MATHEMATICS OF COMPUTATION
VOLUME 41, NUMBER 163
JULY 1983, PAGES 87-102

Runge-Kutta Theory for Volterra and Abel Integral Equations of the Second Kind*

By Ch. Lubich

Abstract. The present paper develops the local theory of general Runge-Kutta methods for a broad class of weakly singular and regular Volterra integral equations of the second kind. Further, the smoothness properties of the exact solutions of such equations are investigated.

1. Introduction. We consider the Volterra integral equation of the second kind

$$(1)\quad y(x)=f(x)+\int_0^x (x-s)^\alpha K(x,s,y(s))\,ds, \qquad x\in I:=[0,\bar{x}],\ \alpha>-1.$$

The function $f\colon I\to \mathbf{R}^n$ is assumed to be (at least) continuous, the kernel $K\colon S\times\mathbf{R}^n \to \mathbf{R}^n$ with $S=\{(x,s)\,|\,0\leqslant s\leqslant x\leqslant \bar{x}\}$ is to be sufficiently differentiable.

For $-1<\alpha<0$ the integral equation (1) is weakly singular and sometimes called an Abel integral equation of the second kind. The special case $\alpha=-\frac{1}{2}$ (Abel equation in the proper sense) often arises in physical problems (see the references in [13] or [7]). Positive values of α are encountered in various biological models [2] and in statistics [14].

There exist general local existence and uniqueness theorems, and we suppose that the existence interval of $y(x)$ is the whole of I. In Section 2 of this paper, we shall give smoothness and analyticity properties of the solution.

For many proofs it will be convenient to assume that the kernel $K(x,s,y)$ is independent of s, i.e. $K(x,s,y)=K(x,y)$. This is no restriction of generality, since otherwise we may take $(x,y(x))$ as the solution of the integral equation

$$\begin{pmatrix} x \\ y(x)\end{pmatrix}=\begin{pmatrix} x \\ f(x)\end{pmatrix}+\int_0^x (x-s)^\alpha \begin{pmatrix} 0 \\ K(x,(s,y(s)))\end{pmatrix} ds.$$

The simple relation

$$(2)\qquad \int_0^h (h-s)^\alpha s^\beta\,ds = B(\alpha+1,\beta+1)\cdot h^{1+\alpha+\beta}\qquad (\alpha,\beta>-1),$$

where B denotes the Beta-function [1], will often be used in this paper. As an almost immediate consequence, product quadrature rules are of the form

$$\int_0^h (h-s)^\alpha g(s)\,ds \approx h^{1+\alpha}\sum_{i=1}^m \omega_i g(c_i h),$$

Received August 5, 1982; revised November 5, 1982.
1980 *Mathematics Subject Classification*. Primary 65R20.
* This work has been supported by the Deutsche Forschungsgemeinschaft.

where the ω_i, c_i do not depend on h. This suggests considering the following type of Runge-Kutta methods for the numerical solution of (1):

$$(3)\qquad Y_i^{(n)} = \tilde{F}_n(x_n + c_i h) + h^{1+\alpha} \sum_{j=1}^{m} a_{ij} K\left(x_n + d_{ij}h, x_n + c_j h, Y_j^{(n)}\right) \qquad (i = 1, \ldots, m),$$

$$y_{n+1} = \tilde{F}_n(x_n + h) + h^{1+\alpha} \sum_{i=1}^{m} b_i K\left(x_n + e_i h, x_n + c_i h, Y_i^{(n)}\right),$$

where $x_n = nh$ and $\tilde{F}_n(x)$ denotes an approximation to the lag term

$$F_n(x) = f(x) + \int_0^{x_n} (x - s)^\alpha K(x, s, y(s))\, ds.$$

The method is explicit if $a_{ij} = 0$ for $1 \leqslant i \leqslant j \leqslant m$. For $\alpha = -\frac{1}{2}$ such methods have first been used by Oules [11]. For $\alpha = 0$ Brunner, Hairer and Nørsett [3] have characterized the order of the local error of (3) in terms of the coefficients of the method. Their paper has in many ways been a model for the present work (far beyond the choice of the title). However, in the case of noninteger α an inherent lack of smoothness does not permit a direct extension of the results and techniques of [3]. So a basically different approach to the order conditions is given in Section 3. Finally, Section 4 contains a variety of examples of explicit and implicit Runge-Kutta methods (3).

2. Smoothness Properties of the Solution. In order to construct numerical methods for the approximate solution of integral equations (1), knowledge of the smoothness properties of the exact solution is indispensable.

The following theorem states that the solution $y(x)$ of (1) is smooth in any closed interval *bounded away from* 0. It is a straightforward extension of a result in Miller and Feldstein [9], and we state it without proof.

THEOREM 1. *Consider the integral equation* (1). *Assume that* $f(x)$ *is continuous in* $[0, \bar{x}]$ *and real analytic in* $(0, \bar{x})$, *and let the kernel* $K(x, s, y)$ *be real analytic in* $S \times \mathbf{R}^n$. *Then the solution* $y(x)$ *of* (1) *is real analytic in the open interval* $(0, \bar{x})$.

However, in general, $y(x)$ will not be analytic at $x = 0$. Apparently a complete answer to the behavior at 0 is as yet unknown in the literature (see, e.g., the recent papers [4], [5]). For example, Picard iteration shows that the integral equation

$$y(x) = 1 + \int_0^x (x - s)^{-1/3} y(s)\, ds$$

has the solution $y(x) = 1 + \frac{3}{2}x^{2/3} + O(x^{4/3})$ as $x \to 0$. The structure of these singularities is well understood for the special case $\alpha = -\frac{1}{2}$ (see Miller and Feldstein [9], de Hoog and Weiss [7]). The following result characterizes the behavior of the solution near 0 for arbitrary $\alpha > -1$.

THEOREM 2. *Consider the integral equation* (1). *Suppose that* $f(x) = F(x, x^{1+\alpha})$, *and assume that both* $F(z_1, z_2)$ *and the kernel* K *are real analytic at the origin. Then there is a function* $Y(z_1, z_2)$, *real analytic at* $(0,0)$, *such that* $y(x) = Y(x, x^{1+\alpha})$.

REMARK. The smoothness of $y(x)$ at 0 is not improved if $f(x)$ itself is real analytic. On the contrary, it is easily seen that $f(x)$ and $y(x)$ cannot be smooth at 0 simultaneously (excluding, of course, the trivial case where α is an integer).

Proof. Without loss of generality we may assume $K(x, s, y) = K(x, y)$ and $f(0) = 0$. We first give the proof for the one-dimensional case. Let $K(x, y) = \sum_{k \geq 0} K_k(x) y^k$. We take an arbitrary analytic function $A(z_1, z_2) = \sum_n a_n z^n$ (where $n = (n_1, n_2)$ ranges over $\mathbf{N}_0^2 \setminus \{(0,0)\}$, and $z = (z_1, z_2)$) and insert $A(x, x^{1+\alpha})$ for $y(x)$ into the integral of (1):

$$\int_0^x (x-s)^\alpha K(x, A(s, s^{1+\alpha}))\, ds = \int_0^x (x-s)^\alpha \sum_k K_k(x) \Big(\sum_n a_n s^{n_1} (s^{1+\alpha})^{n_2} \Big)^k ds$$
$$= \sum_k K_k(x) \sum_n Q_{kn}(A) \int_0^x (x-s)^\alpha s^{n_1} (s^{1+\alpha})^{n_2}\, ds,$$

where $Q_{kn}(A)$ is a polynomial in $a_{00}, a_{10}, a_{01}, \ldots, a_{n_1 n_2}$ having only nonnegative coefficients. (The sums and integrals can be interchanged because of uniform convergence.)

We now use formula (2) and write

$$I(n) = B(1+\alpha, 1 + n_1 + n_2(1+\alpha)) = \int_0^1 (1-t)^\alpha t^{n_1} (t^{1+\alpha})^{n_2}\, dt,$$

so that the expression above reduces to

$$\int_0^x (x-s)^\alpha K(x, A(s, s^{1+\alpha}))\, ds = x^{1+\alpha} \sum_n I(n) \sum_k K_k(x) Q_{kn}(A) x^{n_1} (x^{1+\alpha})^{n_2}. \tag{4}$$

This and formula (1) indicate how we have to choose $Y(z_1, z_2)$: We define Y as the *formal* power series in $z = (z_1, z_2)$ given by

$$Y(z_1, z_2) = F(z_1, z_2) + z_2 \sum_n I(n) \sum_k K_k(z_1) Q_{kn}(Y) z^n. \tag{5}$$

The factor z_2 at the right-hand side of (5) allows the recursive computation of the coefficients y_n of $Y(z) = \sum_n y_n z^n$.

As a next step we proceed to demonstrate that the formal solution $Y(z)$ defined in (5) actually represents a *convergent* power series and hence a (real) analytic function in a neighborhood of $(0,0)$: Let $\tilde{F}$ and $\tilde{K}$ denote convergent majorants of F and K, respectively. Define the formal power series $\tilde{Y}$ by

$$\tilde{Y}(z_1, z_2) = \tilde{F}(z_1, z_2) + z_2 I(0) \sum_n \sum_k \tilde{K}_k(z_1) Q_{kn}(\tilde{Y}) z^n. \tag{6}$$

Observing $|I(n)| \leq I(0)$ for all n and the nonnegativity of the coefficients of the polynomials Q_{kn}, an easy induction argument shows that $\tilde{Y}$ is a majorant of Y.

Moreover, we may rewrite (6) as

$$\tilde{Y}(z) = \tilde{F}(z) + z_2 I(0) \tilde{K}(z_1, \tilde{Y}(z)),$$

and the analytic version of the implicit function theorem implies that $\tilde{Y}(z)$, and hence also $Y(z)$, are analytic in a neighborhood of $(0,0)$.

So we can finally use (4) and (5) to conclude that $y(x) = Y(x, x^{1+\alpha})$ is indeed a solution (and so, by uniqueness, *the* solution) of the integral equation (1) near 0.

In the higher-dimensional case the $K_k(x)$ are symmetric k-linear forms, and expressions like $K_k(x)y^k$ have to be interpreted as $K_k(x)(y,\dots,y)$. Then the above proof carries immediately over to the general case. □

COROLLARY 3. *If the function F with $f(x) = F(x, x^{1+\alpha})$ and the kernel K are only assumed to be sufficiently differentiable, then the solution $y(x)$ of* (1) *has an asymptotic expansion in mixed powers of x and $x^{1+\alpha}$ as $x \to 0$.*

Proof. We construct a truncated power series $Y_N(z_1, z_2)$ as far as possible (say, of degree N) according to (5) and put $y_N(x) = Y_N(x, x^{1+\alpha})$. Then (4) shows that the defect

$$\delta(x) = y_N(x) - f(x) - \int_0^x (x-s)^\alpha K(x, y_N(s))\, ds$$

is of magnitude $O(x^N) + O((x^{1+\alpha})^N)$ as $x \to 0$.

We may interpret the integral equation (1) as a nonlinear operator equation in $C[0, \bar{x}]$ (equipped with the supremum norm):

$$y = f + T(y) \quad \text{and correspondingly} \quad y_N = f + \delta + T(y_N).$$

The estimate

$$\|T(y) - T(z)\| \leqslant \|y - z\| L \int_0^{\bar{x}} (\bar{x} - s)^\alpha\, ds,$$

where L denotes a Lipschitz constant of the kernel K, shows that the Lipschitz constant of T can be made smaller than one if $\bar{x}$ is chosen small enough. Subtracting the two equations, we obtain that the error $y(x) - y_N(x)$ is of the same magnitude as the defect. □

3. Order Conditions. The first part of this section is devoted to the study of the local error of Runge-Kutta methods (3) in an interval bounded away from 0.

Without loss of generality (also with respect to (3)) we may assume that the kernel K in (1) is independent of s. We fix x_0 in the open interval $(0, \bar{x})$ and rewrite (1) as

$$y(x) = F(x) + \int_{x_0}^x (x-s)^\alpha K(x, y(s))\, ds \quad \text{for } x \in [x_0, \bar{x}], \tag{7}$$

where $F(x) = f(x) + \int_0^{x_0}(x-s)^\alpha K(x, y(s))\, ds$. Note that by Theorem 1 the solution $y(x)$ is smooth at x_0. Applying one step of the Runge-Kutta method (3) to the integral equation (7) we obtain

$$Y_i = F(x_0 + c_i h) + h^{1+\alpha} \sum_{j=1}^m a_{ij} K(x_0 + d_{ij} h, Y_j) \qquad (i = 1,\dots,m), \tag{8}$$

$$y_1 = F(x_0 + h) + h^{1+\alpha} \sum_{i=1}^m b_i K(x_0 + e_i h, Y_i).$$

The following two definitions will allow us to state in Theorem 6 purely algebraic conditions on the coefficients of the Runge-Kutta method which imply that the local error $y_1 - y(x_0 + h)$ is of a prescribed order.

As in [3], the following set of trees will play a decisive role.

Definition 4. Let TV (Volterra-trees) denote the set of all trees which may or may not have an index x attached to any of their final nodes.

For a tree $t \in TV$ we introduce

$$\mathrm{fin}(t) = \text{number of final nodes of } t,$$
$$\mathrm{int}(t) = \text{number of interior nodes of } t.$$

(The root is counted as an interior node.)

As in [3], we use for $t_1, \ldots, t_q \in TV$ the notation $[\tau_x^k, \tau^l, t_1, \ldots, t_q]$ to designate a new $t \in TV$ which is illustrated in Figures 1 and 2.

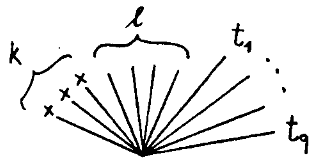

FIGURE 1

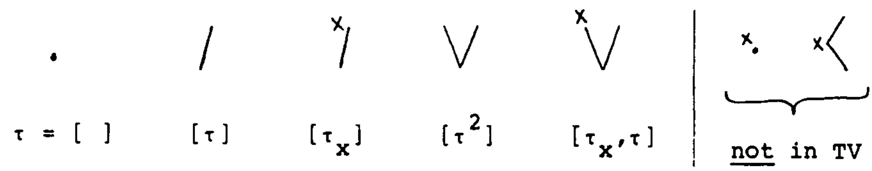

FIGURE 2

In Figure 3 we have marked the final nodes. Here we have $\mathrm{fin}(t) = 7$, $\mathrm{int}(t) = 5$.

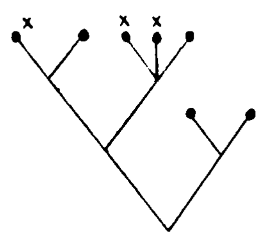

FIGURE 3

Definition 5. Let $J(l) = \int_0^1 (1-s)^\alpha s^l \, ds$ for $l \geq 0$. We define functions φ_i, φ: $TV \to \mathbf{R}$ $(i = 1, \ldots, m)$ recursively by

$$\left.\begin{aligned} \varphi_i([\tau_x^k, \tau^l]) &= \sum_{j=1}^m a_{ij} d_{ij}^k c_j^l - J(l) c_i^{k+l+1+\alpha} \\ \varphi([\tau_x^k, \tau^l]) &= \sum_{i=1}^m b_i e_i^k c_i^l - J(l) \end{aligned}\right. \qquad (k, l \geq 0),$$

and

$$\varphi_i(t) = \sum_{j=1}^m a_{ij} d_{ij}^k c_j^l \varphi_j(t_1) \cdots \varphi_j(t_q),$$
$$\varphi(t) = \sum_{i=1}^m b_i e_i^k c_i^l \varphi_i(t_1) \cdots \varphi_i(t_q),$$

for $t = [\tau_x^k, \tau^l, t_1, \ldots, t_q]$ $(t_i \neq \tau, \tau_x, q \geq 1)$.

In the sequel we shall assume that $\varphi_i(\tau) = 0$, i.e.

$$\sum_{j=1}^{m} a_{ij} = J(0)c_i^{1+\alpha} \quad \text{for } i = 1,\dots,m. \tag{9}$$

(In the special case $\alpha = 0$ this is the familiar condition $\sum_j a_{ij} = c_i$.) We are now in a position to state the main result of this section.

THEOREM 6. *Consider an integral equation* (1) *whose kernel K and solution y are sufficiently smooth at x_0 (cf. Theorem* 1). *Then the condition*

$$\varphi(t) = 0 \quad \text{for all } t \in TV \text{ with } \operatorname{fin}(t) + (1+\alpha)\operatorname{int}(t) \leqslant p \tag{10}$$

implies that the local error of the Runge-Kutta method (3) (*resp.* (8)) *with* (9) *satisfies*

$$y_1 - y(x_0 + h) = O(h^{p+\varepsilon})$$

for some $\varepsilon > 0$ which depends on the exponent α in (1).

Proof. Let $\tilde{K}(h,s) = K(x_0 + h, y(x_0 + s))$, and define the function

$$g(h) = \frac{1}{h^{1+\alpha}} \int_0^h (h-s)^\alpha \tilde{K}(h,s)\,ds = \frac{1}{h^{1+\alpha}} \int_0^h (h-s)^\alpha \sum_{k,l} \frac{1}{k!l!} \partial_h^k \partial_s^l \tilde{K}(0,0) h^k s^l\,ds$$

$$= \sum_{k,l} \frac{J(l)}{k!l!} \partial_h^k \partial_s^l \tilde{K}(0,0) h^{k+l},$$

which is seen to be smooth at $h = 0$.

As in the proof of Theorem 2, the basic idea is now to regard the functions occurring in (8) as functions of two independent variables h, κ. At the end of the proof we shall then insert $h^{1+\alpha}$ for κ. We write formula (8) (with F inserted from (7)) as

$$Y_i(h,\kappa) = y(x_0 + c_i h) - c_i^{1+\alpha}\kappa g(c_i h) + \kappa \sum_{j=1}^{m} a_{ij} K\big(x_0 + d_{ij}h, Y_j(h,\kappa)\big), \tag{11}$$

$$y_1(h,\kappa) = y(x_0 + h) - \kappa g(h) + \kappa \sum_{i=1}^{m} b_i K\big(x_0 + e_i h, Y_i(h,\kappa)\big).$$

We have

$$Y_i = Y_i(h, h^{1+\alpha}), \qquad y_1 = y_1(h, h^{1+\alpha}), \tag{12}$$

$$Y_i(h,0) = y(x_0 + c_i h), \qquad y_1(h,0) = y(x_0 + h), \tag{13}$$

and also

$$\partial_\kappa Y_i(h,0) = -c_i^{1+\alpha} g(c_i h) + \sum_{j=1}^{m} a_{ij} K\big(x_0 + d_{ij}h, y(x_0 + c_j h)\big).$$

This expression can be expanded into a Taylor series in h. This yields

$$\partial_\kappa Y_i(h,0) = \sum_{k,l \geqslant 0} \varphi_i\big([\tau_x^k, \tau^l]\big)\Phi\big([\tau_x^k, \tau^l]\big) h^{k+l},$$

where φ_i is given by Definition 5 and the Φ's are expressions which only contain derivatives of y and K at x_0, but no longer depend on the coefficients of the Runge-Kutta method.

Turning our attention to the higher derivatives of Y_i in (11) with respect to κ, we obtain

$$\partial_\kappa^r Y_i(h,0) = r\sum_{j=1}^{m} a_{ij}\partial_\kappa^{r-1}\Big[K\big(x_0+d_{ij}h, Y_j(h,\kappa)\big)\Big]\Big|_{\kappa=0} \qquad (r \geqslant 2)$$

and observe that the right-hand side of this expression will only depend on the derivatives $\partial_\kappa^\rho Y_i(h,0)$ for $\rho \leqslant r-1$. Consequently, in a step-by-step fashion we may reduce the problem to the case $r=0$, which is already known from (13). (The reduction from $r=1$ to $r=0$ has actually been performed above.) The structure of this reduction process is closely related to the set of Volterra-trees TV. In fact, a tedious induction argument (omitted here), which is based on Faà di Bruno's formula [1, p. 823] and similar to the proof of Theorem 6 in [8], shows

$$\frac{1}{r!}\partial_\kappa^r Y_i(h,0) = \sum_{\substack{t\in TV\\ \operatorname{int}(t)=r}} \varphi_i(t)\Phi(t)h^{\operatorname{fin}(t)} \qquad (r \geqslant 1),$$

where again φ_i is given by Definition 5 and Φ only depends on the integral equation (1).

So we have finally found a factorization of $Y_i(h,\kappa)$ and $y_1(h,\kappa)$ into their "Runge-Kutta parts" φ_i and φ and the "integral equation parts" Φ:

$$(14) \qquad \begin{aligned} Y_i(h,\kappa) &= y(x_0+c_ih) + \sum_{t\in TV} \varphi_i(t)\Phi(t)h^{\operatorname{fin}(t)}\kappa^{\operatorname{int}(t)}, \\ y_1(h,\kappa) &= y(x_0+h) + \sum_{t\in TV} \varphi(t)\Phi(t)h^{\operatorname{fin}(t)}\kappa^{\operatorname{int}(t)}. \end{aligned}$$

Now (10) and (12) complete the proof. □

Remarks. (a) For $\alpha = 0$ condition (10) is equivalent to the order conditions given in [3].

(b) The number of order conditions which have to be satisfied to obtain a prescribed local order strongly depends on the exponent α and tends to infinity as $\alpha \to -1$. (Trees grow into the sky.)

This indicates that the construction of (noncollocation) Runge-Kutta methods becomes increasingly complicated for negative values of α. On the other hand, it will be comparatively easy to construct high-order explicit methods for positive α (see Section 4).

(c) Figure 4 illustrates how the number ε of Theorem 6 depends on α. Consider the straight line L: fin + $(1+\alpha)$int $= p$. Then ε is the smallest vertical distance between L and the points with integer coordinates above L. (This follows from (10) and (14).) We have $0 < \varepsilon \leqslant \min\{1, 1+\alpha\}$.

Special values for ε are:

$$\begin{aligned} \varepsilon &= 1 \quad \text{for integer } \alpha, \\ \varepsilon &= \tfrac{1}{2} \quad \text{for } \alpha = -\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{2}, \ldots. \end{aligned}$$

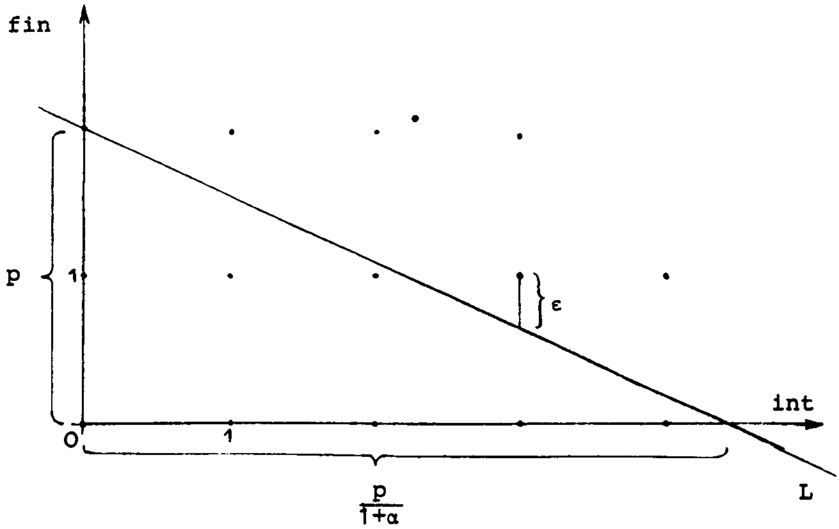

FIGURE 4

The second part of this section is devoted to the study of the local error for the first steps near 0, where the exact solution is usually not smooth. However, the representation of the solution near 0 given by Theorem 2 or Corollary 3 permits essentially the same derivation of the order conditions as before. We shall give these order conditions for the sake of completeness even if their practical value seems a little doubtful.

In this case the order conditions and the coefficients of the method will depend on n, the step-number.

We fix $n \geqslant 0$ and rewrite (1) as

$$(15) \qquad y(x) = F_n(x) + \int_{nh}^{x} (x-s)^\alpha K(x, y(s))\, ds \quad \text{for } x \in [nh, \bar{x}],$$

where $F_n(x) = f(x) + \int_0^{nh} (x-s)^\alpha K(x, y(s))\, ds$.

Applying one step of the Runge-Kutta method (3) to (15), we obtain

$$(16) \qquad \begin{aligned} Y_i &= F_n((n+c_i)h) + h^{1+\alpha} \sum_{j=1}^{m} a_{ij} K\big((n+d_{ij})h, Y_j\big), \\ \bar{y}_{n+1} &= F_n((n+1)h) + h^{1+\alpha} \sum_{i=1}^{m} b_i K\big((n+e_i)h, Y_i\big). \end{aligned}$$

Now the following set of trees will be of importance.

Definition 7. Let TV_0 denote the set of all trees which may or may not have an index x or α attached to any of their final nodes. Trivially we have $TV \subset TV_0$.

The definitions of $\text{fin}(t)$ and $\text{int}(t)$ remain the same as in Definition 4 with the difference that we agree upon counting α-nodes as interior nodes.

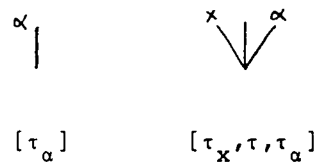

FIGURE 5

For the tree of Figure 6 we have $\text{fin}(t) = 4$, $\text{int}(t) = 8$.

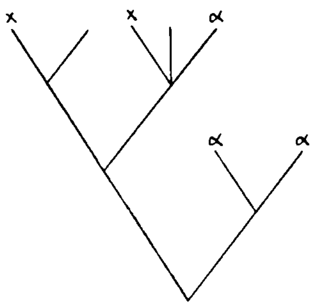

FIGURE 6

The following definition is an extension of Definition 5.

Definition 8. Let

$$J_n(l_1, l_2) = \int_0^1 (1-s)^\alpha s^{l_1}(n+s)^{(1+\alpha)l_2}\, ds,$$

$$\gamma_i = \gamma_i^{(n)} = (n + c_i)^{1+\alpha}, \qquad \gamma = \gamma^{(n)} = (n+1)^{1+\alpha}.$$

We define functions $\varphi_i = \varphi_i^{(n)}$, $\varphi = \varphi^{(n)}$: $TV_0 \to \mathbf{R}$ $(i = 1, \ldots, m)$ recursively by

$$\varphi_i\left(\left[\tau_x^k, \tau^{l_1}, \tau_\alpha^{l_2}\right]\right) = \sum_{j=1}^m a_{ij} d_{ij}^k c_j^{l_1} \gamma_j^{l_2} - J_n(l_1, l_2) c_i^{k+l_1+1+\alpha} \gamma_i^{l_2} \qquad (k, l_1, l_2 \geqslant 0),$$

$$\varphi\left(\left[\tau_x^k, \tau^{l_1}, \tau_\alpha^{l_2}\right]\right) = \sum_{i=1}^m b_i e_i^k c_i^{l_1} \gamma_i^{l_2} - J_n(l_1, l_2)\gamma^{l_2},$$

and

$$\varphi_i(t) = \sum_{j=1}^m a_{ij} d_{ij}^k c_j^{l_1} \gamma_j^{l_2} \varphi_j(t_1) \cdots \varphi_j(t_q),$$

$$\varphi(t) = \sum_{i=1}^m b_i e_i^k c_i^{l_1} \gamma_i^{l_2} \varphi_i(t_1) \cdots \varphi_i(t_q)$$

for $t = [\tau_x^k, \tau^{l_1}, \tau_\alpha^{l_2}, t_1, \ldots, t_q]$ $(t_i \neq \tau_x, \tau, \tau_\alpha, q \geqslant 1)$.

Remark. The restriction of $\varphi_i^{(n)}$, $\varphi^{(n)}$ to TV $(l_2 = 0)$ yields the functions φ_i, φ of Definition 5.

The order conditions near 0 are now given by

THEOREM 9. *Consider an integral equation* (1) *such that the solution* $y(x)$ *has an asymptotic expansion in mixed powers of* x *and* $x^{1+\alpha}$ *as* $x \to 0$ (*cf. Corollary* 3). *Then*

$$\varphi^{(n)}(t) = 0 \quad \textit{for all } t \in TV_0 \textit{ with } \text{fin}(t) + (1+\alpha)\text{int}(t) \leqslant p$$

implies that the local error of the Runge-Kutta method (16) *with* (9) *satisfies*

$$\bar{y}_{n+1} - y((n+1)h) = O(h^{p+\varepsilon})$$

for some $\varepsilon > 0$ *which depends on* α.

Compared to Theorem 6 this result states that the lack of smoothness near 0 can be compensated by satisfying certain additional order conditions.

The proof is similar to that of Theorem 6. Instead of the solution $y(x)$ one uses the smooth function $Y(z_1, z_2)$ with $y(x) = Y(x, x^{1+\alpha})$ of Theorem 2 (or Corollary 3). We omit the details.

4. Examples. In this section we will use the order conditions to derive various examples of Runge-Kutta methods (3).

A Runge-Kutta method (3) (resp. (8)) with (9) will be said to have *local order p* if its coefficients satisfy condition (10).

According to formula (8) the internal stages Y_i $(i = 1, \dots, m)$ can be interpreted as approximations to $y(x_0 + c_i h)$, and y_1 approximates $y(x_0 + h)$. So it appears natural to choose

$$d_{ij} = c_i, \qquad e_i = 1 \qquad (i, j = 1, \dots, m). \tag{17}$$

Runge-Kutta methods whose coefficients satisfy (17) are called *Pouzet-type methods* [3], [12]. The following theorem is an extension of Theorem 3.1 in [3]. Here $T \subset TV$ denotes the set of the Volterra-trees without x-nodes.

THEOREM 10. *Let* a_{ij} *and* b_i $(i, j = 1, \dots, m)$ *represent a Pouzet-type method* (9), (17). *If*

$$\varphi(t) = 0 \quad \text{for all } t \in T \text{ with } \operatorname{fin}(t) + (1+\alpha)\operatorname{int}(t) \leq p \tag{18}$$

(*where* $\varphi(t)$ *is given by Definition* 5), *then the method has local order p*.

Proof. The proof is analogous to the proof of Theorem 3.1 of [3].

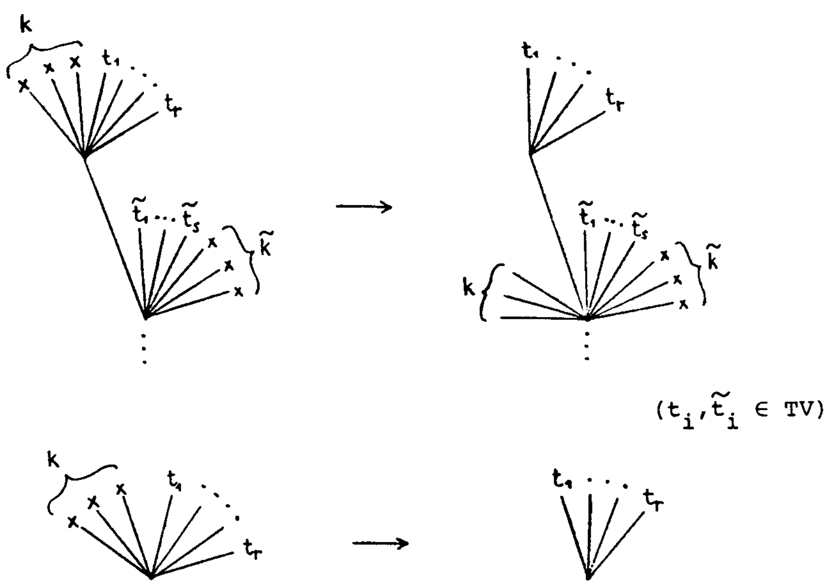

FIGURE 7

Under the condition (17) one can see from Definition 5 that many trees in TV have identical φ. Such pairs are sketched in Figure 7.

Hence, for any tree $t \in TV$ we can construct a tree $t' \in T$ such that $\varphi(t) = \varphi(t')$, $\operatorname{int}(t) = \operatorname{int}(t')$, $\operatorname{fin}(t) \geqslant \operatorname{fin}(t')$. Therefore (18) implies (10). □

Collocation Methods for $x_0 > 0$. We now consider a class of implicit Pouzet-type methods which satisfy the order conditions (10) in a trivial way. Choose distinct c_i ($i = 1,\dots,m$) and determine the coefficients a_{ij}, b_i ($i, j = 1,\dots,m$) from the Vandermonde-type conditions (cf. [6, p. 142])

$$\varphi_i([\tau^l]) = 0, \qquad \varphi([\tau^l]) = 0 \qquad (i = 1,\dots,m;\ l = 0,\dots,m-1),$$

i.e. (see Definition 5)

$$(19) \qquad \sum_{j=1}^{m} a_{ij} c_j^l = J(l) c_i^{l+1+\alpha}, \qquad \sum_{i=1}^{m} b_i c_i^l = J(l) \qquad (l = 0,\dots,m-1).$$

This means that each of the product quadrature formulae in (3) is exact for polynomials of degree $< m$.

Definition 5 shows that the corresponding Pouzet-type method satisfies (18) with $p = m$ and hence, by Theorem 10, has local order m. But we have even

$$(20) \qquad \varphi_i(t) = 0, \qquad \varphi(t) = 0 \quad \text{for all trees } t \in TV \text{ with } \operatorname{fin}(t) \leqslant m-1,$$

and by (12) and (14) this implies (in the notation of Section 3)

$$(21) \qquad \begin{aligned} Y_i - y(x_0 + c_i h) &= O(h^{m+1+\alpha}) \qquad (i = 1,\dots,m), \\ y_1 - y(x_0 + h) &= O(h^{m+1+\alpha}). \end{aligned}$$

Remark. For ordinary differential equations (i.e. the case where $\alpha = 0$ and $K(x, s, y)$ does not depend on x) condition (19) is equivalent to stating that the Runge-Kutta method is a collocation method (cf. [10]). For arbitrary α, if $c_m = 1$, Pouzet-type methods satisfying (19) can be interpreted as collocation methods in the sense of [3, Section 4] and [4].

There is even local superconvergence *en miniature*:

Proposition 11. *Let* $c_1,\dots,c_m$ *be distinct nodes such that the error of the corresponding product quadrature formula is of order*

$$(22) \qquad h^{1+\alpha} \sum_{i=1}^{m} b_i g(c_i h) - \int_0^h (h-s)^\alpha g(s)\, ds = O(h^{q+1+\alpha})$$

for smooth $g(x)$, *where* $q \geqslant m + 1$.

Then the local error of the corresponding Pouzet-type method, whose coefficients are determined by (19) *and* (17), *satisfies*

$$y_1 - y(x_0 + h) = O(h^r), \quad \text{where } r = \begin{cases} m + 2(1+\alpha) \text{ for } \alpha < 0, \\ m + 2 + \alpha \text{ for } \alpha > 0. \end{cases}$$

Proof. The assumption on the product quadrature rule implies

$$\varphi([\tau^l]) = \sum_{i=1}^{m} b_i c_i^l - J(l) = 0 \quad \text{for } l = 0,\dots,q-1.$$

As in the proof of Theorem 10, this condition yields $\varphi(t) = 0$ for all $t \in TV$ with $\operatorname{fin}(t) \leqslant q - 1$, $\operatorname{int}(t) = 1$. Together with (20), this gives the result via (12) and (14).

As an illustration consider Figure 8 where the (fin, int)-coordinates of the trees with nonvanishing φ are marked. The point indicated by "x" is the one for which φ becomes zero because of (22). □

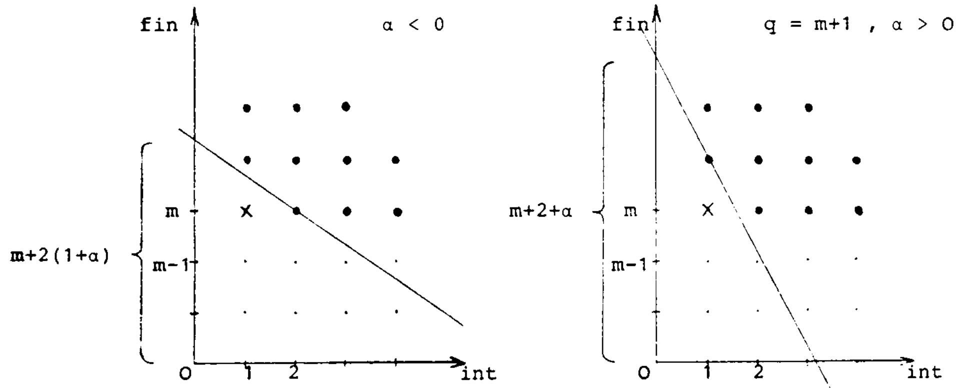

FIGURE 8

Remark. For $\alpha = 0$ the local error is actually $O(h^{q+1})$. (For ordinary differential equations this is proved e.g. in [10]; see also [6, p. 143]. By Theorem 10 the error of the corresponding Pouzet-type method is of the same magnitude.) An analogous statement does *not* hold for arbitrary α. As the following example demonstrates, the result of Proposition 11 can in general not be improved for negative α. (It is obvious from Figure 8 how a stronger result can be obtained for $\alpha > 0$ and $q \geqslant m + 2$.)

Example. Let $\alpha = -\frac{1}{2}$, $m = 2$. Choose c_1, c_2 as the zeros of the polynomial $x^2 - 8/7 \cdot x + 24/105$ (Gauss nodes), and determine b_1, b_2 from (19). Then we have $q = 4$. However, the local error of the corresponding Runge-Kutta method (19), (17) is only $O(h^3)$, because the order condition for the tree $[[\tau^2]]$ is not satisfied. □

Collocation Methods Near 0. For the approximation of the nonsmooth solution near 0 the same concept as above leads to nonpolynomial collocation methods. For $\alpha = -\frac{1}{2}$, such methods have recently been put forward in [13], [5].

Choose distinct c_i $(i = 1,\dots,m)$, and determine the coefficients a_{ij}, b_i $(i, j = 1,\dots,m)$ from the conditions

$$\varphi_i^{(n)}([\tau^{l_1}, \tau_\alpha^{l_2}]) = 0,$$
$$\varphi^{(n)}([\tau^{l_1}, \tau_\alpha^{l_2}]) = 0 \qquad (i = 1,\dots,m;\ l_1 + (1+\alpha)l_2 \leqslant p),$$

i.e. (see Definition 8)

$$\sum_{j=1}^{m} a_{ij} c_j^{l_1} (n + c_j)^{l_2(1+\alpha)} = J_n(l_1, l_2) c_i^{l_1+1+\alpha} (n + c_i)^{l_2(1+\alpha)} \qquad (i = 1,\dots,m),$$

$$\sum_{i=1}^{m} b_i c_i^{l_1} (n + c_i)^{l_2(1+\alpha)} = J_n(l_1, l_2) \quad \text{for } l_1 + (1+\alpha)l_2 \leqslant p,$$

where m and p are related in such a way that the system of linear equations has a unique solution.

If d_{ij}, e_i are chosen according to (17), a similar argument as in the smooth case, which is now based on Theorem 9, yields (the notation is as in formula (16))

$$Y_i - y((n+c_i)h) = O(h^{p+\varepsilon}) \qquad (i = 1, \dots, m),$$
$$\bar{y}_{n+1} - y((n+1)h) = O(h^{p+\varepsilon})$$

for some $\varepsilon > 0$.

Explicit Runge-Kutta Methods for $x_0 > 0$. To begin with, the *explicit Euler method* reads

$$y_{n+1} = \tilde{F}_n(x_{n+1}) + \frac{1}{1+\alpha} h^{1+\alpha} K(x_{n+1}, x_n, y_n).$$

The method has local order 1. It satisfies (19), and (21) shows that the local error is $O(h^{2+\alpha})$.

Since the number of order conditions (10) depends strongly on α, there is no point in constructing high-order explicit methods which have the same local order for *all* α (as it was for Euler's method above). It is more promising to construct methods for special, practically important values of α.

For $\alpha = 0$, various examples are given in [3]. For $\alpha = -\frac{1}{2}$ we begin with a negative result.

PROPOSITION 12. *There is no* 2- (*resp.* 3-, 4-) *stage explicit Runge-Kutta method* (3), (9) *for $\alpha = -\frac{1}{2}$ having local order $p = 2$* (*resp.* $\frac{5}{2}$, 3) (*i.e. local error $O(h^{p+1/2})$*).

(i) (ii) (iii) (iv) (v) (vi) (vii) (viii) (ix)

FIGURE 9

Proof. An explicit method of local order 2 has to satisfy at least the following order conditions (see (18) and Figure 9):

(i) $$\sum_{i=1}^{m} b_i = 2,$$

(ii) $$\sum_{i=2}^{m} b_i c_i = \frac{4}{3},$$

(iii) $$\sum_{i=2}^{m} b_i \left(\sum_{j=2}^{i-1} a_{ij} c_j - \frac{4}{3} c_i^{3/2} \right) = 0.$$

For $m = 2$, (iii) yields $b_2 c_2^{3/2} = 0$ which contradicts (ii). For an explicit method of order $\frac{5}{2}$ the following order conditions also have to be satisfied:

(iv) $$\sum_{i=2}^{m} b_i c_i^2 = \frac{16}{15},$$

(v) $$\sum_{i=3}^{m} \sum_{j=2}^{i-1} b_i a_{ij} \left(\sum_{k=2}^{j-1} a_{jk} c_k - \frac{4}{3} c_j^{3/2} \right) = 0.$$

If $m = 3$, (v) implies $b_3 a_{32} c_2^{3/2} = 0$. Then (iii) reads $b_2 c_2^{3/2} + b_3 c_3^{3/2} = 0$. Inserting this relation in (ii) and (iv), we obtain

$$b_3 c_3 c_2^{-1/2} (c_2^{1/2} - c_3^{1/2}) = \frac{4}{3}, \qquad -b_3 c_3^{3/2} (c_2^{1/2} - c_3^{1/2}) = \frac{16}{15},$$

which is a contradiction.

Finally, for $p = 3$ also the following order conditions have to be satisfied:

(vi) $$\sum_{i=2}^{m} b_i c_i \left(\sum_{j=2}^{i-1} a_{ij} c_j - \frac{4}{3} c_i^{3/2} \right) = 0,$$

(vii) $$\sum_{i=2}^{m} b_i \left(\sum_{j=2}^{i-1} a_{ij} c_j^2 - \frac{16}{15} c_i^{5/2} \right) = 0,$$

(viii) $$\sum_{i=4}^{m} \sum_{j=3}^{i-1} \sum_{k=2}^{j-1} b_i a_{ij} a_{jk} \left(\sum_{l=2}^{k-1} a_{kl} c_l - \frac{4}{3} c_k^{3/2} \right) = 0.$$

If $m = 4$, (viii) implies $b_4 a_{43} a_{32} c_2^{3/2} = 0$, and the contradiction follows in a similar but more technical way as above. □

If we choose $m = 3$, $c_2 = \frac{2}{3}$, $c_3 = 1$, $b_2 = 0$, then (i), (ii), (iii) and Theorem 10 yield

Example 13. The following coefficients represent a 3-stage explicit Pouzet-type method for $\alpha = -\frac{1}{2}$ of local order 2 (i.e. local error $O(h^{5/2})$).

c_i	a_{ij}			
0	0			
2/3	$2\sqrt{6}/3$	0		
1	0	2	0	
	2/3	0	4/3	b_i

In the notation of (3) the method reads

$$\begin{aligned} Y_1 &= \tilde{F}_n(x_n), \\ Y_2 &= \tilde{F}_n(x_n + 2h/3) + 2\sqrt{6}/3 \cdot h^{1/2} \cdot K(x_n + 2h/3, x_n, Y_1), \\ Y_3 &= \tilde{F}_n(x_n + h) + 2h^{1/2} \cdot K(x_n + h, x_n + 2h/3, Y_2), \\ y_{n+1} &= \tilde{F}_n(x_n + h) + 2/3 \cdot h^{1/2} \cdot K(x_n + h, x_n, Y_1) \\ &\quad + 4/3 \cdot h^{1/2} \cdot K(x_n + h, x_n + h, Y_3). \end{aligned}$$

Example 14. The following coefficients represent a 5-stage explicit Pouzet-type method for $\alpha = -\frac{1}{2}$ of local order 3 (i.e. local error $O(h^{7/2})$).

c_i	a_{ij}				
0					
1/2	$\sqrt{2}$	0			
1/2	$\frac{\sqrt{2}}{3}$	$\frac{2\sqrt{2}}{3}$	0		
1	a_{41}	a_{42}	a_{43}	0	
1	$\frac{6-4\sqrt{2}}{45}$	0	$\frac{48+8\sqrt{2}}{45}$	$\frac{36-4\sqrt{2}}{45}$	0
	$\frac{2}{15}$	0	$\frac{16}{15}$	0	$\frac{4}{5}$

where

$$a_{42} = -\frac{a_{53}}{a_{54}} a_{22} = -1.84296978\ldots,$$

$$a_{43} = \frac{8}{3} + \frac{32}{27a_{54}} - a_{42} = 6.267309622\ldots,$$

$$a_{41} = 2 - a_{42} - a_{43} = -2.424339842\ldots.$$

The method was derived in the following way: Choose $c_1 = 0$, $c_2 = c_3 = \frac{1}{2}$, $c_4 = c_5 = 1$, $b_2 = 0$, $b_4 = 0$, $a_{52} = 0$. Then (i), (ii) and (iv) give b_1, b_3 and b_5. (iii) and (vi) imply $a_{32} = 2\sqrt{2}/3$, whence a_{53} and a_{54} can be obtained from (iii) and (vii). Now the value for a_{42} follows from (viii), and (v) gives a_{43}. Finally, the coefficients $a_{21}, \ldots, a_{51}$ are obtained from (9). By Theorem 10 the method has the asserted local order.

Proposition 12 and the foregoing examples indicate that the construction of high order explicit Runge-Kutta methods for negative exponents α is by far more complicated than for $\alpha = 0$. The converse situation holds for positive values of α.

Example 15. The following coefficients represent a 2-stage explicit Pouzet-type method for $\alpha = 1$ of local order 4 (i.e. local error $O(h^5)$).

c_i	a_{ij}		
0	0		
1/2	1/8	0	
	1/6	1/3	b_i

In the notation of (3) the method reads

$$Y_1 = \tilde{F}_n(x_n),$$

$$Y_2 = \tilde{F}_n\left(x_n + \frac{h}{2}\right) + \frac{h^2}{8} K\left(x_n + \frac{h}{2}, x_n, Y_1\right),$$

$$y_{n+1} = \tilde{F}_n(x_n + h) + \frac{h^2}{6} K(x_n + h, x_n, Y_1) + \frac{h^2}{3} K\left(x_n + h, x_n + \frac{h}{2}, Y_2\right).$$

It was derived from (9) and the following order conditions (see Figure 9)

(i) $b_1 + b_2 = \frac{1}{2}$,
(ii) $b_2 c_2 = \frac{1}{6}$,
(iv) $b_2 c_2^2 = \frac{1}{12}$.

By Theorem 10 the method has the asserted local order.

Example 16. The following coefficients represent a 3-stage explicit Pouzet-type method for $\alpha = 1$ of local order 5 (i.e. local error $O(h^6)$).

c_i	a_{ij}			
0	0			
2/5	2/25	0		
1	−1/4	3/4	0	
	1/8	25/72	1/36	b_i

The method was derived from (9) and the following order conditions after choosing $c_3 = 1$ (see Figure 9)

(i) $b_1 + b_2 + b_3 = \frac{1}{2}$,

(ii) $b_2 c_2 + b_3 c_3 = \frac{1}{6}$,

(iv) $b_2 c_2^2 + b_3 c_3^2 = \frac{1}{12}$,

(ix) $b_2 c_2^3 + b_3 c_3^3 = \frac{1}{20}$,

(iii) $b_2(-\frac{1}{6}c_2^3) + b_3(a_{32}c_2 - \frac{1}{6}c_3^3) = 0$.

Acknowledgement. The author would like to thank E. Hairer, P. Kaps and G. Wanner for helpful discussions.

Universität Heidelberg
Institut für Angewandte Mathematik
Im Neuenheimer Feld 293
6900 Heidelberg 1, Federal Republic of Germany

1. M. ABRAMOWITZ & I. A. STEGUN (Editors), *Handbook of Mathematical Functions*, Dover, New York, 1964.

2. U. AN DER HEIDEN, *Analysis of Neural Networks*, Lecture Notes in Biomathematics, Vol. 35, Springer-Verlag, Berlin, Heidelberg, New York, 1980.

3. H. BRUNNER, E. HAIRER & S. P. NØRSETT, "Runge-Kutta theory for Volterra integral equations of the second kind," *Math. Comp.*, v. 39, 1982, pp. 147–163.

4. H. BRUNNER & S. P. NØRSETT, "Superconvergence of collocation methods for Volterra and Abel integral equations of the second kind," *Numer. Math.* v. 36, 1981, pp. 347–358.

5. H. BRUNNER & H. J. J. TE RIELE, *Volterra-Type Integral Equations of the Second Kind with Non-Smooth Solutions: High-Order Methods Based on Collocation Techniques*, Report NW 118, Mathematisch Centrum, Amsterdam, 1982.

6. J. C. BUTCHER, "Implicit Runge-Kutta and related methods," in *Modern Numerical Methods for Ordinary Differential Equations* (G. Hall and J. M. Watt, eds.), Clarendon Press, Oxford, 1976, pp. 136–151.

7. F. DE HOOG & R. WEISS, "High order methods for a class of Volterra integral equations with weakly singular kernels," *SIAM J. Numer. Anal.*, v. 11, 1974, pp. 1166–1180.

8. E. HAIRER & G. WANNER, "On the Butcher group and general multi-value methods," *Computing*, v. 13, 1974, pp. 1–15.

9. R. K. MILLER & A. FELDSTEIN, "Smoothness of solutions of Volterra integral equations with weakly singular kernels," *SIAM J. Math. Anal.*, v. 2, 1971, pp. 242–258.

10. S. P. NØRSETT & G. WANNER, "The real-pole sandwich for rational approximations and oscillation equations," *BIT*, v. 19. 1979, pp. 79–94.

11. H. OULES, "Resolution numérique d'une équation intégrale singulière," *Rev. Française Traitement Information*, v. 7, 1964, pp. 117–124.

12. P. POUZET, "Etude en vue de leur traitement numérique des équations intégrales de type Volterra," *Rev. Française Traitement Information*, v. 6, 1963, pp. 79–112.

13. H. J. J. TE RIELE, *Collocation Methods for Weakly Singular Second Kind Volterra Integral Equations with Non-Smooth Solution*, Report NW 115, Mathematisch Centrum, Amsterdam, 1981.

14. B. FEREBEE, *The Tangent Approximation to One-Sided Brownian Exit Densities*, Univ. Heidelberg, SFB 123, Techn. Rep. Nr. 138, 1981.