/a_0, && n \geq k,\ i = 0(1)k.
\end{aligned}
\tag{A.1}
$$

In view of (A.1) only the weights $w_{k-1,j}^{(s)}$ must be given, or equivalently only the last row of S_k is relevant. Taking the starting quadrature rules given in Table A.1 one can easily verify that the quadrature weights generated by (A.1) are the well-known Gregory quadrature rules. As an illustration, we obtain for k = 2 the weights

$$W = \frac{1}{12}$$



The quadrature error is obtained by application of Theorem 2.1. For the AM formulae the coefficients $a_2,\ldots,a_k$ vanish, and the reader may verify that therefore the quantities $d_n^* = d_n = d_{k-1} = c_{k-1}^{(k)}$ and $s = s_{k-1}$, where $c_{k-1}^{(k)}$ and s_{k-1} are given in Table A.1.

If k is *odd*, then s = k+2 and Theorem 2.1 yields

$$(A.2) \qquad Q_n^{(AM)}[\phi] = - C_{k+2}^* \, h^{k+1} \{\phi^{(k)}(x_n) - \phi^{(k)}(x_0)\} + O(h^{k+2}), \quad k \text{ odd}$$

If k is *even*, then s = k+1 and we obtain after some manipulations

$$(A.3) \qquad Q_n^{(AM)}[\phi] = - C_{k+2}^* \, h^{k+1} \{\phi^{(k)}(x_n) + \phi^{(k)}(x_0)\} + O(h^{k+2}), \quad k \text{ even},$$

The results (A.2) and (A.3) are consistent with those of the Gregory quadrature rules (see e.g. STEINBERG [14]), but are derived here in a completely different fashion.

We also note that only for even orders (k odd) the principal term in the quadrature error is not influenced by the starting rules.

On the relation between the repetition factor and numerical stability of direct quadrature methods for second kind Volterra integral equations

by

P.H.M. Wolkenfelt

ABSTRACT

We consider direct quadrature methods employing quadrature rules which are reducible to linear multistep methods for ordinary differential equations. A simple characterization of both the repetition factor and numerical stability (for small h) is given, which enables us to derive some results with respect to a conjecture of Linz. In particular we show that (i) methods with a repetition factor of one are always numerically stable; (ii) methods with a repetition factor greater than one are not necessarily numerically unstable. Analogous results are derived with respect to the more general notion of asymptotic repetition factor. We also discuss the concepts of strong stability, absolute stability and relative stability and their (dis)connection with the (asymptotic) repetition factor. Some numerical results are presented as a verification.

KEY WORDS & PHRASES: *Numerical analysis, Volterra integral equations of the second kind, reducible quadrature methods, numerical stability, repetition factor.*

1. INTRODUCTION

Consider the second kind Volterra integral equation

$$f(x) = g(x) + \int_0^x K^*(x,y,f(y))dy, \qquad x \geq 0 \tag{1.1}$$

where f is the unknown function and where the forcing function g and the kernel K^* are given smooth functions.

In order to define a discretization of (1.1), let $x_n = nh$ (where h denotes the stepsize) and let $\{w_{nj}\}$ be the weights associated with the quadrature formula

$$\int_0^{x_n} \phi(y)dy \cong h \sum_{j=0}^{n} w_{nj}\phi(x_j). \tag{1.2}$$

Then a direct quadrature method for (1.1) is given by

$$f_n = g(x_n) + h \sum_{j=0}^{n} w_{nj}K^*(x_n,x_j,f_j), \qquad n \geq k. \tag{1.3}$$

Here, f_n denotes a numerical approximation to $f(x_n)$ and k depends on the desired accuracy. If the required starting values $f_0,\ldots,f_{k-1}$ are known, the values $f_k,f_{k+1},\ldots$ can be computed in a step-by-step fashion. For a detailed discussion of such methods we refer to BAKER [1].

It is well-known (see e.g. [8,11,1,2]) that the structure of the quadrature weights w_{nj} is important for the stability analysis of the methods (1.3). In this connection, the following notion is relevant.

DEFINITION 1.1. The weights w_{nj} in (1.3) are said to have an *(exact) repetition factor* r if r is the smallest positive integer such that $w_{n+r,j} = w_{nj}$ for all $n \geq n_0$ and $n_1 \leq j \leq n-n_2$, where n_0, n_1 and n_2 are independent of n.

A method (1.3) is said to have a repetition factor r if the associated weights w_{nj} have an repetition factor r.

This paper has been largely motivated by the following conjecture of LINZ [8, p.27] (see also NOBLE [11]): "We may conjecture that (i) methods with a repetition factor of one tend to be numerically stable, (ii) those with a repetition factor greater than one numerically unstable."

In order to deal with this conjecture in a proper way, it is necessary to have a good understanding of the concept of numerical stability as defined by Linz and Noble. It turns out that numerical stability in the sense of Linz and Noble essentially requires the perturbation sensitivity of the discretization to be "roughly equivalent" to the perturbation sensitivity of the original continuous problem (compare the concept of "strong stability" as discussed by STETTER [13, p.54]). Their analysis is based on the asymptotic expansion of the global discretization error (see also KOBAYASI [6]). An advantage of this approach is its applicability to general equations (1.1), i.e. without any restrictions on the kernel and the forcing function (except for sufficient smoothness). A disadvantage however is that the stepsize h should be sufficiently small so that the conclusions need not hold for large values of h. As a consequence, this kind of stability analysis establishes results with regard to the *suitability of a method for general use* (but with small h). On the other hand it is not assumed that h actually tends to zero. This means that the condition for numerical stability in the sense of Linz and Noble is stronger than the condition for zero-stability which is necessary for convergence.

To gain insight into the relationship between the repetition factor of the quadrature weights and the stability behaviour of the associated direct quadrature method we consider the class of methods which are reducible to linear multistep methods $\{\rho,\sigma\}$ for ordinary differential equations. For this class we derive some properties of the quadrature weights, and, motivated by these results, we introduce the notion of *asymptotic repetition factor* as an extension of Def. 1.1.

We shall characterize:

(i) the exact and asymptotic repetition factor in terms of the location of the essential zeros of the polynomial ρ;

(ii) numerical stability in terms of the growth parameters associated with these zeros.

It turns out that with these characterizations, results with regard to the conjecture of Linz can be derived in a rather elegant, and almost straightforward manner. To be specific, we shall demonstrate that:

(i) methods with an asymptotic repetition factor of one are always numerically stable in the sense of Linz and Noble;

(ii) methods with an exact or asymptotic repetition factor greater than one can still be numerically stable;

(iii) an asymptotic repetition factor of one is necessary and sufficient for strong stability (a concept which we shall define in §5).

Furthermore, we shall indicate that the stability concept of Linz and Noble is almost identical to the concept of relative stability for small h, but that it is has nothing whatever to do with absolute stability.

Finally, we present some numerical experiments which serve as an illustration of the theoretical results.

2. PRELIMINARIES

We assume that for $n \geq k$, $0 \leq j \leq n$ the weights w_{nj} in (1.3) can be generated by the recurrence relation

$$\sum_{i=0}^{k} a_i w_{n-i,j} = \begin{cases} 0 & \text{for } j = 0(1)n-k-1 \\ b_{n-j} & \text{for } j = n-k(1)n, \end{cases} \tag{2.1}$$

where a_i and b_i $(i = 0(1)k)$ are the coefficients of a linear multistep method for ordinary differential equations ([7, p.11]). For the construction of the weights by means of (2.1) we set $w_{nj} = 0$ for $j > \max(n,k-1)$ and define a set of starting weights $\{w_{nj} \mid n,j = 0(1)k-1\}$ (see [14] for details). The quadrature rules generated in this way are called ([9]) (ρ,σ)-*reducible*. The direct quadrature method (1.3) employing such quadrature rules is also called (ρ,σ)-reducible. Here, ρ and σ denote the first and second characteristic polynomial associated with the linear multistep method, that is

$$\rho(\zeta) := \sum_{i=0}^{k} a_i \zeta^{k-i}, \quad \sigma(\zeta) := \sum_{i=0}^{k} b_i \zeta^{k-i}.$$

From (2.1) it can be derived that

$$w_{nj} = \omega_{n-j} \qquad \text{for } n-j \geq 0,\ j \geq k, \tag{2.2}$$

where the sequence $\{\omega_n\}_{n=0}^{\infty}$ satisfies

$$
\begin{aligned}
& a_0\omega_0 && = b_0 \\
& a_0\omega_1 + a_1\omega_0 && = b_1 \\
& \cdots && \cdots \\
& a_0\omega_k + a_1\omega_{k-1} + \ldots + a_k\omega_0 && = b_k
\end{aligned}
\tag{2.3a}
$$

$$
a_0\omega_n + a_1\omega_{n-1} + \ldots + a_k\omega_{n-k} = 0, \qquad n \geq k+1. \tag{2.3b}
$$

We also need the following definitions.

DEFINITION 2.1. (from [13, p.206]). A polynomial is said to *satisfy the root condition* if it has no zeros outside the closed unit disk and only simple zeros on the unit circle. It is said to *satisfy the strong root condition* if it satisfies the root condition and 1 is its only zero on the unit circle.

DEFINITION 2.2. A nonvanishing zero ζ of a polynomial P is called *essential* if $|\zeta| = 1$ and *nonessential* if $|\zeta| < 1$. A possible vanishing zero of P is called the *trivial* zero of P.

Furthermore, we shall assume throughout this paper that ρ and σ have no common factors and that the method $\{\rho,\sigma\}$ is convergent (that is $\rho(1) = 0$, $\rho'(1) = \sigma(1)$ and ρ satisfies the root condition).

An obvious extension of (2.1) is to define quadrature rules which are reducible to cyclic linear multistep methods. Occasionally, we shall state some results with respect to such reducible quadrature methods, but for reasons of clarity our results are mainly related to methods satisfying (2.1).

3. PROPERTIES OF THE QUADRATURE WEIGHTS ω_n

We shall derive some properties of the sequence $\{\omega_n\}$ defined in (2.3). This sequence satisfies a homogeneous difference equation with characteristic polynomial ρ. Since, by assumption, ρ satisfies the root condition, the essential zeros of ρ are simple. In order to simplify the presentation of the results and their proofs we assume subsequently that the nonessential zeros of ρ are also simple. Without this assumption our results remain true*) however, unless the assumption is given explicitly in the statement of the

*) In this case the proofs need some modification; details can be found in [14].

Theorems.

First we give the explicit form of the solution of a difference equation with constant coefficients.

LEMMA 3.1. *Let the sequence* $\{y_n\}_{n=0}^{\infty}$ *satisfy the difference equation*

$$\sum_{i=0}^{k} a_i y_{n-i} = 0, \qquad n \geq k \quad (a_0 \neq 0), \tag{3.1}$$

with starting values $y_0,\ldots,y_{k-1}$. *Assume that the characteristic polynomial* $\rho(\zeta) = \Sigma_{i=0}^{k} a_i \zeta^{k-i}$ *has* t *nonvanishing simple zeros and a zero* $\zeta = 0$ *of multiplicity* m_0 ($m_0 = 0$ *is allowed*). *Furthermore, let the coefficients* $\alpha_j^{(i)}$ *be defined by*

$$\sum_{j=0}^{k-1} \alpha_j^{(i)} \zeta^{k-1-j} := \rho(\zeta)/(\zeta-\zeta_i), \qquad i = 1,2,\ldots,t, \tag{3.2}$$

Then the solution $\{y_n\}$ is given by

$$y_n = \sum_{i=1}^{t} \zeta_i^n \Delta_i / \rho'(\zeta_i), \qquad n \geq m_0 \tag{3.3}$$

where

$$\Delta_i = \sum_{j=0}^{k-1} \alpha_j^{(i)} y_{k-1-j}. \tag{3.4}$$

PROOF. Along the lines indicated by HENRICI [3, p.238]. □

In view of (3.2) the coefficients $\alpha_j^{(i)}$ can be expressed in ζ_i and the coefficients $a_0,\ldots,a_k$; to be specific

$$\alpha_j^{(i)} = \sum_{\nu=0}^{j} a_\nu \zeta_i^{j-\nu}, \qquad i = 1,2,\ldots,t. \tag{3.5}$$

We now return to the recurrence relation (2.3b). Due to the special structure of the starting values $\omega_1,\ldots,\omega_k$ defined by (2.3a), we can prove the following basic result.

THEOREM 3.1. *Let the linear multistep method* $\{\rho,\sigma\}$ *be convergent. Assume that the nonvanishing zeros* $\zeta_1 = 1, \zeta_2,\ldots,\zeta_t$ *of* ρ *are simple and let* m_0

denote the multiplicity of the trivial zero $\zeta = 0$ $(m_0 \geq 0)$. *Then the solution* $\{\omega_n\}$ *of* (2.3b) *with starting values* (2.3a) *is given by*

$$\omega_n = \sum_{i=1}^{t} \gamma_i \zeta_i^n, \qquad n \geq m_0 + 1 \tag{3.6}$$

where

$$\gamma_i = \sigma(\zeta_i)/\zeta_i \rho'(\zeta_i) \neq 0, \qquad i = 1,2,\ldots,t. \tag{3.7}$$

PROOF. We replace y_n in (3.3) by ω_{n+1} and determine Δ_i. In view of (3.4) $\Delta_i = \Sigma_{j=0}^{k-1} \alpha_j^{(i)} \omega_{k-j}$. Substitution of (3.5) gives $\Delta_i = a_0\omega_k + (a_0\zeta_i + a_1)\omega_{k-1} + \ldots$ $\ldots + (a_0\zeta_i^{k-1} + \ldots + a_{k-1})\omega_1$. Collecting powers of ζ_i and using (2.3a) yields

$$\begin{aligned}\Delta_i &= (b_k - a_k\omega_0) + \zeta_i(b_{k-1} - a_{k-1}\omega_0) + \ldots + \zeta_i^{k-1}(b_1 - a_1\omega_0) \\ &= \sum_{j=1}^{k} b_j\zeta_i^{k-j} - \omega_0 \sum_{j=1}^{k} a_j\zeta_i^{k-j} = \sigma(\zeta_i) - b_0\zeta_i^k - \omega_0\rho(\zeta_i) + a_0\omega_0\zeta_i^k \\ &= \sigma(\zeta_i),\end{aligned}$$

since $a_0\omega_0 = b_0$ and $\rho(\zeta_i) = 0$. As a result $\omega_{n+1} = \Sigma_{i=1}^{t} \zeta_i^n \sigma(\zeta_i)/\rho'(\zeta_i)$, $n \geq m_0$, and its equivalence with (3.6) is readily seen. Since, by assumption ρ and σ have no common factor $\sigma(\zeta_i) \neq 0$, which proves that $\gamma_i \neq 0$. □

Note that $\gamma_1 = \sigma(1)/\rho'(1) = 1$ by virtue of consistency. As a consequence of (3.6) we have

COROLLARY 3.1. *If* ρ *satisfies the strong root condition, then*

$$\lim_{n\to\infty} \omega_n = 1. \tag{3.8}$$

In particular, if $\rho(\zeta) = a_0\zeta^{k-1}(\zeta - 1)$, *then*

$$\omega_n = 1 \qquad \text{for all } n \geq k. \tag{3.9}$$ □

Property (3.9) holds for example for the Adams-Moulton methods (which generate the well-known Gregory quadrature rules). On the other hand, the

backward differentiation methods generate a sequence $\{\omega_n\}$ satisfying (3.8).

From (3.6) we can also derive the following periodicity property.

COROLLARY 3.2. *Let the weights* ω_n *be defined by* (2.3). *Then*

$$\omega_{n+d} = \omega_n \qquad \text{for all } n \geq m_0 + 1 \tag{3.10}$$

if and only if the nonvanishing zeros of ρ *satisfy* $\zeta^d = 1$.

PROOF. In view of (3.6), $\omega_{n+d} - \omega_n = \Sigma_{i=1}^{t} \gamma_i \zeta_i^n (\zeta_i^d - 1)$ for all $n \geq m_0 + 1$. Since $\gamma_i \neq 0$ for $i = 1,2,\ldots,t$, $\omega_{n+d} - \omega_n = 0$ if and only if $\zeta_i^d = 1$, $i = 1,2,\ldots,t$. □

Obviously, the periodicity of the sequence $\{\omega_n\}$ is lost if ρ has a non-essential zero. We can however derive the following asymptotic result.

COROLLARY 3.3. *Let the weights* ω_n *be defined by* (2.3). *Then*

$$\lim_{n\to\infty} (\omega_{n+d} - \omega_n) = 0 \tag{3.11}$$

if and only if the essential zeros of ρ *satisfy* $\zeta^d = 1$.

PROOF. Let $\zeta_1,\ldots,\zeta_s$ denote the essential zeros of ρ. The weights ω_n are given by (3.6) and can be written as $u_n + v_n$ where $u_n = \Sigma_{i=1}^{s} \gamma_i \zeta_i^n$ and where $v_n \to 0$ as $n \to \infty$. Therefore $\lim(\omega_{n+d} - \omega_n) = \lim(u_{n+d} - u_n)$. Using the same argument as in the proof of Cor. 3.2 this limit is zero if and only if $\zeta_i^d = 1$, $i = 1,\ldots,s$. □

The properties derived in this section enable us to characterize the repetition factor in terms of the location of the essential zeros of ρ.

4. CHARACTERIZATION OF THE (ASYMPTOTIC) REPETITION FACTOR

In view of Def. 1.1 and property (2.2) the weights w_{nj} of a (ρ,σ)-reducible quadrature method have an exact repetition factor r if and only if r is *the smallest positive integer* such that $\omega_{n+r} = \omega_n$, $n \geq n_0$. This observation together with Cor. 3.2 yields the following characterization.

THEOREM 4.1. *The weights of a* (ρ,σ)*-reducible quadrature method have an exact repetition factor* r *if and only if* r *is the smallest positive integer such that the nonvanishing zeros of* ρ *satisfy* $\zeta^r = 1$. □

We recall that the polynomial ρ associated with a linear multistep method derived from interpolatory quadrature has the form $\zeta^k - \zeta^{k-r}$ (compare the Adams-family (r = 1) or the Milne-Simpson family (r = 2)). For such methods we have the following result as an immediate consequence of Theorem 4.1.

COROLLARY 4.1. *If* $\rho(\zeta) = a_0(\zeta^k - \zeta^{k-r})$ *then the weights have an exact repetition factor* r. □

We shall now consider the case that ρ has also nonessential zeros. In this case the weights do not have an exact repetition factor r in view of Th. 4.1. We have seen however in Cor. 3.3 that $\omega_{n+d} \simeq \omega_n$ for n sufficiently large, if the essential zeros of ρ satisfy $\zeta^d = 1$. In particular, if the weights are computed using finite-precision arithmetic we have the identity $\omega_{n+d} = \omega_n$ for large n. These observations suggest the following extension of Def. 1.1.

DEFINITION 4.1. The weights w_{nj} in (1.3) are said to have an *asymptotic repetition factor* r if r is the smallest positive integer such that $\lim_{n\to\infty}(w_{n+r,j} - w_{nj}) = 0$ for all j, $n_1 \le j \le n - n_2$, where n_1 and n_2 are independent of n.

With this definition and Cor. 3.3 the following theorem is self-evident.

THEOREM 4.2. *The weights of a* (ρ,σ)*-reducible quadrature method have an asymptotic repetition factor* r *if and only if* r *is the smallest positive integer such that the essential zeros of* ρ *satisfy* $\zeta^r = 1$. □

As an example, the quadrature weights generated by the polynomials $\rho(\zeta) = (\zeta-1)(\zeta^2-\zeta+1)$ and $\rho(\zeta) = (\zeta-1)(\zeta^2+1)(\zeta - 1/2)$ have an exact repetition factor of 6 and an asymptotic repetition factor of 4, respectively.

As an important special case of Th. 4.2 and 4.1 we have the following result which we shall use in §6 in connection with the conjecture of Linz.

COROLLARY 4.2. *The weights of a* (ρ,σ)*-reducible quadrature method have an asymptotic repetition factor of one if and only if* ρ *satisfies the strong root condition. In particular, the weights have an exact repetition factor of one if and only if* $\rho(\zeta) = a_0\zeta^{k-1}(\zeta-1)$. □

5. CHARACTERIZATION OF NUMERICAL STABILITY (FOR SMALL h)

In the following numerical stability in the sense of Linz and Noble will be called numerical stability (for small h).

We touched upon the concept of numerical stability (for small h) already in §1 in connection with the conjecture of Linz. For the sake of completeness we repeat here the stability definitions of both Linz and Noble.

DEFINITION 5.1. (LINZ [8, p.20]). A step-by-step method for (1.1) is *numerically stable* if the error growth is roughly equivalent to that of the solution of the variational equation of (1.1). If there exist some equations for which the error grows much faster than the solution of the variational equation of (1.1) then the method must be considered *numerically unstable*.

DEFINITION 5.2. (NOBLE [11, p.25], see also [1, p.823]). A step-by-step method for solving a Volterra integral equation is said to be unstable if the error in the computed solution has dominant spurious components introduced by the numerical scheme.

We shall now explain how these definitions must be interpreted. For a (ρ,σ)-reducible quadrature method (of order p) the asymptotic expansion of the global discretization error $e(x_n) = f_n - f(x_n)$ assumes the form ([4])

$$e(x_n) = h^p \sum_{i=1}^{s} \zeta_i^n e_p^{(i)}(x) + O(h^{p+1}) \tag{5.1}$$

where $\zeta_1 = 1, \zeta_2,\ldots,\zeta_s$ are the essential zeros of ρ and where $e_p^{(i)}(x)$ satisfies

$$e_p^{(i)}(x) = g_p^{(i)}(x) + \gamma_i \int_0^x K(x,y)e_p^{(i)}(y)dy, \qquad i = 1,2,\ldots,s. \tag{5.2}$$

Here, $K(x,y) = (\partial/\partial f)K^*(x,y,f(y))$ and the quantities γ_i are the so-called

growth parameters ([3]) defined as

$$\gamma_i = \sigma(\zeta_i)/\zeta_i\rho'(\zeta_i), \qquad i = 1,2,\ldots,s. \tag{5.3}$$

The functions $g_p^{(i)}(x)$ in (5.2) are related to the (local) quadrature errors and to the errors in the starting values.

The component $e_p^{(1)}(x)$ associated with $\zeta_1 = 1$ is called the *principal error component*. Since $\gamma_1 = 1$, this component satisfies, in view of (5.2), an equation which is identical to the variational equation of the continuous problem (1.1). The remaining components (if any) $e_p^{(2)}(x),\ldots,e_p^{(s)}(x)$ associated with $\gamma_2,\ldots,\gamma_s$ are called the *spurious error components* introduced by the discretization method. These components satisfy equations (5.2) which are different from the variational equation of (1.1), unless $\gamma_i = 1$. If $|e_p^{(i)}(x)| >> |e_p^{(1)}(x)|$ for some i $(2 \le i \le s)$, then $e_p^{(i)}(x)$ is *dominant* and the method is numerically unstable (in the sense of Linz and Noble).

From the above explanation we conclude that the values of the growth parameters are crucial for numerical stability. In order to make this even more transparent we consider the integral equation

$$f(x) = g(x) + \lambda \int_0^x \exp(\mu(x-y))f(y)dy, \tag{5.4}$$

whose solution is given by

$$f(x) = g(x) + \lambda \int_0^x \exp((\lambda+\mu)(x-y))g(y)dy. \tag{5.5}$$

Clearly, the problem (5.4) is well-conditioned with respect to bounded perturbations of g if $\mathrm{Re}(\lambda+\mu)$ is non-positive. Suppose that for a given method $\gamma_i \neq 1$ for some i, then, in view of (5.2) and (5.5), the associated spurious error component $e_p^{(i)}(x)$ is given by

$$e_p^{(i)}(x) = g_p^{(i)}(x) + \gamma_i\lambda \int_0^x \exp((\gamma_i\lambda+\mu)(x-y))g_p^{(i)}(y)dy. \tag{5.6}$$

Since $\gamma_i \neq 1$ one can always choose λ and μ such that $\mathrm{Re}(\lambda+\mu) < 0$ and $\mathrm{Re}(\gamma_i\lambda+\mu) > 0$. As a consequence, the global error has a spurious component $e_p^{(i)}(x)$ which is exponentially increasing in general, whereas the continuous

problem (5.4) is well-conditioned.

From the foregoing the following characterization is readily deduced.

THEOREM 5.1. *A reducible quadrature method of the form* (1.3) *is numerically stable (for small* h*) (in the sense of Linz and Noble) if each essential zero of* ρ *has a growth parameter equal to one; the method is weakly stable (for small* h*) (or numerically unstable in the terminology of Linz and Noble) if there exists at least one essential zero of* ρ *whose growth parameter is different from one.* □

Essentially, this theorem is an equivalent, but more quantitative definition of the numerical stability concept. We have used the term weak stability rather than numerical instability, because a weakly stable method displays not always an unstable behaviour.

We recall that in the numerical treatment of ordinary differential equations a linear multistep method is weakly stable if ρ has an essential zero with $\gamma_i < 0$ (cf. [13, p.246]). In the context of integral equations however, *weak stability can also occur for positive values of the growth parameters*!

For the expansion (5.1) we also observe that in general the terms ζ_i^n will cause the global error to be non-smooth at consecutive grid-points. This situation cannot occur if $\zeta_1 = 1$ is the only essential zero of ρ. In order to emphasize and distinguish this important feature we give the following definition.

DEFINITION 5.3. A numerically stable reducible quadrature method is called *strongly stable* (for small h) if the associated polynomial ρ satisfies the strong root condition.

REMARKS.

5.1. The terms strong and weak stability are adopted from HENRICI [3], STETTER [13]. Numerical stability (for small h) which is not strong is sometimes called harmless weak stability (cf. [12]).

5.2. The growth parameters of (ρ,σ)-reducible quadrature methods were defined in (5.3). Since Th. 5.1 is not restricted to this class of methods, we shall now briefly indicate how the values of the growth parameters can be obtained for more general quadrature methods:

In general, the application of a (step-by-step) direct quadrature method to the test equation $f(x) = 1 + \lambda \int_0^x f(y)dy$ (cf. [2]) is equivalent to the application of an m-cyclic linear multistep method to the ODE test equation $f' = \lambda f$. Let $P(\bar{h};\zeta)$ ($\bar{h} = mh\lambda$) be the associated characteristic polynomial and let $\zeta_1(0),\ldots,\zeta_s(0)$ be the essential zeros of $\rho(\zeta) := P(0;\zeta)$, then the growth parameters γ_i are given by the expansion

$$\zeta_i(\bar{h}) = \zeta_i(0)(1 + \gamma_i\bar{h}) \qquad \text{as } h \to 0.$$

For m = 1 the equivalence with (5.3) is well-known.

6. NUMERICAL STABILITY VERSUS REPETITION FACTOR

In §4 we have characterized the asymptotic repetition factor in terms of the location of the essential zeros of the polynomial ρ, and in §5 numerical stability was characterized in terms of the growth parameters associated with these zeros. In other words, numerical stability is determined by the rate of change (relative to $\bar{h}$) of the essential zeros and not so much by their location. It is intuitively clear therefore that numerical stability cannot be characterized completely by the repetition factor. We can indicate however some connections between the two concepts.

THEOREM 6.1. (NOBLE [11]). *Step-by-step methods* (1.3) *with an exact repetition factor of one are numerically stable (for small* h*).* □

With the more general notion of asymptotic repetition factor introduced in §4, the above result can be extended.

THEOREM 6.2. *A* (ρ,σ)*-reducible quadrature method with an asymptotic repetition factor of one is numerically stable (for small* h*).* □

PROOF. In view of Cor. 4.2 the polynomial ρ satisfies the strong root condition, or equivalently, $\zeta_1 = 1$ is the only essential zero. Its growth parameter is equal to one by virtue of consistency. Application of Th. 5.1 yields the result. □

The reverse statements of the theorems above are not true; that is

THEOREM 6.3. *Methods with an exact or asymptotic repetition factor greater than one can be numerically stable.*

PROOF. It is sufficient to consider specific examples. Consider the (ρ,σ)-reducible quadrature method with $\rho(\zeta) = (\zeta^2-1)(\zeta-1/3)$ and $\sigma(\zeta) = \zeta(\zeta^2-2/3\zeta+1)$. In view of Th. 4.2 the weights have an asymptotic repetition factor of two. The method is numerically stable since the growth parameters associated with the essential zeros $\zeta_1 = 1$ and $\zeta_2 = -1$ are both equal to one. An example of a numerically stable method which has an exact repetition factor of two is obtained by taking $\rho(\zeta) = \zeta^2 - 1$ and $\sigma(\zeta) = \zeta^2 + 1$. □

We emphasize however that there exists an *equivalence* between an asymptotic repetition factor of one and strong stability in the sense of Def. 5.3. This important result is given in the following theorem.

THEOREM 6.4. *A (ρ,σ)-reducible quadrature method for solving second kind Volterra integral equations is strongly stable (for small* h*) if and only if the quadrature weights have an asymptotic repetition factor of one.*

PROOF. See the proof of Th. 6.2. □

We remark that Th. 6.4 does not hold if asymptotic repetition factor is replaced by exact repetition factor. This clearly shows the relevance of the former notion.

We conjecture that for more general quadrature methods (e.g. methods which are reducible to cyclic linear multistep methods) a result analogous to that of Th. 6.4 can be derived. Such a derivation however is beyond the scope of this paper.

7. ABSOLUTE AND RELATIVE STABILITY

McKEE and BRUNNER [10] have interpreted the stability concept of Linz and Noble in a different way. With reference to the test equation (cf. [2])

$$(7.1) \qquad f(x) = 1 + \lambda \int_0^x f(y)dy, \qquad \lambda < 0$$

(whose solution $f(x) = \exp(\lambda x)$ is decaying to zero as $x \to \infty$), they give the following definition.

DEFINITION 7.1. (from [10]). A method for (1.1) is called numerically stable if when applied to (7.1) the discretized solution f_n tends to zero as $n \to \infty$ for some fixed h.

Note that this definition is reminiscent of the definition of absolute stability in the numerical treatment of ODEs.

With this definition of numerical stability McKee and Brunner give the following example to demonstrate that the conjecture of Linz is incorrect. They consider the (second order) method generated by the quadrature weights

$$W_0 = \frac{1}{6}\begin{bmatrix} 0 & & & & & & & & & \\ 3 & 3 & & & & & & & & \\ 4 & 4 & 4 & & & & & & & \\ 3 & 6 & 6 & 3 & & & & & & \\ 4 & 4 & 8 & 4 & 4 & & & & & \\ & & \cdots & & & & & & & \\ 3 & 6 & 6 & 6 & 6 & 6 & \cdots & 6 & 3 & \\ 4 & 4 & 8 & 4 & 8 & 4 & \cdots & 8 & 4 & 4 \end{bmatrix}. \tag{7.2}$$

The weights in (7.2) are *not* (ρ,σ)-reducible, but reducible to a 2-cyclic linear multistep method. Clearly, W_0 has a repetition factor of two. Furthermore, McKee and Brunner show that the method has a non-vanishing interval of absolute stability of the form $(-\alpha,0)$, and therefore (7.2) is numerically stable in the sense of Def. 7.1.

We recall from §1, that the asymptotic analysis of Linz and Noble is applicable to general second kind Volterra equations. Since the stability definition of McKee and Brunner refers to one special test equation, we state here that *their interpretation of the stability concept of Linz and Noble is incorrect*. As a consequence, the method (7.2) of McKee and Brunner is *not* a proper counterexample. To strengthen these statements, we have determined (cf. Remark 5.2) the values of the growth parameters γ_i of the method (7.2) and obtained $\gamma_1 = 1$ and $\gamma_2 = 1/6$. Therefore their method must be considered weakly stable (or numerically unstable) in view of Th. 5.1. Indeed we shall see in §8 that the method applied to an equation different from (7.1) will display a conspicuously unstable behaviour. Clearly, absolute

stability with respect to (7.1) is only a necessary condition for numerical stability in the sense of Linz and Noble.

KEECH [5] employs essentially the same stability definition as McKee and Brunner, and gives the following example

$$(7.3) \qquad W_1 = \frac{1}{2}\begin{bmatrix} 0 & & & & & & & & & \\ 1 & 1 & & & & & & & & \\ 2 & 0 & 2 & & & & & & & \\ 0 & 4 & 1 & 1 & & & & & & \\ 2 & 0 & 4 & 0 & 2 & & & & & \\ & & \cdots & & & & & & & \\ 0 & 4 & 0 & 4 & \cdots & 0 & 4 & 1 & 1 & \\ 2 & 0 & 4 & 0 & \cdots & 4 & 0 & 4 & 0 & 2 \\ & & \cdots & & & & & & & \end{bmatrix}.$$

His method is reducible to a 2-cyclic linear multistep method. It has repetition factor two and Keech shows that the interval of absolute stability is $(-2,0)$. Clearly, also his arguments are based on an incorrect interpretation of the stability concept of Linz and Noble.

It turns out however that the growth parameters associated with (7.3) are both equal to one so that the method of Keech is indeed numerically stable in the sense of Linz and Noble. Clearly, the method is *not* strongly stable.

Instead of looking at absolute stability as was done by McKee and Brunner and Keech, we can also adopt the concept of relative stability of a method with respect to (7.1) with $\lambda \in \mathbb{R}$. That is we require all roots of $P(\bar{h};\zeta) = 0$ (see Remark 5.2) to satisfy

$$(7.4) \qquad |\zeta_i(\bar{h})| \leq |\zeta_1(\bar{h})|, \qquad i = 2,3,\ldots$$

where $\zeta_1(\bar{h})$ corresponds to the principal root (i.e. $\zeta_1(\bar{h}) = \exp(\bar{h}) + \mathcal{O}(\bar{h}^{p+1})$ for a method of order p). For the weakly stable method (7.2) the interval of relative stability has the form $(0,\beta)$, $\beta > 0$, whereas for the stable method (7.3) this interval is approximately $(-3/4,5/4)$. It is known (see [12]) that the existence of an interval of relative stability of the form $(-\alpha,\beta)$, $\alpha,\beta > 0$ implies that all growth parameters associated with the essential zeros are equal to one. This yields

THEOREM 7.1. *A reducible quadrature method is numerically stable (for small* h*) if there exists an interval* $(-\alpha,\beta)$, $\alpha,\beta > 0$ *such that the method is relatively stable for all* $\bar{h} \in (-\alpha,\beta)$. □

If a method is numerically stable and not relatively stable for $\bar{h} \in (-\alpha,\beta)$ then the violation of (7.4) for some i is caused only by the $\bar{h}^{-2}$ or higher order terms in the expansion of the essential zero $\zeta_i(\bar{h})$. Therefore for small h, the existence of an interval of relative stability of the form $(-\alpha,\beta)$ is also "almost" necessary for numerical stability in the sense of Linz and Noble.

8. NUMERICAL ILLUSTRATION

In this section we present numerical results partly as an illustration of the various stability concepts discussed in §5 and partly as a verification of our theoretical results.

For our experiments we have constructed the following quadrature method parameterized by γ $(\gamma \neq 0,1)$

$$W_2(\gamma) = \frac{1}{2}\begin{bmatrix} 0 & & & & & \\ 1 & 1 & & & \bigcirc & \\ 1+\gamma & 2-2\gamma & 1+\gamma & & & \\ 1 & 2+\gamma & 2-2\gamma & 1+\gamma & & \\ 1+\gamma & 2-2\gamma & 2+2\gamma & 2-2\gamma & 1+\gamma & \\ 1 & 2+\gamma & 2-2\gamma & 2+2\gamma & 2-2\gamma & 1+\gamma \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix} \tag{8.1}$$

The quadrature weights in (8.1) are reducible to the linear multistep method $\{\rho,\sigma\}$ with $\rho(\zeta) = \zeta^2 - 1$ and $\sigma(\zeta) = \zeta^2(1+\gamma)/2 + \zeta(1-\gamma) + (1+\gamma)/2$. In view of Corollary 4.1 the weights have an exact repetition factor of two. Furthermore, the method is second order convergent and the growth parameters associated with $\zeta_1 = 1$ and $\zeta_2 = -1$ are $\gamma_1 = 1$ and $\gamma_2 = \gamma$, respectively. The method has an interval of absolute stability $(-\infty,0)$ if $\gamma > 0$. It has an interval of relative stability $(0,\infty)$ if $\gamma < 1$, and $(-\infty,0)$ if $\gamma > 1$. Since $\gamma \neq 1$, the method is weakly stable in view of Th. 5.1.

We have solved the integral equation of the form (5.4)

$$(8.2) \qquad f(x) = 1 + \lambda \int_0^x \exp(\mu(x-y))f(y)dy,$$

whose exact solution is, in view of (5.5), given by

$$(8.3) \qquad f(x) = (\mu+\lambda \exp(\lambda+\mu)x)/(\lambda+\mu).$$

We took the values $(\lambda,\mu) = (1,-2)$ and $(\lambda,\mu) = (-2,1)$. Seven different methods were used, to be specific: the method of McKee and Brunner given by (7.2) and denoted by W_0; the method of Keech given by (7.3) and denoted by W_1; the method (8.1) with $\gamma = 1/6$ and $\gamma = 3$ and denoted by $W_2(1/6)$ and $W_2(3)$, respectively; the methods employing quadrature weights which are reducible to the second and third order backward differentiation method and to the third order Adams-Moulton method and denoted by BD_2, BD_3 and AM_3, respectively. (Note that the method AM_3 is identical to the quadrature method employing the third order Newton-Gregory quadrature rules.)

Since the polynomial ρ associated with the methods BD_2, BD_3 and AM_3 satisfies the strong root condition, these methods have an asymptotic repetition factor of one (cf. Corollary 4.2) and are strongly stable (cf. Th. 6.4). The method W_1 has an exact repetition factor of two and is stable but not strongly stable. The remaining methods also have an exact repetition factor of two but are weakly stable (see Th. 5.1). In view of the values of the growth parameters we expect that for $(\lambda,\mu) = (1,-2)$ all methods except $W_2(3)$ yield stable results, whereas for $(\lambda,\mu) = (-2,1)$ the method W_0 and $W_2(1/6)$ are expected to behave unstable.

To demonstrate clearly this unstable behaviour of some of the methods it is necessary to integrate over a rather long time-interval. We have integrated the problem (8.2) on the interval [0,25] with stepsizes $h = 0.1$ and $h = 0.05$. In the Tables 8.1 and 8.2 we have listed the true error only for $h = 0.05$ (the results for $h = 0.1$ show the same behaviour).

x	W_0	$W_2(1/6)$	$W_2(3)$	W_1	BD_2	BD_3	AM_3
5.0	$-3.0_{10}-3$	$-2.5_{10}-3$	$-6.7_{10}-2$	$-6.6_{10}-3$	$-6.2_{10}-3$	$-4.4_{10}-4$	$-8.0_{10}-5$
15.0	$-3.0_{10}-3$	$-2.5_{10}-3$	$-1.3_{10}+3$	$-6.7_{10}-3$	$-6.2_{10}-3$	$-4.4_{10}-4$	$-8.0_{10}-5$
25.0	$-3.0_{10}-3$	$-2.5_{10}-3$	$-3.1_{10}+7$	$-6.7_{10}-3$	$-6.2_{10}-3$	$-4.4_{10}-4$	$-8.0_{10}-5$

Table 8.1. True error for (8.2) with $\lambda=1$, $\mu=-2$ and $h=0.05$

x	W_0	$W_2(1/6)$	$W_2(3)$	W_1	BD_2	BD_3	AM_3
5.0	$1.5_{10}{-2}$	$5.3_{10}{-4}$	$-3.0_{10}{-3}$	$-1.2_{10}{-3}$	$-1.2_{10}{-3}$	$2.9_{10}{-5}$	$5.7_{10}{-6}$
15.0	$1.2_{10}{+1}$	$7.7_{10}{-1}$	$-4.1_{10}{-3}$	$-1.7_{10}{-3}$	$-1.7_{10}{-3}$	$6.6_{10}{-5}$	$1.1_{10}{-5}$
25.0	$9.5_{10}{+3}$	$6.0_{10}{+2}$	$-4.1_{10}{-3}$	$-1.7_{10}{-3}$	$-1.7_{10}{-3}$	$6.6_{10}{-5}$	$1.1_{10}{-5}$

Table 8.2. True error for (8.2) with $\lambda=-2$, $\mu=1$ and $h=0.05$

From these tables we conclude that dependent on the values λ and μ the methods with a growth parameter different from one (that is W_0, $W_2(1/6)$ and $W_2(3)$) are unstable, whereas the strongly stable methods (BD_2, BD_3 and AM_3) and the stable method of Keech (W_1) yield stable results for both problems. Although not included in the tables of results, we also noticed that for the stable method of Keech the true error changes sign at every mesh point, whereas the strongly stable methods yield a smooth global error. Clearly, the numerical results are in full agreement with the theory.

In order to eliminate the effect of the quadrature errors (which may be quite large when solving (8.2) with $\lambda = -2$ and $\mu = 1$) we have also investigated the effect of an *isolated perturbation* (see [2]). The methods were applied to (8.2) yielding values f_n; next the value of f_1 was perturbed by an amount of 0.01 and the method was applied once again yielding perturbed values $\tilde{f}_n$. In the Tables 8.3 and 8.4 we have listed the difference $|\tilde{f}_n - f_n|$ at some meshpoints. The tables show that for both problems the perturbation

x	W_0	$W_2(1/6)$	$W_2(3)$	W_1	BD_2	BD_3	AM_3
5.0	$4.7_{10}{-6}$	$5.6_{10}{-6}$	$2.7_{10}{-1}$	$1.0_{10}{-5}$	$4.4_{10}{-6}$	$8.8_{10}{-6}$	$6.3_{10}{-6}$
15.0	$2.2_{10}{-10}$	$2.6_{10}{-10}$	$9.4_{10}{+3}$	$4.8_{10}{-10}$	$2.1_{10}{-10}$	$4.0_{10}{-10}$	$2.9_{10}{-10}$
25.0	$1.4_{10}{-14}$	$1.4_{10}{-14}$	$3.3_{10}{+8}$	$1.4_{10}{-14}$	$1.4_{10}{-14}$	$1.4_{10}{-14}$	$1.4_{10}{-14}$

Table 8.3. Effect of an isolated perturbation ($\lambda=1$, $\mu=-2$; $h=0.1$)

x	W_0	$W_2(1/6)$	$W_2(3)$	W_1	BD_2	BD_3	AM_3
5.0	$8.5_{10}{-3}$	$8.3_{10}{-3}$	$-6.7_{10}{-6}$	$4.4_{10}{-5}$	$1.3_{10}{-5}$	$3.7_{10}{-5}$	$1.9_{10}{-5}$
15.0	$6.7_{10}{+0}$	$6.5_{10}{+0}$	$-1.5_{10}{-10}$	$1.5_{10}{-9}$	$4.1_{10}{-10}$	$1.8_{10}{-9}$	$8.9_{10}{-10}$
25.0	$5.2_{10}{+3}$	$5.1_{10}{+3}$	0	$5.0_{10}{-14}$	0	$6.4_{10}{-14}$	$5.0_{10}{-14}$

Table 8.4. Effect of an isolated perturbation ($\lambda=-2$, $\mu=1$; $h=0.1$)

is damped by the strongly stable and stable methods, whereas it is amplified by the weakly stable methods (dependent on the values of λ and μ). We remark that for the method of Keech we have perturbed f_2 instead of f_1, since it can be seen from (7.3) that a perturbation of f_1 has no effect on the even-numbered gridpoints which are displayed in the tables.

All calculations were performed on a CDC-CYBER 750 Computer system using single precision (60 bit wordlength with a 48 bit mantissa).

9. CONCLUDING REMARKS

Motivated by a conjecture of Linz we have investigated for a special class of quadrature methods the relationship between the (asymptotic) repetition factor and numerical stability. We have shown that the methods with an (asymptotic) repetition factor of one are strongly stable, which implies numerical stability in the sense of Linz and Noble. However, if a method has a repetition factor greater than one, we *need additional information* in order to determine whether that method is numerically stable or not. To be specific, we have to check that the values of the growth parameters associated with the essential zeros of the polynomial ρ are equal to one. In general, these values can be determined from the stability polynomial associated with the method when applied to the test equation (7.1), and in this connection the analysis of BAKER and KEECH [2] can be used although that analysis was developed for a different type of stability.

On the other hand, it is the rule rather than the exception that for a non-artificially constructed method, the growth parameters associated with the essential zeros ($\neq 1$) are different from one (see e.g. [13, p.247]), so that we share the general opinion that methods with an (asymptotic) repetition factor greater than one should not be generally employed for the solution of second kind Volterra integral equations.

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Modified multilag methods for Volterra functional equations*)

by

P.H.M. Wolkenfelt

ABSTRACT

Linear multistep methods for ordinary differential equations in conjunction with a family of computationally efficient quadrature rules are employed to define a class of so-called multilag methods for the solution of Volterra integral and integro-differential equations. In addition, modified multilag methods are proposed which have the property that the stability behaviour is independent of the choice of the quadrature rules. High-order convergence of the methods is established. In particular, a special class of high-order convergent methods is presented for the efficient solution of first kind Volterra equations. Numerical experiments are reported.

KEY WORDS & PHRASES: *Numerical analysis, Volterra integral and integro-differential equations, multilag methods, convergence and stability*

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*) This report will be submitted for publication elsewhere.

1. INTRODUCTION

Consider the second kind Volterra integral equation

$$f(x) = g(x) + \int_0^x K(x,y,f(y))dy, \quad 0 \le x \le X, \tag{1.1}$$

whose kernel K and forcing function g are assumed to be sufficiently smooth.

In order to discretize (1.1) at $x = x_n$ we need an approximation of the Volterra integral operator at $x = x_n$. A conventional approach is to consider a family of quadrature rules W with weights w_{nj} which yields the direct quadrature methods

$$f_n = g(x_n) + h \sum_{j=0}^{n} w_{nj} K(x_n,x_j,f_j). \tag{1.2}$$

Here, h denotes the stepsize, $x_j = jh$ are equidistant gridpoints and f_j denotes a numerical approximation to $f(x_j)$. A wide variety of specific methods (1.2) is discussed e.g. in [2].

The stability behaviour of a numerical method for (1.1) is analyzed by applying that method with a fixed positive stepsize h to the test equation (cf. [3])

$$f(x) = 1 + \lambda \int_0^x f(y)dy, \qquad \lambda \in \mathbb{C}. \tag{1.3}$$

Thus applying (1.2) to (1.3) yields the equations

$$f_n = 1 + h\lambda \sum_{j=0}^{n} w_{nj} f_j. \tag{1.4}$$

It is well-known that the weights w_{nj} frequently display a certain structure which makes it possible to reduce the discrete Volterra equation (1.4) to a finite term recurrence relation. Particular attention has been paid (cf. [16,20]) to the class of (ρ,σ)-reducible quadrature methods which have the property that the equations (1.4) reduce to the relations

$$\sum_{i=0}^{k} a_i f_{n-i} = h\lambda \sum_{i=0}^{k} b_i f_{n-i}. \tag{1.5}$$

In (1.5) a_i and b_i represent the coefficients of a linear multistep (LM) method for ordinary differential equations (see e.g. [14]) which we shall denote by (ρ,σ). Here, ρ and σ are polynomials defined as

$$(1.6) \qquad \rho(\zeta) := \sum_{i=0}^{k} a_i \zeta^{k-i}, \qquad \sigma(\zeta) := \sum_{i=0}^{k} b_i \zeta^{k-i}.$$

The main advantage of constructing methods for (1.1) which reduce to (1.5), lies in the fact that the stability behaviour, determined by the stability polynomial $\rho(\zeta) - h\lambda\sigma(\zeta)$, can be prescribed by choosing a suitable LM method. For example, the backward differentiation methods generate highly stable quadrature rules (cf. [20]). A disadvantage of (ρ,σ)-reducible quadrature methods however concerns their implementation. For instance in the case of the backward differentiation methods just mentioned, either the weights must be generated numerically (cf. [20]) in each integration step which results in a rather awkward implementation and extra overhead costs, or the methods must be implemented following the imbedding approach described in [18] (see also §2) at the cost of a rather large number of additional arithmetic operations.

In this paper, we propose two new classes of methods which are more efficient than the (ρ,σ)-reducible quadrature methods since they can be constructed and implemented in a simple and straightforward fashion. The methods, which we have called *multilag methods* and *modified multilag methods*, are composed of an LM method (ρ,σ) and a family of efficient quadrature rules W.

It turns out, however, that the stability behaviour of the multilag methods is not identical to that of the (ρ,σ)-reducible quadrature methods. In fact, stability is determined by (ρ,σ) as well as by the quadrature rules W[*]. Adopting the idea of "modification" proposed by VAN DER HOUWEN [11,12] in connection with mixed Runge-Kutta methods for (1.1), we change the multilag methods by adding suitable perturbation terms (residuals) to obtain the modified multilag methods the stability behaviour of which is determined only by (ρ,σ) *irrespective of the choice of the quadrature rules* W. As a result the modified multilag methods combine the advantages of the multilag methods

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*) We intend to report on the stability behaviour of the multilag methods for various choices of W in future work.

and the (ρ,σ)-reducible quadrature methods. To be specific, the methods are easy to construct, simple to implement and computationally efficient. Moreover, they reduce to (1.5) when applied to (1.3).

The derivation of the multilag methods for (1.1) is essentially based on an appropriate approximation of the Volterra integral operator (see §2) and therefore it is not surprising that the same approximations can also be employed in connection with the numerical solution of other types of Volterra equations. To demonstrate this, we shall apply our techniques also to derive numerical methods for Volterra integro-differential equations

$$f'(x) = F(x,f(x), \int_0^x K(x,y,f(y))dy), \quad f(0) = f_0, \tag{1.7}$$

and for first kind Volterra integral equations

$$\int_0^x K(x,y,f(y))dy = g(x), \qquad g(0) = 0. \tag{1.8}$$

We shall establish, in §3 and 4, the order of convergence of the multilag methods as well as their modification for the solution of (1.1) and (1.7).

It is well-known that for the solution of first kind equations (1.8) by means of direct quadrature methods special stabilized quadrature rules must be constructed (see e.g. [1,6]). In §5, we shall present a class of high-order convergent modified multilag methods which combine *conventional* quadrature rules with a highly stable LM method.

To illustrate the theoretical results we have included in §6 some numerical experiments with modified multilag methods in which we chose for (ρ,σ) the highly stable backward differentiation methods and for W the Gregory quadrature rules.

2. PRELIMINARIES AND NOTATIONS

In this section we shall derive approximations of the Volterra integral operator $\int_0^x K(x,y,f(y))dy$, which occurs in the functional equations (1.1), (1.7) and (1.8). For this derivation it is convenient to introduce the function $\Psi(t,x)$ defined as

$$(2.1) \qquad \Psi(t,x) = \int_0^t K(x,y,f(y))dy,$$

where (for the moment) f is a given function. Following Pouzet (see e.g. [2]), we regard $\Psi(t,x)$ as the solution of the ordinary differential equation (with parameter x)

$$(2.2) \qquad \frac{d}{dt}\Psi(t,x) = K(x,t,f(t))$$

with initial condition $\Psi(0,x) = 0$. This observation suggests the use of methods for ordinary differential equations (cf. [9,18]). Using an LM method (ρ,σ) (with normalization $a_0 = 1$), we may define an approximation $\hat{\psi}_n(x)$ of $\psi_n(x)$ ($\psi_n(x) := \Psi(hh,x)$) by the recurrence relation

$$(2.3) \qquad \hat{\psi}_\nu(x) = -\sum_{i=1}^{k} a_i\hat{\psi}_{\nu-i}(x) + h\sum_{i=0}^{k} b_iK(x,x_{\nu-i},f(x_{\nu-i})),$$

$$\nu = k(1)n,$$

provided that the starting values $\hat{\psi}_0(x),\ldots,\hat{\psi}_{k-1}(x)$ are given. In the treatment of second kind Volterra equations WOLKENFELT et al. [18] discuss methods employing such approximations and indicate the equivalence with (ρ,σ)-reducible quadrature methods. A disadvantage of this approach is that for the computation of $\hat{\psi}_n(x)$ the recurrence relation (2.3) must be evaluated for $\nu = k(1)n$, which may give a considerable amount of overhead, especially when dealing with systems of Volterra integral equation. This drawback can be avoided by the following approach: instead of defining starting values $\hat{\psi}_0(x),\ldots,\hat{\psi}_{k-1}(x)$ followed by a recursive evaluation of (2.3), we compute approximations $\tilde{\psi}_{n-k}(x),\ldots,\tilde{\psi}_{n-1}(x)$ by means of *computationally efficient* quadrature rules followed by *one single application* of (ρ,σ). To be specific, we define

$$(2.4) \qquad \hat{\psi}_n(x) := -\sum_{i=1}^{k} a_i\tilde{\psi}_{n-i}(x) + h\sum_{i=0}^{k} b_iK(x,x_{n-i},f(x_{n-i}))$$

where

$$(2.5) \qquad \tilde{\psi}_n(x) := h\sum_{j=0}^{n} w_{nj}K(x,x_j,f(x_j)).$$

Here, $W = \{w_{nj} | n \geq n_0,\ 0 \leq j \leq n\}$ denotes a family of quadrature rules. The value of n_0 depends on the accuracy of these rules. Obviously, (2.4) can only be applied for $n \geq n_k = n_0 + k$.

REMARK. Examples of computationally efficient quadrature rules are the rules with a finite repetition factor (see e.g. [3]). In the case of a repetition factor of one the weights satisfy

$$w_{nj} - w_{n-1,j} = \begin{cases} 0 & \text{if } 0 \leq j < n-\kappa, \\ \\ \nabla w_{nj} & \text{if } n-\kappa \leq j \leq n, \end{cases}$$

so that $\tilde{\psi}_{n-k+1}(x),\ldots,\tilde{\psi}_{n-1}(x)$ defined in (2.5) can be computed recursively as follows

$$\tilde{\psi}_m(x) = \tilde{\psi}_{m-1}(x) + h \sum_{j=m-\kappa}^{m} \nabla w_{mj} K(x,x_j,f(x_j)),\quad m = n-k+1(1)n-1. \tag{2.6}$$

Specific examples are the Gregory quadrature rules ([2]). It is easily verified that for the evaluation of $\hat{\psi}_n(x)$ by means of (2.4), (2.5) and (2.6) roughly $2nk$ multiplications and additions are saved in comparison with (2.3). □

So far we assumed that the function f is known. Now assume that only approximations f_j to $f(x_j)$ are available. In this case we replace in (2.4) and (2.5), $f(x_j)$ by f_j, $\hat{\psi}_n(x)$ by $\hat{I}_n(x)$ and $\tilde{\psi}_n(x)$ by $\tilde{I}_n(x)$ to obtain the approximations

$$\hat{I}_n(x) := -\sum_{i=1}^{k} a_i \tilde{I}_{n-i}(x) + h \sum_{i=0}^{k} b_i K(x,x_{n-i},f_{n-i}),\quad n \geq n_k \tag{2.7}$$

where

$$\tilde{I}_n(x) := h \sum_{j=0}^{n} w_{nj} K(x,x_j,f_j),\qquad n \geq n_0. \tag{2.8}$$

Since the function $\tilde{I}_n(x)$ which depends on all previously computed f_j-values, is usually called a *lag term* (or history term), we shall call the function $\hat{I}_n(x)$ a multilag approximation to $\psi_n(x)$.

For the convergence analysis of our methods we need the local truncation error $T_n(h;x)$ of (2.4) at $t = nh$ defined as

$$\psi_n(x) = -\sum_{i=1}^{k} a_i \psi_{n-i}(x) + h \sum_{i=0}^{k} b_i K(x, x_{n-i}, f(x_{n-i})) + T_n(h;x). \tag{2.9}$$

Note that for an LM method of order p

$$T_n(h;x) = C_{p+1} h^{p+1} \frac{d^p}{dt^p} K(x,t,f(t))\Big|_{t=nh} + O(h^{p+2}) \text{ as } h \to 0 \tag{2.10}$$

where $C_{p+1} \neq 0$ denotes the error constant of (ρ,σ) (cf. [8]). For the rules (2.5) we define the quadrature error

$$Q_n(h;x) := \psi_n(x) - \tilde{\psi}_n(x). \tag{2.11}$$

Furthermore we assume that the quadrature weights w_{nj} are uniformly bounded, i.e. $|w_{nj}| \leq \bar{w}$ for all n and j.

In our theorems we shall establish a bound on the global discretization error in terms of quadrature errors, local truncation errors and errors in the starting values using the following notation:

$$\delta_1(h) = \max\{|f(x_j)-f_j|: 0 \leq j \leq n_0-1\}; \tag{2.12}$$

$$\delta_2(h) = \max\{|f(x_j)-f_j|: n_0 \leq j \leq n_k-1\}; \tag{2.13}$$

$$T_N(h) = \max\{|T_n(h;x_n)|: n_k \leq n \leq N\}; \tag{2.14}$$

$$Q_N(h) = \max\{|Q_{n-i}(h;x_n)|: n_k \leq n \leq N,\ 1 \leq i \leq k\}; \tag{2.15}$$

$$\Delta Q_N(h) = \max\{|Q_{n-i}(h;x_n) - Q_{n-i}(h;x_{n-i})|: n_k \leq n \leq N,\ 1 \leq i \leq k\} \tag{2.16}$$

In order not to distract the reader's attention from the main results, all theorems are stated without proof. However, for those interested, the technical details can be found in the Appendix of [21].

3. METHODS FOR SECOND KIND VOLTERRA INTEGRAL EQUATIONS

The second kind Volterra equation (1.1) can be written as

$$f(x) = g(x) + \Psi(x,x), \qquad 0 \le x \le X, \tag{3.1}$$

where we have used the notation (2.1).

3.1. Multilag methods

In order to discretize (3.1) at $x = x_n$, we replace $f(x_n)$ by f_n and $\Psi(x_n,x_n) = \psi_n(x_n)$ by $\hat{I}_n(x_n)$ defined in (2.7) to obtain the *multilag method*

$$f_n = g(x_n) - \sum_{i=1}^{k} a_i \tilde{I}_{n-i}(x_n) + h \sum_{i=0}^{k} b_i K(x_n,x_{n-i},f_{n-i}), \quad n \ge n_k \tag{3.2}$$

where $\tilde{I}_n(x)$ is defined in (2.8). The required starting values are f_j, $j = 0(1)n_k-1$.

For the global error $f(x_n)-f_n$ the following result can be derived.

THEOREM 3.1. *Assume that* K *satisfies the Lipschitz condition*

$$|K(x,y,\phi_1) - K(x,y,\phi_2)| \le L_1|\phi_1-\phi_2|. \tag{3.3}$$

Let $f(x)$ *be the solution of* (3.1) *and let* f_n *be defined by* (3.2). *Then for* h *sufficiently small* ($X = Nh$)

$$\max_{n_k \le n \le N} |f(x_n)-f_n| \le C \max\{h\delta_1(h),h\delta_2(h),Q_N(h),T_N(h)\} \tag{3.4}$$

where C *is a constant independent of* N *and* h, *and where* $\delta_1(h),\delta_2(h),Q_N(h)$ *and* $T_N(h)$ *are defined in* (2.12) *to* (2.15). □

Using this theorem high-order convergence of the methods (3.2) is now readily established.

THEOREM 3.2. *Let the condition* (3.3) *be satisfied and assume that* g *and* K *are sufficiently smooth. In addition, let*

(i) *the* LM *method* (ρ,σ) *be convergent of order* p;

(ii) *the quadrature rules* W *be of order* q;

(iii) *the errors in the starting values be of order* s.

Then the multilag method (3.2) *is convergent of order* r, *where*

$r = \min\{s+1, q, p+1\}$. *To be specific*

$$\max_{n_k \le n \le N} |f(x_n) - f_n| \le Ch^r \text{ as } h \to 0,\ N \to \infty,\ Nh = X$$

where C *is a constant independent of* N *and* h. □

With respect to the stability analysis we remark that the application of (3.2) to the basic test equation (1.3) yields the relations

$$\begin{aligned} f_n &= 1 - \sum_{i=1}^{k} a_i \tilde{I}_{n-i} + h\lambda \sum_{i=0}^{k} b_i f_{n-i}, \\ \tilde{I}_n &= h\lambda \sum_{j=0}^{n} w_{nj} f_j. \end{aligned} \tag{3.5}$$

which clearly indicates that the stability behaviour of (3.2) depends on (ρ,σ) as well as on the quadrature rules W. Under suitable assumptions on the quadrature weights (e.g. reducibility [20] or finite repetition factor [3]) the relations (3.5) can be reduced to a recurrence relation in terms of f_n-values only and the stability behaviour is then determined by a root condition on the associated stability polynomial. A systematic study along these lines for various choices of quadrature rules W will be the subject of future research.

In this paper we concentrate on a modification of (3.2) which has been constructed in such a way that the stability behaviour with respect to (1.3) is independent of the choice of the quadrature rules W used for the lag terms $\tilde{I}_n(x)$.

3.2. Modified multilag methods

In [12] a modification of mixed Runge-Kutta methods was proposed (see also [11]) with the aim of improving the stability behaviour. This modified method was derived by modifying the lag term by a suitable perturbation term which can be regarded as a residual (see [13]). Motivated by this approach, we present the following modification of (3.2)

$$f_n = g(x_n) - \sum_{i=1}^{k} a_i \{\tilde{I}_{n-i}(x_n) + r_{n-i}\} + h \sum_{i=0}^{k} b_i K(x_n, x_{n-i}, f_{n-i}), \quad n \ge n_k \tag{3.6a}$$

(3.6b) $$r_n = f_n - g(x_n) - \tilde{I}_n(x_n), \qquad n \geq n_0,$$

where $\tilde{I}_n(x)$ is defined in (2.8). The *modified multilag method* (3.6) requires the starting values f_j, $j = 0(1)n_k-1$. Note that r_n defined in (3.6b) can be regarded as a residual.

We remark that the class (3.6) includes as a special case the methods proposed by VAN DER HOUWEN [11] (who chose, in the notation (3.6), $a_1 = -1$, $a_2 = \ldots = a_k = 0$).

It is easily verified that application of (3.6) to the test equation (1.3) yields, due to cancellation of the $\tilde{I}_n$ terms, the recurrence relation (1.5). Thus the stability behaviour of (3.6) is determined only by (ρ,σ), and therefore identical to that of the (ρ,σ)-reducible quadrature methods.

Before establishing the high-order convergence of the modified methods (3.6) we first state the following result.

THEOREM 3.3. *Let* K *satisfy the Lipschitz condition*

$$\begin{aligned} &|K(x,y,\phi_1) - K(x,y,\phi_2) - K(x_n,y,\phi_1) + K(x_n,y,\phi_2)| \leq \\ &\leq L_1^* |x-x_n||\phi_1-\phi_2|, \end{aligned} \tag{3.7}$$

and let the LM *method* (ρ,σ) *be convergent. Furthermore let* f(x) *be the solution of* (3.1) *and let* f_n *be defined by* (3.6). *Then for* h *sufficiently small*

$$\max_{n_k \leq n \leq N} |f(x_n)-f_n| \leq C \max\{h\delta_1(h), \delta_2(h), h^{-1}\Delta Q_N(h), h^{-1}T_N(h)\} \tag{3.8}$$

where C *is a constant independent of* N *and* h *and where* $\delta_1(h)$, $\delta_2(h)$, $\Delta Q_N(h)$ and $T_N(h)$ *are defined in* (2.12) *to* (2.16). □

The Lipschitz condition (3.7) required in the above theorem is satisfied if, for example, K_x satisfies a Lipschitz condition with respect to f. We then may write the left-hand side of (3.7) as

$$\left| \int_{x_n}^{x} \{K_x(t,y,\phi_1) - K_x(t,y,\phi_2)\}dt \right|$$

from which the right-hand side of (3.7) is immediate. It can also be shown that $h^{-1}\Delta Q_N(h)$ has the same order of accuracy as $Q_N(h)$ provided that K and K_x are sufficiently smooth. This fact together with Theorem 3.3 yields

THEOREM 3.4. *Let the assumptions of Theorem* 3.3 *and* 3.2 *be valid. Then the modified multilag method* (3.6) *is convergent of order* r^*, *where* $r^* = \min\{s,q,p\}$. □

Comparison of the results of Theorem 3.2 and 3.4 clearly shows the effect of the modification on the order of convergence: if $s \geq p+1$ and $q \geq p+1$, the order of the modified methods is lowered by one.

4. METHODS FOR VOLTERRA INTEGRO-DIFFERENTIAL EQUATIONS

Using (2.1), equation (1.7) can be written as

$$f'(x) = F(x,f(x),\Psi(x,x)), \qquad 0 \leq x \leq X \tag{4.1}$$

with initial condition $f(0) = f_0$. Application of an LM method for ordinary differential equations to (4.1) in which $\Psi(x_n,x_n)$ is replaced by a numerical approximation yields a wide class of numerical methods (cf. [5,15,16,20]).

4.1. Multilag methods

We shall employ a linear k^*-step method (ρ^*,σ^*) with coefficients a_i^* and b_i^*, and numerical approximations $\hat{I}_n = \hat{I}_n(x_n)$ as defined in (2.7) to obtain the methods

$$\sum_{i=0}^{k} a_i^* f_{n-i} = h \sum_{i=0}^{k} b_i^* F(x_{n-i},f_{n-i},\hat{I}_{n-i}), \qquad n \geq n_k = n_0 + k \tag{4.2a}$$

$$\hat{I}_n = -\sum_{i=1}^{k} a_i \tilde{I}_{n-i}(x_n) + h \sum_{i=0}^{k} b_i K(x_n,x_{n-i},f_{n-i}), \qquad n \geq n_k \tag{4.2b}$$

$$\hat{I}_n = \tilde{I}_n(x_n) \text{ if } n_0 \leq n \leq n_k-1, \tag{4.2c}$$

where $\tilde{I}_n(x)$ is defined in (2.8). Note that we have assumed, without loss of generality, that $k^* = k$. The required starting values for (4.2) are

f_j, $j = 0(1)n_k-1$.

A bound for the global discretization error is established in the following theorem.

THEOREM 4.1. *Let* K *satisfy the condition* (3.3) *and let* F *satisfy the Lipschitz conditions*

$$|F(x,\phi_1,z) - F(x,\phi_2,z)| \le L_2|\phi_1-\phi_2|, \tag{4.3a}$$

$$|F(x,\phi,z_1) - F(x,\phi,z_2)| \le L_3|z_1-z_2|, \tag{4.3b}$$

and assume that the LM *method* (ρ^*,σ^*) *is convergent. Let* $f(x)$ *be the solution of* (4.1) *and let* f_n *be defined by* (4.2). *Then for* h *sufficiently small*

$$\max_{n_k\le n\le N} |f(x_n)-f_n| \le C \max\{h\delta_1(h),\delta_2(h),h\delta_3(h),Q_N(h),T_N(h),h^{-1}T_N^*(h)\} \tag{4.4}$$

where C *is a constant independent of* N *and* h *and where* $\delta_1(h),\delta_2(h),Q_N(h)$ *and* $T_N(h)$ *are defined in* (2.12) *to* (2.15). *Furthermore*

$$\delta_3(h) = \max\{|Q_n(h;x_n)|: n_0 \le n \le n_k-1\}, \tag{4.5}$$

$$T_N^*(h) = \max\{|T_n^*(h;x_n)|: n_k \le n \le N\}, \tag{4.6}$$

where $T_n^*(h;x_n)$ *denotes the local truncation error at* $x = x_n$ *of the* LM *method* (ρ^*,σ^*) *when applied to* (4.1). □

An immediate consequence of the above theorem is

THEOREM 4.2. *Let the conditions* (3.3) *and* (4.3) *be satisfied and assume that* F *and* K *are sufficiently smooth. In addition, let*

(i) *the* LM *method* (ρ^*,σ^*) *be convergent of order* p^*;

(ii) *the* LM *method* (ρ,σ) *be convergent of order* p;

(iii) *the quadrature rules* W *be of order* q;

(iv) *the errors in the starting values be of order* s.

Then the multilag method (4.2) *is convergent of order* r, *where* $r = \min\{s,q,p+1,p^*\}$. □

Concerning the stability behaviour we note that the application of (4.2) to the basic test equation (cf. [16])

$$f'(x) = \xi f(x) + \eta \int_0^x f(y)dy, \qquad \xi,\eta \in \mathbb{C} \tag{4.7}$$

yields relations which depend also on the quadrature rules W. In order to eliminate the effect of these quadrature rules on the stability behaviour we construct a modification of (4.2).

4.2. Modified multilag methods

Along the same lines as in §3.2 we define the modified multilag methods by

$$\sum_{i=0}^{k} a_i^* f_{n-i} = h \sum_{i=0}^{k} b_i^* F(x_{n-i}, f_{n-i}, \hat{I}_{n-i}), \qquad n \geq n_k, \tag{4.8a}$$

$$\hat{I}_n = -\sum_{i=1}^{k} a_i \{\tilde{I}_{n-i}(x_n) + r_{n-i}\} + h \sum_{i=0}^{k} b_i K(x_n, x_{n-i}, f_{n-i}), \quad n \geq n_k \tag{4.8b}$$

$$r_n = \hat{I}_n - \tilde{I}_n(x_n), \qquad n \geq n_k. \tag{4.8c}$$

(4.8d) $\tilde{I}_n(x) = h \sum_{j=0}^{n} \omega_{nj} k(x, x_j, f_j)$

As in (4.2c) we define $\tilde{I}_n = \hat{I}_n(x_n)$ if $n_0 \leq n \leq n_k - 1$, which implies that $r_n = 0$ if $n_0 \leq n \leq n_k - 1$.

Due to this modification the method (4.8) applied to (4.7) yields the recurrence relations

$$\begin{aligned} \sum_{i=0}^{k} a_i^* f_{n-i} &= h \sum_{i=0}^{k} b_i^* (\xi f_{n-i} + \eta \hat{I}_{n-i}), \\ \sum_{i=0}^{k} a_i \hat{I}_{n-i} &= h \sum_{i=0}^{k} b_i f_{n-i}. \end{aligned} \tag{4.9}$$

Elimination of $\hat{I}_n$ yields a recurrence relation in f_n-values only whose characteristic (or stability) polynomial is given by

$$\rho(\zeta)[\rho^*(\zeta) - h\xi\sigma^*(\zeta)] - h^2\eta\sigma(\zeta)\sigma^*(\zeta), \tag{4.10}$$

which is independent of W. Note that the same stability polynomials were found by MATTHYS [16] who considered (ρ,σ)-reducible quadrature rules.

We shall now deal with the convergence of (4.8). First we give the following bound for the global error.

THEOREM 4.3. *Let* K *satisfy the condition* (3.7) *and let* F *satisfy* (4.3) *and let the* LM *methods* (ρ^*,σ^*) *and* (ρ,σ) *be convergent. Further, let* $f(x)$ *be the solution of* (4.1) *and let* f_n *be defined by* (4.8). *Then for* h *sufficiently small*

$$(4.11)\qquad \max_{n_k\le n\le N} |f(x_n)-f_n| \le C \max\{h\delta_1(h),\delta_2(h),\delta_3(h),h^{-1}\Delta Q_N(h), h^{-1}T_N(h),h^{-1}T_N^*(h)\}$$

where C *is a constant independent of* N *and* h, *where* $\delta_1(h),\delta_2(h)$, $T_N(h)$ *and* $\Delta Q_N(h)$ *are defined in* (2.12) *to* (2.16) *and where* $\delta_3(h)$ *and* $T_N^*(h)$ *are defined in* (4.5),(4.6). □

As a consequence we have

THEOREM 4.4. *Let the assumptions of Theorem* 4.3 *and* 4.2 *be valid. Then the modified multilag method* (4.8) *is convergent of order* r^*, *where* $r^* = \min\{s,q,p,p^*\}$. □

From the results of Theorem 4.2 and 4.4 it is evident that the modified methods may lose one order of accuracy (cf. §3.2).

5. MODIFIED MULTILAG METHODS FOR FIRST KIND VOLTERRA INTEGRAL EQUATIONS

In section 3 and 4 we considered general LM methods in conjunction with general quadrature rules. It turned out that convergent LM methods together with convergent quadrature rules generate convergent methods for second kind Volterra equations and integro-differential equations.

It is well known, however, that for the solution of first kind equations convergence of the quadrature rules does not generally imply convergence of the associated direct quadrature method and additional assumptions are necessary (see e.g. [1,6,7,10,17,19]).

In this section we do not pursue complete generality and present the convergence results of a particular class of modified multilag methods. To be specific, we consider the methods

$$(5.1a) \qquad -\sum_{i=1}^{k} a_i\{\tilde{I}_{n-i}(x_n) + r_{n-i}\} + hb_0K(x_n,x_n,f_n) = g(x_n), \qquad n \geq n_k,$$

$$(5.1b) \qquad r_n = g(x_n) - \tilde{I}_n(x_n), \qquad n \geq n_0,$$

where $\tilde{I}_n(x)$ is defined in (2.8). The required starting values are f_j, $j = 0(1)n_k-1$.

The methods (5.1) can be derived as follows. Using (2.1) the first kind Volterra equation (1.8) can be written as

$$(5.2) \qquad \Psi(x,x) = g(x), \qquad 0 \leq x \leq X.$$

Discretization of (5.2) at $x = x_n$ using the approximation (2.7) in which we take $b_2=\ldots=b_k = 0$, and modification by the "residual approach" then yields (5.1). Note that we have chosen a particular class of LM methods (i.e. $\sigma(\zeta) = b_0\zeta^k$) which includes the well-known backward differentiation methods. We emphasize that the quadrature rules W are still free to choose.

For the global error the following bound can be derived.

THEOREM 5.1. *In addition to the condition* (3.7) *assume that*

$$(5.3) \qquad |K(x,x,\phi_1) - K(x,x,\phi_2)| \geq L_4|\phi_1-\phi_2|, \qquad (L_4 > 0).$$

Let the LM *method* (ρ,σ) *with* $\sigma(\zeta) = b_0\zeta^k$ *be convergent. Furthermore let* $f(x)$ *be the solution of* (1.8) *and let* f_n *be defined by* (5.1). *Then for* h *sufficiently small*

$$(5.4) \qquad \max_{n_k\leq n\leq N} |f(x_n)-f_n| \leq C \max\{h\delta_1(h),h\delta_2(h),h^{-1}\Delta Q_N(h),h^{-1}T_N(h)\}$$

where C *is a constant independent of* N *and* h, *and where* $\delta_1(h),\delta_2(h),\Delta Q_N(h)$ *and* $T_N(h)$ *are defined in* (2.12) *to* (2.16). □

We remark that the Lipschitz condition (5.3) is implied by the condi-

tions for the existence of a unique continuous solution to (1.8) given in [7]. To be specific, one of the conditions is that $|\frac{\partial K}{\partial f}(x,x,f)|$ should be bounded away from zero.

As an immediate consequence of Theorem 5.1 we have.

THEOREM 5.2. *Let the assumptions of Theorem* 5.1 *be valid and let* K *and* g *be sufficiently smooth. In addition, let*

(i) *the* LM *method* (ρ,σ) *with* $\sigma(\zeta) = b_0\zeta^k$ *be convergent of order* p;

(ii) *the quadrature rules* W *be of order* q;

(iii) *the errors in the starting values be of order* s.

Then the method (5.1) *is convergent of order* r^*, *where* $r^* = \min\{s+1,q,p\}$. □

It is easily verified that the methods (5.1) applied to the test equation

$$(5.5) \qquad \int_0^x f(y)dy = g(x)$$

reduce to $f_n = (hb_0)^{-1}\Sigma_{i=0}^{k} a_i g(x_{n-i})$, *irrespective of the choice of the quadrature rules* W. As a result, the methods (5.1) correspond to "local differentiation formulae" which is a desirable property with respect to stability (see e.g. [17,p.417]).

6. NUMERICAL EXPERIMENTS

In this section we report on numerical experiments with modified multilag methods (3.6), (4.8) and (5.1). For the LM method (ρ,σ) and the quadrature rules W we chose, for p = 2(1)6, the pth order backward differentiation (BD) methods ([14]) and the pth order Gregory quadrature rules, respectively. In the methods (4.8) we took (ρ^*,σ^*) identical to (ρ,σ). The methods are denoted by BDGp (p=2(1)6).

The methods were applied to test problems (taken from [5],[6] and [20]) with known exact solution. Integration was performed with a constant stepsize, and the necessary starting values were computed from the exact solution. In consequence of the Theorems 3.4, 4.4 and 5.2 the methods BDGp are of order p, asymptotically.

In the tables of results we have tabulated for different orders and

a sequence of stepsizes, the number of correct decimal digits cd (defined by $-^{10}\log$ (absolute error)) at the endpoint of integration. Moreover we have listed in the convergence experiments the computed order p^* (defined by $\{cd(h) - cd(2h)\}/^{10}\log 2$).

All calculations have been performed on a CDC CYBER 750 installation using 14 significant digits.

6.1. Second kind Volterra integral equations

In order to test their high-order convergence we have applied the BDG methods to the following problem

$$(6.1.1) \qquad f(x) = \tfrac{1}{2}x^2 \exp(-x) + \tfrac{1}{2}\int_0^x (x-y)^2 \exp(y-x) f(y)dy, \qquad 0 \le x \le 6,$$

with exact solution $f(x) = \frac{1}{3} - \frac{1}{3}\exp(-3x/2)\{\cos(\tfrac{1}{2}x\sqrt{3}) + \sqrt{3}\sin(\tfrac{1}{2}x\sqrt{3})\}$. In Table 6.1.1 the results are tabulated for various choices of h.

h^{-1}	p=2	p=3	p=4	p=5	p=6
4	1.89	1.86	2.34	2.97	3.51
8	$2.22^{1.1}$	$2.57^{2.4}$	$3.25^{3.0}$	$4.21^{4.1}$	$4.92^{4.7}$
16	$2.70^{1.6}$	$3.37^{2.7}$	$4.31^{3.5}$	$5.60^{4.6}$	$6.55^{5.4}$
32	$3.25^{1.8}$	$4.23^{2.9}$	$5.44^{3.8}$	$7.05^{4.8}$	$8.28^{5.8}$
64	$3.83^{1.9}$	$5.11^{2.9}$	$6.61^{3.9}$	$8.53^{4.9}$	$10.10^{6.1}$

Table 6.1.1. Number of correct digits at x=6 and the computed order p^* for the BDG methods applied to (6.1.1).

From this table it is obvious that the computed order tends to the theoretical order of convergence.

The favourable stability behaviour of the BDG methods is demonstrated in the following example:

$$(6.1.2) \qquad f(x) = g(x) - \lambda\int_0^x \frac{1+x}{1+y} f^2(y)dy, \qquad 0 \le x \le xe,$$

with exact solution $f(x) = [1+(1+x)\exp(-x)]^{\frac{1}{2}}$ if we choose $g(x) = f(x) + \lambda(1+x)[\ln(1+x) + 1-\exp(-x)]$. We considered the values $\lambda = 1,10,100,1000$ and 10000 which makes (6.1.2) increasingly stiff. The endpoint of integration was 192h. The results are given in Table 6.1.2.

h^{-1}	λ	p=2	p=3	p=4	p=5	p=6
	1	3.23	3.83	4.97	5.10	5.84
	10	3.23	3.84	4.98	5.11	5.85
4	100	3.24	3.84	4.98	5.11	5.85
	1000	3.24	3.84	4.98	5.11	5.85
	10000	3.24	3.84	4.98	5.11	5.85
	1	3.84	4.93	6.19	7.01	8.21
	10	3.87	4.96	6.22	7.04	8.24
16	100	3.87	4.97	6.23	7.05	8.24
	1000	3.87	4.97	6.23	7.05	8.24
	10000	3.87	4.97	6.23	7.05	8.24
	1	5.18	6.41	8.06	9.29	10.46
	10	4.99	6.42	8.08	9.35	10.65
64	100	4.99	6.42	8.09	9.37	10.36
	1000	4.99	6.42	8.09	9.43	10.63
	10000	4.99	6.42	8.09	9.40	10.44

Table 6.1.2. The number of correct digits at x = 192h for problem (6.1.2)

The results show that for fixed h the accuracy is hardly affected by increasing stiffness and justify the conclusion that the BDG methods are highly-stable.

6.2. Volterra integro-differential equations

To test high-order convergence we applied the BDG methods to

$$(6.2.1)\qquad \begin{cases} z(x) = \int_0^x \dfrac{dy}{1+(1+x)f(y)} \\ f'(x) = -x - (1+x)^{-2} + \dfrac{1}{f(x)} \ln\dfrac{2+2x}{2+x} + \int_0^x \dfrac{dy}{1+(1+x)f(y)}, \quad 0\le x\le 10. \end{cases}$$

Taking $f(0) = 1$ yields the exact solution $f(x) = (1+x)^{-1}$. The results summarized in Table 6.2.1 clearly show that the computed order tends to the theoretical order of convergence, except for the sixth order method.

h^{-1}	p=2		p=3		p=4		p=5		p=6	
4	5.85	0.8	5.76	1.4	6.32	1.8	7.00	2.0	7.60	2.3
8	6.10	1.0	6.19	2.2	6.86	2.7	7.59	3.2	8.30	3.4
16	6.40	1.6	6.84	2.6	7.67	3.3	8.51	3.9	9.33	4.4
32	6.89	1.9	7.61	2.8	8.65	3.6	9.67	4.3	10.65	7.1
64	7.45		8.45		9.73		10.97		12.79	

Table 6.2.1. Number of correct digits at x=10 and computed order p^* for the BDG methods applied to (6.2.1).

For the stability test we applied the methods to

$$(6.2.2)\qquad \begin{cases} f'(x) = [d(x) - \alpha f(x) - \beta z(x)]^3 - 1, & f(0) = 1 \\ z(x) = \int_0^x (x+\gamma y)^{\delta} f^3(y)\,dy. \end{cases}$$

Choosing $d(x) = 1 + \alpha + \gamma^{-1}(1+\delta)^{-1}\beta x^{\delta+1}\{(1+\gamma)^{\delta+1}-1\}$ yields the exact solution $f(x) \equiv 1$. As in [20] we considered the values $\alpha = 40$, $\beta = 15$, $\gamma = 2$ and $\delta = 3/2$, and integration was performed with $h = 1/8$. On the basis of the stability regions of the BDG methods (which are identical to those of the [BD;BD] methods given in [20]), we expect the methods to yield stable results. In Table 6.2.2 the results are given at some gridpoints.

x	p=2	p=3	p=4	p=5	p=6
1.0	3.23	4.37	5.44	6.17	*
3.0	4.25	6.07	6.72	8.54	7.72
5.0	4.45	6.93	7.06	8.47	8.25
7.0	4.60	7.49	7.28	8.68	8.15
16.0	5.00	8.15	7.79	9.23	9.82

Table 6.2.2. Number of correct digits for problem (6.2.2) obtained with the BDG methods with h = 1/8.

The asterisk in this table indicates that x = 1 is a point where an exact starting value was given. The numerical results clearly display the stable behaviour of the BDG methods.

6.3. First kind Volterra integral equations

We applied the BDG methods to the following problems taken from [6]

$$(6.3.1) \qquad 2\int_0^x \cos(x-y)f(y)dy = \exp(x) + \sin(x) - \cos(x),$$

$$(6.3.2) \qquad \int_0^x \exp(y-x)f(y)dy = \sinh(x).$$

Both problems have the exact solution f(x) = exp(x). The endpoint of integration was x = 4. The correct order of convergence of the BDG methods up to order five is shown by the Tables 6.3.1 and 6.3.2.

h^{-1}	p=2		p=3		p=4		p=5		p=6	
10	0.87	2.3	1.50	2.8	2.20	3.9	3.20	4.9	4.55	6.6
20	1.55	2.2	2.33	2.9	3.36	3.9	4.68	5.0	6.54	6.5
40	2.20	2.1	3.20	3.0	4.54	4.0	6.18	5.0	8.50	3.5
80	2.83		4.09		5.73		7.68		9.54	

Table 6.3.1. Number of correct digits at x=4 and the computed order p^* of the BDG methods applied to (6.3.1)

h^{-1}	p=2		p=3		p=4		p=5		p=6	
10	-0.02	1.9	0.81	2.8	1.64	3.8	2.45	4.7	1.81	1.4
20	0.54	1.9	1.66	2.9	2.77	3.9	3.87	4.8	2.23	13.9
40	1.12	2.0	2.54	3.0	3.94	3.9	5.32	4.9	6.40	6.8
80	1.71		3.43		5.12		6.80		8.43	

Table 6.3.2. Number of correct digits at x=4 and computed order p* of the BDG methods applied to (6.3.2)

Although not displayed in the tables of results, the global error turns out to be a smooth function except for the sixth order method when h is small (h = 1/40, 1/80). This may explain the uncertain behaviour of BDG6.

7. CONCLUDING REMARKS

The results of section 6 justify the conclusion that the construction presented in this paper yields high order convergent methods which can be made highly stable by choosing a highly stable LM method.

To emphasize we repeat that the modified multilag methods applied to the basic test equations of (1.1), (1.7) and (1.8) yield exactly the same stability polynomials as those obtained with (ρ,σ)-reducible quadrature methods. As a consequence, all stability results previously derived for (ρ,σ)-reducible quadrature methods (e.g. A-stability results [16], stability regions [4,5,20]) also hold for the modified multilag methods.

Finally we remark that the class of methods presented here can easily be extended by considering cyclic LM methods for ordinary differential equations. In this case the method (3.6) for example takes the form

$$(7.1)\qquad f_n = g(x_n) - \sum_{i=1}^{k} a_i^{(n)}\{\tilde{I}_{n-i}(x_n)+r_{n-i}\} + h\sum_{i=0}^{k} b_i^{(n)}K(x_n,x_{n-i},f_{n-i}),$$

with r_n defined as in (3.6b) and where $a_i^{(n)}$ and $b_i^{(n)}$ are periodic functions of n. The proof of high-order convergence of (7.1) will probably be more complicated than for the methods presented in this paper. On the other hand, the stability properties of cyclic LM methods are well-known for ODE-theory

and thus can be exploited to construct in a straightforward fashion highly accurate, highly stable modified multilag methods for the efficient solution of Volterra equations.

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APPENDIX *Proofs of the theorems*

In our proofs we shall apply the following well-known lemmas.

LEMMA 1. *If* $|v_n| \le hA\sum_{j=0}^{n} |v_j| + B$ *for* $n = m(1)N$, *where* $h > 0$, $A > 0$, $B > 0$ *and* $|v_j| \le V$ *for* $j = 0(1)m-1$, *then for* h *sufficiently small*

$$\max_{m\le n\le N} |v_n| \le (hA^*mV + B^*)\exp(A^*x),$$

where $Nh = X$, $A^* = (1-hA)^{-1}A$ *and* $B^* = (1-hA)^{-1}B$.

PROOF. See e.g. BAKER [2, p.925]. □

LEMMA 2. *Let the sequence* $\{v_n\}_{n=m}^{N}$ *satisfy*

$$\sum_{i=0}^{k} a_i v_{n-i} = z_n \quad \text{for } n \ge m+k, \qquad (a_0 \ne 0)$$

where $v_m,\ldots,v_{m+k-1}$ *are given and where* $\{z_n\}_{n=m+k}^{N}$ *is an arbitrary sequence. Let the polynomial* $\rho(\zeta) = \Sigma_{i=0}^{k} a_i \zeta^{k-i}$ *satisfy the root condition, then*

$$|v_n| \le C \sum_{j=m+k}^{n} |z_j| + D \sum_{j=m}^{m+k-1} |v_j|, \qquad m+k \le n \le N,$$

where C *and* D *are uniformly bounded constants independent of* N.

PROOF. Along the lines indicated in HENRICI [8, p.243]. □

Note that z_n may depend on $v_0,\ldots,v_n$, i.e. $z_n = z_n(v_0,\ldots,v_n)$. We shall frequently use this convenient property in our proofs.

To save space, we also introduce the following notation:

(A.1) $e_n := f(x_n) - f_n;$

(A.2) $\Delta K_{nj} := K(x_n,x_j,f(x_j)) - K(x_n,x_j,f_j);$

(A.3) $\Delta\tilde{I}_n(x_m) := \psi_n(x_m) - \tilde{I}_n(x_m), \quad m = n-k(1)n-1;$

(A.4) $\Delta F_n^{(1)} := F(x_n,f(x_n),\hat{I}_n) - F(x_n,f_n,\hat{I}_n);$

(A.5) $\Delta F_n^{(2)} := F(x_n,f(x_n),\psi_n(x_n)) - F(x_n,f(x_n),\hat{I}_n);$

(A.6) $\Delta\hat{I}_n := \psi_n(x_n) - \hat{I}_n$

For the quantities defined above, the following useful inequalities can be derived. In view of the Lipschitz conditions (3.3) and (3.7)

$$|\Delta K_{nj}| \le L_1 |e_j|, \tag{A.7}$$

$$|\Delta K_{nj} - \Delta K_{n-i,j}| \le L_1^* ih|e_j|. \tag{A.8}$$

Since $\Delta\tilde{I}_n(x_m) = \psi_n(x_m) - \tilde{I}_n(x_m) = \psi_n(x_m) - \tilde{\psi}_n(x_m) + \tilde{\psi}_n(x_m) - \tilde{I}_n(x_m)$, where $\tilde{\psi}_n(x)$ is defined in (2.5), we may write using (2.11) and (A.2)

$$\Delta\tilde{I}_n(x_m) = Q_n(h;x_m) + h \sum_{j=0}^{n} w_{nj}\Delta K_{mj}.$$

As a consequence

$$|\Delta\tilde{I}_n(x_m)| \le Q_N(h) + hL_1\bar{w} \sum_{j=0}^{n} |e_j|, \tag{A.9}$$

where $Q_N(h)$ is defined in (2.15) and $\bar{w}$ is the uniform bound of $|w_{nj}|$.

Analogously we can derive, using (A.8), that

$$|\Delta\tilde{I}_{n-i}(x_n) - \Delta\tilde{I}_{n-i}(x_{n-i})| \le \Delta Q_N(h) + h^2 L_1^* \bar{w} \sum_{j=0}^{n-i} |e_j|, \tag{A.10}$$

where $\Delta Q_N(h)$ is defined in (2.16).

From the Lipschitz conditions (4.3) it follows that

$$|\Delta F_n^{(1)}| \le L_2|e_n|, \quad |\Delta F_n^{(2)}| \le L_3|\Delta\hat{I}_n|. \tag{A.11}$$

We remark that C_i occurring in the proofs below denotes a generic uniformly bounded constant.

PROOF OF THEOREM 3.1. The solution of the continuous problem (3.1) satisfies $f(x_n) = g(x_n) + \psi_n(x_n)$, or using (2.9),

$$f(x_n) = g(x_n) - \sum_{i=1}^{k} a_i\psi_{n-i}(x_n) + h \sum_{i=0}^{k} b_i K(x_n, x_{n-i}, f(x_{n-i})) + T_n(h;x_n). \tag{A.12}$$

Subtract f_n defined by (3.2) from (A.12) to obtain the equation for the global error e_n

$$(A.13) \qquad e_n = -\sum_{i=1}^{k} a_i \Delta\tilde{I}_{n-i}(x_n) + h\sum_{i=0}^{k} b_i \Delta K_{n,n-i} + T_n(h;x_n), \quad n_k \le n \le N,$$

where $\Delta\tilde{I}_n(x)$ and ΔK_{nj} are defined in (A.3) and (A.2). Using (A.9), (A.7) and (2.14) yields

$$(A.14) \qquad |e_n| \le hC_1 \sum_{j=0}^{n} |e_j| + C_2 Q_N(h) + C_3 T_N(h), \quad n_k \le n \le N.$$

Finally, application of Lemma 1 to (A.14) yields the result (3.4). □

PROOF OF THEOREM 3.3. Analogous to (A.12) the solution of the continuous problem (3.1) satisfies

$$(A.15) \qquad f(x_n) = g(x_n) - \sum_{i=1}^{k} a_i\{\psi_{n-i}(x_n) + f(x_{n-i}) - g(x_{n-i}) - \psi_{n-i}(x_{n-i})\}$$
$$+ h\sum_{i=0}^{k} b_i K(x_n, x_{n-i}, f(x_{n-i})) + T_n(h;x_n),$$

where we have used that $f(x_{n-i}) = g(x_{n-i}) + \psi_{n-i}(x_{n-i})$. Subtract f_n defined by (3.6) from (A.15) to obtain after some manipulations

$$(A.16) \qquad \sum_{i=0}^{k} a_i\, e_{n-i} = -\sum_{i=1}^{k} a_i\{\Delta\tilde{I}_{n-i}(x_n) - \Delta\tilde{I}_{n-i}(x_{n-i})\}$$
$$+ h\sum_{i=0}^{k} b_i \Delta K_{n,n-i} + T_n(h;x_n), \quad n_k \le n \le N.$$

Let z_n denote the right-hand side of (A.16) then $|z_n|$ can be bounded by

$$(A.17) \qquad |z_n| \le h^2 C_1 \sum_{j=0}^{n-1} |e_j| + C_2 \Delta Q_N(h) + hC_3 \sum_{i=0}^{k} |e_{n-i}| + T_N(h),$$

where we have used (A.10), (A.7) and (2.14). Now equation (A.16) can be written as $\Sigma_{i=0}^{k} a_i e_{n-i} = z_n$ $(n \ge n_k = n_0 + k)$ and application of Lemma 2 yields the inequality

$$(A.18) \qquad |e_n| \le C_4 \sum_{j=n_0+k}^{n} |z_j| + C_5 \sum_{j=n_0}^{n_0+k-1} |e_j|, \quad n_k \le n \le N.$$

Substitution of (A.17) into (A.18) yields

$$(A.19) \qquad |e_n| \le hC_6 \sum_{j=0}^{n} |e_j| + C_7 h^{-1} \Delta Q_N(h) + C_8 h^{-1} T_N(h) + C_9 \delta_2(h)$$

where we have used that $nh \le X$ and where $\delta_2(h)$ is defined in (2.13). Finally, application of Lemma 1 to (A.19) yields the result (3.8). □

PROOF OF THEOREM 4.1. The solution of the continuous problem (4.1) satisfies

$$(A.20) \qquad \sum_{i=0}^{k} a_i^* f(x_{n-i}) = h \sum_{i=0}^{k} b_i^* F(x_{n-i}, f(x_{n-i}), \psi_{n-i}(x_{n-i})) + T_n^*(h;x_n)$$

where $T_n^*(h;x_n)$ denotes the local truncation error at $x=x_n$ of (ρ^*,σ^*). Subtract (4.2a) from (A.20) to obtain

$$(A.21) \qquad \sum_{i=0}^{k} a_i^* e_{n-i} = h \sum_{i=0}^{k} b_i^* \{\Delta F_{n-i}^{(1)} + \Delta F_{n-i}^{(2)}\} + T_n^*(h;x_n), \quad n_k \le n \le N,$$

where we have used the notation (A.4) and (A.5). Let z_n denote the right-hand side of (A.21), then $|z_n|$ can be bounded by

$$(A.22) \qquad |z_n| \le hC_1 \sum_{i=0}^{k} \{|e_{n-i}| + |\Delta \hat{I}_{n-i}|\} + T_N^*(h),$$

where we have used (A.11) and (4.6). Writing equation (A.21) as $\Sigma_{i=0}^{k} a_i^* e_{n-i} = z_n$ $(n_0+k \le n \le N)$ and applying Lemma 2 yields the inequality

$$(A.23) \qquad |e_n| \le C_2 \sum_{j=n_k}^{n} |z_j| + C_3 \sum_{j=n_0}^{n_k-1} |e_j|, \qquad n_k \le n \le N.$$

Substitution of (A.22) in (A.23) gives the inequality

$$(A.24) \qquad |e_n| \le hC_4 \sum_{j=n_0}^{n} \{|e_j| + |\Delta \hat{I}_j|\} + C_5 h^{-1} T_N^*(h) + C_6 \delta_2(h).$$

Next we derive an inequality for $\Delta \hat{I}_n := \psi_n(x_n) - \hat{I}_n$, where $\hat{I}_n$ is defined by (4.2b). Thus subtracting (4.2b) from (2.9) gives

$$\Delta \hat{I}_n = - \sum_{i=1}^{k} a_i \Delta \tilde{I}_{n-i}(x_n) + h \sum_{i=0}^{k} b_i \Delta K_{n,n-i} + T_n(h;x_n).$$

Use of (A.9) and (A.7) then yields the inequality

$$|\Delta\hat{I}_n| \le C_7 Q_N(h) + hC_8 \sum_{j=0}^{n} |e_j| + T_N(h), \quad n_k \le n \le N. \tag{A.25}$$

Furthermore we have, in view of (4.2c), $\Delta\hat{I}_n = \Delta\tilde{I}_n(x_n)$ if $n_0 \le n \le n_k - 1$, which yields using (A.9)

$$|\Delta\hat{I}_n| \le |Q_n(h;x_n)| + hC_9 \sum_{j=0}^{n} |e_j|, \qquad n_0 \le n \le n_k - 1. \tag{A.26}$$

Substitution of (A.25) and (A.26) into (A.24) gives

$$\begin{aligned} |e_n| \le\ & hC_{10} \sum_{j=0}^{n} |e_j| + C_{11} h\delta_3(h) + C_{12} Q_N(h) + C_{13} T_N(h) \\ & + C_5 h^{-1} T_N^*(h) + C_6 \delta_2(h), \qquad n_k \le n \le N, \end{aligned} \tag{A.27}$$

where $\delta_3(h)$ is defined in (4.5). Application of Lemma 1 to (A.27) yields the result (4.4). □

PROOF OF THEOREM 4.3. The error equation for e_n is the same as in the proof of Theorem 4.1. (equation (A.16)), so that we arrive at the inequality (A.24). The error equation for $\Delta\hat{I}_n$, however, is different and is derived as follows. Write (2.9) as

$$\begin{aligned} \psi_n(x_n) = & - \sum_{i=1}^{k} a_i \{\psi_{n-i}(x_n) + \psi_{n-i}(x_{n-i}) - \psi_{n-i}(x_{n-i})\} \\ & + h \sum_{i=0}^{k} b_i K(x_n, x_{n-i}, f(x_{n-i})) + T_n(h;x_n), \quad n_k \le n \le N. \end{aligned} \tag{A.28}$$

Substitute r_n defined by (4.8c) into (4.8b) and subtract the resulting equation from (A.28). We then obtain

$$\begin{aligned} \sum_{i=0}^{k} a_i \Delta\hat{I}_{n-i} = & - \sum_{i=1}^{k} a_i \{\Delta\tilde{I}_{n-i}(x_n) - \Delta\tilde{I}_{n-i}(x_{n-i})\} \\ & + h \sum_{i=0}^{k} b_i \Delta K_{n,n-i} + T_n(h;x_n), \quad n_k \le n \le N. \end{aligned} \tag{A.29}$$

Let z_n denote the right-hand side of (A.29), then

$$|z_n| \le C_7 \Delta Q_N(h) + h^2 C_8 \sum_{j=0}^{n-1} |e_j| + hC_9 \sum_{i=0}^{k} |e_{n-i}| + T_N(h), \tag{A.30}$$

where we have used (A.10) and (A.7). Writing (A.29) as $\Sigma_{i=0}^{k} a_i \Delta\hat{I}_{n-i} = z_n$ $(n_k \le n \le N)$ and applying Lemma 2 yields

$$|\Delta\hat{I}_n| \le C_{10} \sum_{j=n_k}^{n} |z_j| + C_{11} \sum_{j=n_0}^{n_k-1} |\Delta\hat{I}_j|, \quad n_k \le n \le N. \tag{A.31}$$

Since $\hat{I}_n = \tilde{I}_n(x_n)$ for $n = n_0(1)n_k-1$, $\Delta\hat{I}_n$ equals $\Delta\tilde{I}_n(x_n)$ which yields

$$|\Delta\hat{I}_n| \le |Q_n(h;x_n)| + hC_{12} \sum_{j=0}^{n} |e_j|, \quad n_0 \le n \le n_k-1. \tag{A.32}$$

Substitution of (A.30) and (A.32) into (A.31) yields after some manipulations

$$|\Delta\hat{I}_n| \le C_{13}h^{-1}\Delta Q_N(h) + hC_{14} \sum_{j=0}^{n} |e_j| + C_{15}h^{-1}T_N(h) + \delta_3(h), \tag{A.33}$$

$$n_k \le n \le N.$$

Next we substitute (A.32) and (A.33) into (A.24) to obtain

$$|e_n| \le hC_{16} \sum_{j=0}^{n} |e_j| + C_{17}h^{-1}\Delta Q_N(h) + C_{18}h^{-1}T_N(h) + \tag{A.34}$$

$$+ C_{19}\delta_3(h) + C_5 h^{-1} T_N^*(h) + C_6\delta_2(h), \quad n_k \le n \le N.$$

Finally, application of Lemma 1 to (A.34) yields the result (4.11). □

PROOF OF THEOREM 5.1. The solution of the continuous problem (5.2) satisfies

$$-\sum_{i=1}^{k} a_i\{\psi_{n-i}(x_n) + g(x_{n-i}) - \psi_{n-i}(x_{n-i})\} + hb_0K(x_n,x_n,f(x_n)) + \tag{A.35}$$

$$T_n(h;x_n) = g(x_n).$$

Subtract (5.1) to obtain

$$hb_0\Delta K_{nn} = \sum_{i=1}^{k} a_i\{\Delta\tilde{I}_{n-i}(x_n) - \Delta\tilde{I}_{n-i}(x_{n-i})\} - T_n(h;x_n).$$

which yields the inequality

$$(A.36) \qquad h|b_0|L_4|e_n| \le C_1\Delta Q_N(h) + C_2h^2\sum_{j=0}^{n-1}|e_j| + T_N(h), \quad n_k \le n \le N,$$

where we have used (A.10) and (2.14) and the fact that $|\Delta K_{nn}| \ge L_4|e_n|$ (see condition (5.3)). Dividing through by $h|b_0|$ and applying Lemma 1 yields the result (5.4). □

SAMENVATTING

Dit proefschrift handelt over de convergentie- en stabiliteitsanalyse van numerieke methoden voor het oplossen van Volterra integraalvergelijkingen van de tweede soort

$$(V2) \qquad f(x) = g(x) + \int_0^x K(x,y,f(y))dy.$$

Hierin stelt f de onbekende functie voor en zijn g en K (de kern) gegeven functies. Bovendien worden numerieke methoden voor verwante vergelijkingen, te weten Volterra integraalvergelijkingen van de eerste soort en Volterra integro-differentiaalvergelijkingen, onderzocht. Het proefschrift bestaat uit een inleiding en uit zes artikelen ([A] t/m [F]), die in wetenschappelijke tijdschriften verschenen zijn of eventueel nog zullen verschijnen.

Vergelijkingen van het Volterra type treden op in zowel wetenschappelijke als technische toepassingen en beschrijven dynamische systemen, waarvan het gedrag niet alleen van de toestand op dat moment afhangt, maar ook van de toestanden waarin het systeem zich in het verleden heeft bevonden. In het algemeen kan men dergelijke vergelijkingen niet exact oplossen. Een benadering van de exacte oplossing kan echter worden bepaald met behulp van numerieke technieken.

Een belangrijke klasse van numerieke methoden ontstaat door de integraal in (V2) in vaste roosterpunten $x_n = nh$ te benaderen door middel van kwadratuurformules. Dit resulteert in een stelsel niet-lineaire vergelijkingen dat eenvoudig door voorwaartse substitutie opgelost kan worden. In dit proefschrift wordt in het bijzonder een belangrijke deelklasse beschouwd. Deze zogenaamde (ρ,σ)-reducibele kwadratuurformules hebben een directe relatie tot lineaire meerstapsmethoden (ρ,σ) voor het oplossen van beginwaardeproblemen.

De constructie van (ρ,σ)-reducibele kwadratuurformules wordt uitgebreid besproken in [D]. Tevens wordt een uitdrukking voor de kwadratuurfout gegeven. Voorts wordt het gebruik van dergelijke kwadratuurformules voor het oplossen van (V2) en Volterra integro-differentiaalvergelijkingen onderzocht en worden convergentie- en stabiliteitsresultaten

afgeleid.

Het is bekend dat een groot aantal kwadratuurformules die convergente methoden opleveren voor vergelijkingen van de tweede soort, divergente methoden geven voor eerste soort vergelijkingen. Met betrekking tot de laatstgenoemde vergelijkingen worden in artikel [C] voor de klasse van (ρ,σ)-reducibele kwadratuurformules de extra voorwaarden gegeven, die convergentie garanderen. Bovendien worden resultaten betreffende de orde van convergentie bewezen.

Aanleiding tot artikel [F] was de inefficiënte implementatie van sommige interessante (ρ,σ)-reducibele kwadratuurformules. In dit artikel wordt een nieuwe klasse van numerieke methoden geconstrueerd, die enerzijds efficiënt geimplementeerd kunnen worden, anderzijds de gewenste stabiliteitseigenschappen van (ρ,σ)-reducibele kwadratuurformules intact laten. Ook hier worden convergentieresultaten bewezen.

In zowel [C], [D] als [F] worden numerieke experimenten besproken uitgevoerd met kwadratuurformules waarin (ρ,σ) correspondeert met de achterwaartse differentiatieformules.

De klassieke stabiliteitsanalyse van numerieke methoden voor (V2) is gebaseerd op een eenvoudige testvergelijking waarin het Volterra karakter onvoldoende tot uitdrukking komt. In artikel [A] wordt aangetoond dat een stabiliteitsanalyse ook mogelijk is met betrekking tot een meer algemene klasse van testvergelijkingen.

In [B] wordt een relatie gelegd tussen de oplossing van de integraalvergelijking (V2) en de oplossing van een differentiaalvergelijking met een parameter. Enerzijds kunnen hiermee numerieke methoden voor (V2) afgeleid worden. Anderzijds kan de stabiliteitsanalyse van methoden voor (V2) uitgevoerd worden via de stabiliteitsanalyse van methoden voor differentiaalvergelijkingen.

Aanleiding tot het onderzoek in [E] was het vermoeden van Linz, dat de structuur van de coefficienten in de kwadratuurformules (de repetitiefactor) bepalend is voor de stabiliteit van de corresponderende numerieke methode. In dit artikel wordt, voor de klasse van (ρ,σ)-reducibele kwadratuurformules, een karakterisering afgeleid van de repetitiefactor en numerieke stabiliteit, waarmee vervolgens resultaten met betrekking tot bovenstaand vermoeden worden bewezen.

Jaka Blom

STELLINGEN

bij het proefschrift

THE NUMERICAL ANALYSIS OF REDUCIBLE QUADRATURE METHODS FOR VOLTERRA INTEGRAL AND INTEGRO-DIFFERENTIAL EQUATIONS

van

P.H.M. WOLKENFELT

30 september 1981

I

De in artikel [A] van dit proefschrift beschreven technieken kunnen, onder dezelfde aannamen, ook gebruikt worden in de stabiliteitsanalyse van numerieke methoden voor Volterra integro-differentiaalvergelijkingen.

P.J. van der Houwen, H.J.J. te Riele and P.H.M. Wolkenfelt, *On the stability of multistep formulas for systems of Volterra integro-differential equations*, Report NW 63/78, Mathematisch Centrum, Amsterdam (1978).

II

Een (ρ,σ)-reducibele kwadratuurmethode voor het oplossen van Volterra integraalvergelijkingen van de tweede soort kan niet V_0-stabiel zijn.

P.H.M. Wolkenfelt, *Stability analysis of reducible quadrature methods for Volterra integral equations of the second kind*, Report NW 79/80, Mathematisch Centrum, Amsterdam (1980); to appear in ZAMM (1981).

III

De trapeziumregel als directe kwadratuurmethode voor Volterra integraalvergelijkingen van de tweede soort is A-stabiel; diezelfde trapeziumregel geformuleerd als Runge-Kuttamethode is niet A-stabiel.

IV

Evenals voor de lineaire meerstapsmethode voor gewone differentiaalvergelijkingen geldt voor de gemengde Runge-Kuttamethode voor Volterra integraalvergelijkingen van de tweede soort (gespecificeerd in [IV]) een Dahlquistbarrière.

[IV] P.J. van der Houwen, P.H.M. Wolkenfelt and C.T.H. Baker, *Convergence and stability analysis for modified Runge-Kutta methods in the numerical treatment of second kind Volterra integral equations*, Report NW 96/80, Mathematisch Centrum, Amsterdam (1980); to appear in IMA Journal on Numerical Analysis.

V

De integraalrepresentatie van de functie $\beta(x)$ gegeven in [V, p.947, formule 8.371.1] is niet correct en dient vervangen te worden door

$$\beta(x) = \int_0^1 \frac{t^{x-1}}{1+t}\, dt \qquad [\mathrm{Re}\ x > 0].$$

[V] I.S. Gradshteyn and I.M. Ryzhik, *Table of integrals, series and products* (corrected and enlarged edition), Academic Press, New York, 1980.

VI

De in [VI, p.123] gegeven representatie van de kwadratuurfout met behulp van de Peano-kern is slechts geldig, indien wordt aangenomen dat de steunpunten binnen het integratie-interval liggen.

[VI] J. Stoer and R. Bulirsch, *Introduction to numerical analysis*, Springer-Verlag, New York, 1980.

VII

Beschouw voor het numeriek oplossen van het stelsel gewone differentiaalvergelijkingen $y' = f(y)$ de "one-leg" versie van de trapeziumregel toegepast met staplengte $2h$:

$$y_{n+1} = y_{n-1} + 2h\, f(\tfrac{1}{2}y_{n-1} + \tfrac{1}{2}y_{n+1}), \qquad n = 1,2,\ldots .$$

Indien in bovenstaande methode

(i) f verkregen is uit semi-discretisering van de parabolische partiële differentiaalvergelijking $u_t = u_{xx}$ met behulp van centrale differenties;

(ii) een benaderende oplossing van het resulterende stelsel lineaire vergelijkingen bepaald wordt door toepassing van één iteratie met het Jacobi-proces, waarin als beginschatting $y_{n+1}^{(0)} = 2y_n - y_{n-1}$ wordt gekozen,

dan is het resulterende schema identiek aan de bekende methode van DuFort en Frankel.

VIII

Teneinde de beoordelaars van manuscripten, bedoeld voor publicatie in wetenschappelijke tijdschriften, zo weinig mogelijk te beïnvloeden, dient in de beoordelingsfase ook de auteur van het desbetreffende manuscript anoniem te blijven.

IX

De mogelijke restitutie aan de werknemer van een door de (overheids) werkgever teveel afgedragen premie AOW/AWW is een verkapte vorm van extra loon; de hieruit voortvloeiende onbillijkheden kunnen worden opgeheven door de teveel betaalde premie aan de werkgever te restitueren.

X

Een uitbreiding van de overigens uitstekende dienstverlening van het faculteitsbureau in de vorm van de beschikbaarheid van een in de Engelse taal gesteld promotiereglement is geenszins overbodig.

XI

Voor vele wetenschappers verdient het aanbeveling om kennis te nemen van het rapport [XI] waarin adviezen worden gegeven voor het schrijven van wetenschappelijke publicaties zoals:

(i) "add plenty of colorful and descriptive qualifiers (such as mostly, frequently, and usually). These qualifiers can absolutely save your reputation if you have published something that is later proven wrong";

(ii) "make each sentence exceed 20 words. Studies indicate a drop in reading comprehension when this is done";

het satirische karakter van dergelijke adviezen moet echter terdege onderkend worden.

[XI] N. Tredennick and B. Shimamoto, *On systematic generation of scientific papers (or how to write a crummy paper)*, Research Report RC 8425, IBM T.J. Watson Research Center (1980).