- Z. Jackiewicz State University, Tempe Arizona
- M. KWAPISZ Gdańsk

The numerical solution of functional differential equations, a survey

(Praca wpłynęła do Redakcji 6.11.1989)

Abstract. Significant progress has been made in the last few years in the numerical solution of functional differential equations. It is the purpose of this paper to review the results in this area. Special attention is given to implementation of one-step methods and predictor corrector methods for functional differential equations including equations of neutral type and to the stability theory of numerical methods for these equations.

1. Introduction. It is the purpose of this paper to review the results, algorithms and problems in the numerical solution of functional differential equations (FDEs)

(1.1)
$$\begin{cases} y'(t) = f(t, y(\cdot)), & t \in [a, b], \\ y(t) = g(t), & t \in [\overline{a}, a], \end{cases}$$

and neutral functional-differential equations (NFDEs)

(1.2)
$$\begin{cases} y'(t) = f(t, y(\cdot), y'(\cdot)), & t \in [a, b], \\ y(t) = g(t), & t \in [\overline{a}, a], \end{cases}$$

 $\overline{a} \leq a \leq b$. Here, g is a given initial function and f is a Volterra operator, i.e. f in (1.1) depends on y(s) and f in (1.2) depends on y(s) and y'(s) for $s \leq t$. It is usually assumed that f is continuous and satisfies Lipschitz condition with respect to the arguments $y(\cdot)$ and $y'(\cdot)$ (compare [44–47, 49, 56]). However, these equations have been also studied under weaker hypotheses such as, for example, Perron type conditions appearing in the theory of differential equations (see [43, 53, 54]).

The work of the first author was supported by the National Science Foundation under grant DMS-8900411

Equations (1.1) and (1.2) include as special cases ordinary differential equations (ODEs), delay differential equations (DDEs) (including equations with state-dependent delays) and Volterra integro-differential equations (VI-DEs). These equations have found applications in many areas of science and engineering such as control theory, oscillation theory, electrodynamics, biomathematics, pharmacokinetics, theory of learning and medical science (see [14, 28, 29, 37, 59]).

In our review of numerical methods particular emphasis will be given to the methods which are analogues of discrete variable methods for ODEs. These methods include as important special cases Runge-Kutta methods and linear multistep methods.

In the next section we introduce quasilinear multistep methods for NFDEs. This is a very general class of methods which includes as special cases most of the methods for the numerical solution of these equations. In section 3 we review some problems of implementation of one-step and linear multistep methods such as the choice of appropriate representation of underlying formulas, local error estimation and step and order changing strategies. We also review specific algorithms for FDEs and NFDEs. In section 4 we review stability properties of one-step methods and linear multistep method for FDEs and NFDEs. Finally, in section 5 we briefly mention other approaches to the numerical solution of FDEs such as extrapolation methods, methods based on Kato-Trotter theorem for semigroups of operators and techniques based on Lanczos-Tau method.

An extensive survey of developments in the area of numerical solution of FDEs up to the year 1972 was given by Cryer [22]. A more recent survey is due to Bellen [11]. In this paper we concentrate mainly on the results obtained in the last few years.

2. Quasilinear multistep methods for NFDEs. Let there be a stepsize $h \in (0, h_0], h_0 > 0$, and integers $k \geq 1, \theta \geq 0$, and define the grid $t_i := a + ih, i = 0, 1, \ldots, N$, where Nh = b - a. Suppose the functions $a_j : [0,1] \to R, j = 0, 1, \ldots, k-1$, and $\phi, \psi : [a,b] \times C_n[\overline{a},b] \times \tilde{C}_n[\overline{a},b] \times [0,1] \times [0,h_0] \to R^n$ are given, where $C_n[\overline{a},b](\tilde{C}_n[\overline{a},b])$ is the space of continuous (piecewise continuous) functions from $[\overline{a},b]$ into R^n . The quasilinear multistep method for the numerical solution of (1.2) is defined by

$$(2.1) \quad \begin{cases} y_h(t_{i+k-1} + rh) + \sum_{j=0}^{k-1} a_j(r) y_h(t_{i+j}) = h\phi(t_i, y_h(\cdot), z_h(\cdot), r, h), \\ z_h(t_{i+k-1} + rh) = \psi(t_i, y_h(\cdot), z_h(\cdot), r, h), \end{cases}$$

 $i = \theta, \theta + 1, \ldots, N - k, r \in (0, 1]$. Usually, $\theta = 0$ or $\theta = 1$. Here y_h and z_h are approximations to Y and Y' respectively, where Y is the solution to (1.2). It is assumed that these approximations are given on the initial interval $[\overline{a}, t_{k-1+\theta}]$. These initial approximations could be obtained by, for example,

one-step methods considered in [47, 72]. It is easy to avoid this starting problem if $\overline{a} < a$. It is also possible to avoid the starting problem if $\overline{a} = a$ by some modification of NFDE under consideration or by implementing these methods in variable step/variable order mode.

Methods of type (2.1) include as special cases most of the discrete variable methods for the numerical solution of (1.1) and (1.2). In particular, they include one-step methods and linear multistep methods. The former class includes collocation methods and Runge-Kutta methods and the latter class includes Adams-Bashfort, Adams-Moulton, and backward differentiation methods. As explained in [49] the methods (2.1) also include predictor-corrector methods.

Quasilinear multistep methods have been investigated in [53] in the context of ODEs and in [43] in the context of FDEs. In these papers very general convergence results were obtained under Perron type conditions imposed on the function f which define the initial-value problem and on the increment functions of the method. In [49] convergence and order properties of (2.1) for NFDEs were investigated under the Lipschitz-type conditions imposed on f, ϕ and ψ . To formulate these results assume that:

- H₁. For any $y \in C_1[\overline{a}, b]$ the mapping $t \to f(t, y(\cdot), y'(\cdot))$ is continuous on [a, b].
- H₂. The Lipschitz condition holds

$$||f(t, y_1(\cdot), z_1(\cdot)) - f(t, y_2(\cdot), z_2(\cdot))|| \le L_1(||y_1 - y_2||_{[\overline{a}, t]} + ||z_1 - z_2||_{[\overline{a}, t - \delta]}) + L_2||z_1 - z_2||_{[\overline{a}, t]},$$

with $L_1 \geq 0, 0 \leq L_2 < 1, \delta > 0$, for $t \in [a, b], y_1, y_2 \in C_n^1[\overline{a}, b], z_1, z_2 \in C_n[\overline{a}, b]$. Here, $C_n^1[\overline{a}, b]$ denotes the space of functions of class C^1 from $[\overline{a}, b]$ into R^n and $||x||_{[\overline{a}, t]}$ stands for $\sup\{||x(s)|| : \overline{a} \leq s \leq t\}$, where $||\cdot||$ is some norm in R^n . These conditions guarantee the existence of a unique solution Y to (1.2) (compare [56]). We also impose the following conditions on the functions a_j, ϕ and ψ :

H₃. The functions $a_j, j = 0, 1, ..., k-1$, are continuous, $a_{k-1}(0) = -1$ and $a_j(0) = 0$ for j = 0, 1, ..., k-2.

 H_4 . $\phi(t, y(\cdot), z(\cdot), 0, 0) = 0$ and

$$\|\phi(t, y_1(\cdot)z_1(\cdot), r, h) - \phi(t, y_2(\cdot)z_2(\cdot), r, h)\| \le$$

$$\le M(\|y_1 - y_2\|_{[\overline{a}, t+kh]} + \|z_1 - z_2\|_{[\overline{a}, t+kh]}),$$

with $M \ge 0$, for $t \in [a, b], y_1, y_2 \in C_n[\overline{a}, b], z_1, z_2 \in \tilde{C}_n[\overline{a}, b], r \in (0, 1], h \in (0, h_0].$

 $\begin{aligned} & \text{H}_{5}. \quad \|\psi(t,y_{1}(\cdot)z_{1}(\cdot),r,h) - \psi(t,y_{2}(\cdot)z_{2}(\cdot),r,h)\| \\ & \leq L_{1}(\|y_{1}-y_{2}\|_{[\overline{a},t+kh]} + \|z_{1}-z_{2}\|_{[\overline{a},t+kh-\delta]}) + L_{2}\|z_{1}-z_{2}\|_{[\overline{a},t+kh]}, \\ & \text{with } L_{1} \geq 0, 0 \leq L_{2} < 1, \delta > 0, \text{ for } t \in [a,b], y_{1}, y_{2} \in C_{n}[\overline{a},b], \end{aligned}$

 $z_1, z_2 \in \tilde{C}_n[\overline{a}, b], r \in (0, 1], h \in (0, h_0].$ Define the local discretization errors of (2.1) by

$$\eta(t,r,h) := Y(t + (k-1+r)h) + \sum_{j=0}^{k-1} a_j(r)Y(t+jh) - h\phi(t,Y(\cdot),Y'(\cdot),r,h),$$

$$\nu(t, r, h) := Y'(t + (k - 1 + r)h) - \psi(t, Y(\cdot), Y'(\cdot), r, h),$$

 $t \in [a, b - kh], r \in (0, 1], \text{ and put}$

$$\eta(h) := \sup\{\|\eta(t,r,h)\| : t \in [a,b-kh], r \in (0,1]\},
\mu(h) := \sup\{\|\eta(t,1,h)\| : t \in [a,b-kh]\},
\nu(h) := \sup\{\|\nu(t,r,h)\| : t \in [a,b-kh], r \in (0,1]\}.$$

The method (2.1) is said to be consistent if $\eta(h) = o(1), \mu(h) = o(h)$, and $\nu(h) = o(1)$ as $h \to 0$. This method is said to be of order p if $\eta(h) = O(h^p), \mu(h) = O(h^{p+1})$ and $\nu(h) = O(h^p)$ as $h \to 0$. The method (2.1) is said to be stable if no root of the polynomial

$$\rho(z) = z^k + \sum_{j=0}^{k-1} a_j(1)z^j$$

has modulus greater than one and every root with modulus one is simple.

Denote the global error functions of the method (2.1) by $\epsilon_h := y_h - Y$ and $e_h := z_h - Y'$. We have the following convergence theorem.

THEOREM 2.1 ([49], compare also [44, 46, 47]). Assume that H_1-H_5 hold, the method (2.1) is consistent and stable, and that $\|\epsilon_h\|_{[\overline{a},t_{k-1+\theta}]} = o(1)$ and $\|e_h\|_{[\overline{a},t_{k-1+\theta}]} = o(1)$ as $h \to 0$. Then the method (2.1) is convergent. Moreover, if the method is of order p and the starting errors satisfy $\|\epsilon_h\|_{[\overline{a},t_{k-1+\theta}]} = O(h^p)$ and $\|e_h\|_{[\overline{a},t_{k-1+\theta}]} = O(h^p)$ as $h \to 0$ then the order of convergence is also p, i.e. $\|\epsilon_h\|_{[\overline{a},b]} = O(h^p)$, $h \to 0$.

The conditions given in the above theorem are minimal conditions which ensure the convergence of order p of the method (2.1). To obtain additional properties of this method such as, for example, smooth behaviour of the global discretization error, we must impose rather strong assumptions about the functions $f, g, Y, \phi, \psi, \epsilon$, and e, where ϵ and e are solutions to variational equations defined below in the formulation of Theorem 2.2. Moreover, we must assume more about the initial errors and the method (2.1). This method is said to be of strong order p if $\eta(h) = O(h^{p+1})$ and $\nu(h) = O(h^{p+1})$ as $h \to 0$. We have the following theorem:

THEOREM 2.2 ([49], see also [52]). Assume that $\epsilon_h(t) = O(h^{p+1})$ and $e_h(t) = O(h^{p+1})$ as $h \to 0$ for $t \in [\overline{a}, t_{k-1+\theta}]$; the method (2.1) is stable and

has strong order p; and there exist a function $u \in C_n[\overline{a}, b]$ such that

$$\eta(t, 1, h) = h^{p+1}u(t) + O(h^{p+2})$$

for $t \in [a, b]$ as $h \to 0$. Assume also that the functions $f, g, Y, \phi, \psi, \epsilon$, and e are sufficiently smooth, where ϵ and e satisfy the system of equations

$$\begin{split} \epsilon'(t) - e(t) &= -u(t), & t \in [a, b], \\ e(t) &= \frac{\partial f}{\partial Y(\cdot)}(t, Y(\cdot), Y'(\cdot))\epsilon(\cdot) + \frac{\partial f}{\partial Y'(\cdot)}(t, Y(\cdot), Y'(\cdot))e(\cdot), & t \in [a, b], \\ \epsilon(t) &= e(t) = 0, & t \in [\overline{a}, a]. \end{split}$$

Then

$$\epsilon_h(t) = y_h(t) - Y(t) = h^p \epsilon(t) + O(h^{p+1}),$$

 $\epsilon_h(t) = z_h(t) - Y'(t) = h^p \epsilon(t) + O(h^{p+1}),$

for $t \in [\overline{a}, b]$ as $h \to \infty$.

This theorem forms a basis for local error estimation and stepsize and order changing strategies of many algorithm based on one-step methods and predictor-corrector methods. These algorithms will be discussed in Section 3.

3. Some problems of implementation of one-step and predictor-corrector methods. The solutions to (1.1) and (1.2) usually have discontinuities in their derivatives at some points in the interval of integration which may lead to order-breakdown of numerical methods for these equations. It is therefore not surprising that most of the early efforts to develop fixed-step formulas which are analogues of discrete variable methods for ODEs were concerned with methods of low orders. Feldstein [32] in his doctoral dissertation considered many different variants of Euler method for FDEs. He proved the convergence of this method for constant stepsizes and investigated the asymptotic behaviour of the global discretization error. Further analysis of continuous extension of Euler method was given by Cryer and Tavernini [24]. Hornung [41] and Castleton and Grimm [21] considered some variants of Euler methods for DDEs of neutral type (including equations with statedependent delays).

Higher order methods for DDEs were first investigated by Zverkina [85]. She considered analogues of Adams-Moulton methods for ODEs and used the technique of correcting for derivative jumps to obtain high order of convergence. Tavernini [71–73] established convergence and order theory of one-step and linear multistep methods for FDEs which is the extension of the corresponding theory for ODEs (see [25, 38, 60]). In [74] and [33] this theory was further extended to include DDEs with state-dependent delays. Jackiewicz [43] established the convergence theory of general class of quasilinear multistep methods for FDEs which unifies the convergence theory

for one-step methods and linear multistep methods for these equations. In [44-47, 49] this theory was extended to NFDEs and in [52] to DDEs of neutral type with state-dependent delays.

In the papers mentioned above the convergence and order properties of numerical methods were investigated under the assumption that the stepsize h of the method is constant. Moreover, it was usually assumed that the solution to the problem under consideration is sufficiently smooth. Since this is usually not the case, the efficient implementation of numerical methods requires special techniques for accurate determination of the location of jump discontinuities (breaking points) in lower order derivatives of the solution. If these discontinuities can be predicted in advance, which is the case for example, for DDEs which are not state dependent

(3.1)
$$\begin{cases} y'(t) = f(t, y(t), y(\alpha(t))), & t \in [a, b], \\ y(t) = g(t), & t \in [\overline{a}, a], \end{cases}$$

 $\overline{a} \leq \alpha(t) \leq t$, then the interval of integration can be divided into subintervals on which the solution to (3.1) is sufficiently smooth and a numerical method could be employed with fixed stepsize on each such subinterval. To improve efficiency some step control strategy could be used between the breaking points or we could use the constrained mesh (see [10, 11, 13]), i.e. the mesh that includes the breaking points of the solution and such that for any grid point t_i the point $\alpha(t_i)$ is again a grid point if $\alpha(t_i) > \overline{a}$. This approach was mostly used for one-step methods (compare [10–13, 83, 84]). A different approach must be employed for equations for which the location of breaking points cannot be predicted in advance. This is the case, for example, for DDEs with state dependent delays

(3.2)
$$\begin{cases} y'(t) = f(t, y(t), y(\alpha(t, y(t)))), & t \in [a, b], \\ y(t) = g(t), & t \in [\overline{a}, a], \end{cases}$$

 $\overline{a} \leq \alpha(t,y) \leq t$. Neves [61, 62] proposed a variable-step fourth order algorithm DMRODE for the solution of (3.2) which is combination of the Runge-Kutta-Merson formula of the fourth order for ODEs and interpolation formula of the third degree. In this algorithm only the "integration part" of the local discretization error was estimated, using the formulas from ODEs theory and the detection of jump discontinuities was left to the step-control mechanism based on this estimate. It was later demonstrated [63] that this approach is not always reliable and that the actual error can be badly underestimated. (It was shown by the example that if the second derivative jump occurs 3/7 into the step, the local error estimator will return the value zero no matter how big the actual error is.) Behaviour of the same nature was also demonstrated in [63] for the generalization of the Runge-Kutta-Fehlberg formula coupled with an interpolation formula of the third degree. Similar

conclusions were also reached for different algorithms by Arndt [4], de Gee and Jackiewicz [45]. The understanding of this phenomenon made it possible to take some corrective measures to make the local error estimation reliable. Two different approaches are proposed by Neves [63]. The first consists in comparing the approximate solution $y_h(\alpha(t_{i+1}, y_h(t_{i+1})))$ computed by the existing interpolation formula with the corresponding value obtained by extrapolation from mesh points outside the interval spanned by $\alpha(t_i, y_h(t_i))$ and $\alpha(t_{i+1}, y_h(t_{i+1}))$. The big discrepancy between this values indicates that α crosses the previous jump point. Repeating the process of cutting the stepsize in half until this discrepancy is small would result in locating the approximation P_h to the previous jump point P_h and it would make it possible to compute the approximation Q_h to the new jump point P_h . It was proved by Feldstein and Neves [33] that the new jump point P_h is a root of even multiplicity P_h of the nonlinear equation

$$\alpha(Q, Y(Q)) = P,$$

where Y is the solution to (4.2). Since Y and P are in general, not known in advance, we solve instead the equation

$$\alpha(Q_h, y_h(Q_h)) = P_h,$$

by some iterative technique. Assuming that the approximation y_h to Y is of order p and that the approximation P_h to a previous jump point is sufficiently accurate, Feldstein and Neves [33] have shown that the computed approximation Q_h to Q is, in general, of order $Q(h^{p/m})$ only. Therefore, if the multiplicity m is large, the order of accuracy of Q_h can be low. However, it was demonstrated in [33] that this will not prevent the method from attaining the pth order of accuracy on the whole interval [a, b].

The above approach is based on theoretical results on the propagation of discontinuities in the derivatives of the solution Y to (3.2) described in [64]. There are initial attempts to describe such propagation for systems of DDEs (see [82]). This approach to location of breaking points cannot be carried over, at least for the time being, to neutral DDEs with state dependent delays because of the lack of results on propagation of discontinuities in the solution to such equations.

The second approach proposed by Neves [63] consist in monitoring the occurrence of a current jump point by comparing the approximate solution $y_h(t)$ obtained by interpolation with the corresponding values obtained by extrapolation over the interval of the last successful step. Neves remarked that this approach can be used for ODEs with discontinuities. This approach seems to carry over also to NFDEs.

In the DMRODE algorithm by Neves [61, 62], the algorithm based on Runge-Kutta-Merson formulas described in [2], and the algorithm by Arndt

[4], the principal part of the local error consists of the local integration error and local interpolation error since both of these errors are of the same order. To get a reliable local error estimate both errors must be taken into account. However, employing the interpolation formula of order greater than the order of the underlying method for ODEs, in a sufficiently smooth situation, the principal part of the local error consists only of the local integration error, since the local interpolation error is of higher order. This was already observed by Oppelstrup [66] and employed in his RKFHB4 algorithm based on Runge-Kutta-Fehlberg formulas of orders 4 and 5 and Hermite-Birkhoff interpolation of degree 4. However, even in this case it is recommended to monitor the local interpolation error because it can be dominant for larger stepsize. Similar ideas were used for RKFR4 and RKFR7 algorithms by Oberle and Pesch [65], a variable step algorithm [52], based on fully implicit one-step methods discussed in [47], with local error estimated by local extrapolation, a variable-step algorithm [49], and variable-step variable order algorithms [50, 51, 55] based on Adams-Bashforth Adams-Moulton predictor-corrector methods with local error estimated by Milne's device. As shown in [49], local error estimators based on Milne's device are asymptotically correct in a sufficiently smooth situation. This follows from the results on the asymptotic expansions of the global discretization error (compare Theorem 2.2). Unfortunately, when the solution to (1.1) or (2.1) has derivative jumps these estimators are not always efficient. To deal with derivative discontinuities the following approaches are possible. One consists in including the jump points in a mesh and using smooth formulas to interpolate the delay functions on the whole interval $[t_i, t_{i+1}]$. This procedure, which makes the local error estimators asymptotically correct, was employed by Oberle and Pesch [65], Bock and Schlöder [17], and Arndt [4] for DDEs. Unfortunately, this procedure is not applicable to NFDEs with state dependent delays, for which the propagation of jump points is not known. Another approach was proposed recently by de Gee [26] for predictor-corrector methods with local error estimated by Milne's device. This approach, applicable also to ODEs, can be briefly summarized as follows. Denote by $s_{\nu}, \nu = 1, 2, \dots, q$, the jumps in the p+1 derivative of the solution Y to (4.1). Then, as shown in [26], the local error δ_h at the point t of linear multistep method of order p with error constant C_{p+1} is given by

$$\delta_h(t) = C_{p+1} h^{p+1} Y^{(p+1)}(t) + h^{p+1} \sum_{\nu} \gamma((t-s_{\nu})/h) \Delta_{\nu}^{(p+1)} + O(h^{p+2}),$$

where the sum is taken over all ν such that $s_{\nu} < t$. Here, $\Delta_{\nu}^{(p+1)}$ denotes the jump of $Y^{(p+1)}$ at s_{ν} and γ is some function which depends on the coefficients of the linear multistep method. The plots of γ are given in [26]. Denote by $\tilde{C}_{k+1}, \tilde{\gamma}, \tilde{y}_h$ and C_{k+1}, γ, y_h the quantities corresponding respec-

tively to Adams-Bashforth predictor and Adams-Moulton corrector of the same order k. Then, as shown in [26], Milne's device takes the form

(3.3)
$$\frac{C_{k+1}}{C_{k+1} - \tilde{C}_{k+1}} (y_h(t_i) - \tilde{y}_h(t_i))
= h^{k+1} \Big[C_{k+1} Y^{(k+1)}(t_i) \\
+ \sum_{\nu} C_{k+1} \frac{\gamma((t_i - s_{\nu})/h - \tilde{\gamma}((t_i - s_{\nu})/h)}{C_{k+1} - \tilde{C}_{k+1}} \Delta_{\nu}^{(k+1)} \Big] + O(h^{k+2}).$$

This result means that Milne's device, instead of monitoring the local discretization error $\delta_h(t_i)$ of predictor-corrector method

$$\delta_h(t_i) = h^{k+1} \left[C_{k+1} Y^{(k+1)}(t_i) + \sum_{\nu} \gamma((t_i - s_{\nu})/h) \Delta_{\nu}^{(k+1)} \right] + O(h^{(k+2)}),$$

monitors the quantity on the right-hand side of (3.3). Comparing the graph of γ with the graph of $C_{k+1}(\gamma - \tilde{\gamma})/(C_{k+1} - \tilde{C}_{k+1})$ (see [26]), we see that Milne's device does detect the jump in $Y^{(k+1)}$, but one step later than it should. This observation can be used to modify the step-changing strategy based on Milne's device. After a rejected step from t_i to t_{i+1} it is recommended that the previous step from t_{i-1} to t_i , which can contain the jump in $Y^{(p+1)}$, also be rejected, and the integration started with decreased step from t_{i-1} . A similar strategy was also recommended by Gottwald and Wanner [36] for Rosenbroch methods for stiff systems of ODEs.

As mentioned above the algorithms for the numerical solution of FDEs and NFDEs based on predictor-corrector methods with local error estimation based on Milne's device have been presented in [50, 51, 55]. The algorithm described in [50] is based on, using the terminology of Shampine and Bogacki [68], quasi-constant stepsize implementation of Adams formulas. This means that we are using Adams-Bashforth predictor and Adams-Moulton corrector of the same order with constant coefficients to advance the step from t_i to $t_{i+1} = t_i + h_i$, while all necessary back values at $t_i - h_i, t_i - 2h_i, \dots, t_i - kh_i$, are computed by interpolation. On the other hand the algorithm described in [55] is based on fully variable stepsize implementation of Adams formulas. This means that the coefficients of underlying formulas are defined for the nonuniform mesh and must, in general, be recomputed at every step. This leads to significant overhead, especially for systems of DDEs of low order. The corresponding error constants of Adams-Bashforth and Adam-Moulton formulas, which appear in Milne's formulas for error estimates, depend only on the order which is used to advance the step in case of algorithm [50]; they depend on the order and the sequence of stepsizes in case of algorithm [55]. This means that in the latter case these "constants" must be recomputed, in general, at every step which

further increases the overhead of this method. However, the extensive numerical experiments presented in [55] demonstrate that the algorithm based on a fully variable stepsize implementation of Adams formulas is more accurate and much more reliable than the algorithm based on quasi constant stepsize implementation of these formulas. These numerical experiments were performed on a broad spectrum of test examples ranging from single DDEs with constant delays and DDEs of the second order, to VIDEs. They include real-life examples from many areas of science as those listed, for example, in Oberle and Pesch [65] and Bellen and Zennaro [13]. These experiments demonstrate that the stepsize and order changing strategy based on estimation of local error by Milne's device can automatically detect the discontinuities in the solution and reduce its stepsize and order accordingly to pass it, the stepsize and order are increased automatically later on until the next discontinuity is detected. The typical graphs of stepsize versus abacissa and order versus abacissa are presented in [55]. These graphs illustrate that the dependence of stepsize and order on abacissa may be very erratic with many rejected steps which results in increased cost of computations. Therefore, it seems reasonable to combine the algorithms [50, 55] with some method of locating discontinuities; once the location and order of the discontinuity are detected, the method should step to it and restart. The methods of locating discontinuities are discussed, for example, by Stetter [70] or Gear and Østerby [35] in the context of ODEs, by Tavernini [75, 76] for FDEs, and by Feldstein and Neves [33] for DDEs with state-dependent delays.

Recently, a new approach to the implementation of Runge-Kutta methods for ODEs has been proposed by Enright [30, 31]. Since this approach has the potential of applications to FDEs and NFDEs we will briefly describe it below. Assume that the discrete solution obtained by Runge-Kutta method has been extended by some local interpolation scheme to the whole interval of integration. Local means that the interpolation polynomial on the interval $[t_i, t_{i+1}]$ is defined only in terms of quantities computed at this step so that the one-step nature of Runge-Kutta methods is preserved. The evaluation of these interpolants may entail additional computational cost but they provide an approximation y_h which is defined on the whole interval of integration. Define the local defect δ by

$$\delta(t) = y_h'(t) - f(t, y_h(t)), \quad t \in [t_i, t_{i+1}].$$

This is the amount by which y_h fails to satisfy the original problem. The new error control and stepsize changing strategy proposed by Enright [30, 31] is based on monitoring and attempting to bound the local defect rather than the local discretization error on each step to integration. He demonstrated that the approximate solution y_h computed by using this strategy satisfies exactly an initial-value problem which is small perturbation of the original

problem. As a consequence, the relationship between the error $y_h - Y$ and the tolerance used to bound the local defect depends only on the sensitivity of the original problem but is independent of the numerical method. This is the main advantage of this approach—separation of the numerical stability of the method from the mathematical conditioning of the problem. In [31] Enrigth defines and compares different strategies for estimating the local defect δ . Enrigth's approach was further modified and improved by Higham [39] who constructed interpolants for Runge-Knutta methods for which the asymptotic behaviour of the corresponding defect is known a priori. These interpolants were constructed following the approach of [30, 31] and the corresponding local defect δ on $[t_i, t_{i+1}]$ has the form

$$\delta(t_i + rh) = h^p \phi(r) K + O(h^{p+1}), \quad r \in (0, 1],$$

where p is the order of the method, K is some constant independent of r and h and ϕ is some polynomial. It follows from this relation that we can estimate δ by sampling at the point r^* which maximizies $|\phi(r)|$ over [0,1] and this process is optimal for any problem. In further report [40] Higham applied Enright's approach to Adams'predictor-corrector methods. He has considered variable-step variable-order code due to Shampine and Gordon [69] with local interpolant defined by Watts and Shampine [79] and he has shown that the shape of the associated defect is determined only by the local stepsize pattern. As a consequence, also, in this case, the defect δ over $[t_i, t_{i+1}]$ can be estimated by sampling at a single point $t_i + r^*h_i$. He has proved that for k = 1, $r^* = \frac{1}{2}$ and for $k \geq 2$, r^* is the solution in (0,1) of the equation

$$\frac{1-2r}{r(r-1)} = \sum_{j=2}^k \frac{1}{r-\sigma_j},$$

where $\sigma_j = (t_{i+1-j} - t_i)/h$, j = 2, 3, ..., k, define the stepsize pattern.

Application of Enright [30, 31] technique requires the development of interpolants which can be associated with discrete approximations generated by numerical methods. For this reason this approach seems to be ideally suited for FDEs and NFDEs since, by the nature of the problem, the numerical approximation must be generated on the whole interval of the integration anyway. Since the definition of the local defect δ is affected both by the formula to advance the step and the corresponding interpolation scheme, this step control strategy should be more reliable than the strategy based on the estimation of the local discretization error alone.

We conclude this section by mentioning the recent algorithm by Wiener and Strehemel [80] which can automatically detect stiffness in DDEs.

4. Stability properties of numerical methods for FDEs and NFDEs. To investigate stability properties of numerical methods for (1.1)

and (1.2), these methods are usually applied, with a fixed positive stepsize h, to various test equations with known region of stability. The simplest test equation is

(4.1)
$$\begin{cases} y'(t) = by(t-\tau), & t \le 0, \\ y(t) = g(t), & t \in [-\tau, 0], \end{cases}$$

 $\tau > 0$, where b is real, and it is known (see Bellman and Cooke [14]) that the solution to this equation tends to zero as $t \to \infty$ for all g if and only if $b \in (-\pi/2\tau, 0)$. The numerical method, with stepsize $h = \tau/m$, where m is positive integer, which inherits this property is said to be DA₀-stable and Cryer [23] gives some necessary and sufficient conditions for linear multistep method to be DA₀-stable. He also introduced a more general notion of GDA₀-stability which relaxes to condition $h = \tau/m$ to $h = \tau/(m-u)$, where $u \in [0,1)$, and investigated the properties of linear multistep methods with respect to this concept. Barwell [9] generalized some of Cryer's results to the case where b is complex and also considered a more general test equation

(4.2)
$$\begin{cases} y'(t) = ay(t) + by(t-\tau), & t \ge 0, \\ y(t) = g(t), & t \in [-\tau, 0], \end{cases}$$

with a and b complex. He introduced the notion of Q- and GQ-stability related to (4.1) (with b complex) and P- and GP-stability related to (4.2) which are analogues of Cryer's concepts of DA_0- and GDA_0- stability and investigated stability properties of some simple multistep methods coupled with Lagrange interpolation. Still more general concepts of stability with respect to (4.1) were introduced by van der Houwen and Sommeijer [78] and stability criteria were derived for a class of linear multistep methods.

Stability analysis of numerical methods for DDEs is difficult since it is necessary to consider difference equations of arbitrarily high order. To illustrate this point suppose that the linear multistep method for (3.1) (4.3)

$$\begin{cases} \sum_{j=0}^{k} \alpha_j y_h(t_{i+k-j}) = h \sum_{j=0}^{k} \beta_j f(t_{i+k-j}, y_h(t_{i+k-j}), y_h(\alpha(t_{i+k-j}))), \\ y_h(s) = g_h(s), \quad s \in [t_0 - \tau, t_0], \end{cases}$$

 $i=0,1,\ldots$, coupled with Lagrange interpolation of sufficiently high order, and stepsize h=r/m, where m is a positive integer, is applied to (4.2). Here, $t_i=a+ih, i=0,1,\ldots,y_h$ is an approximate solution, and y_h is an approximation to y. This leads to the difference equation

(4.4)
$$\begin{cases} \sum_{j=0}^{k} \alpha_j y_h(t_{i+k-j}) = h \sum_{j=0}^{k} \beta_j (ay_h(t_{i+k-j}) + by_h(t_{i+k-j-m}), \\ y_h(s) = g_h(s), \quad s \in [t_0 - \tau, t_0], \end{cases}$$

 $i=0,1,\ldots$, of order m+k. Now in order to establish some stability properties of (4.3) we should be able to decide whether or not the solution y_h of (4.4) is bounded (or tends to zero as $t\to\infty$). This is, in general, a nontrivial task and first results in this area were obtained only for simplest

numerical methods. Barwell [9] established P- and GP-stability for first and second order backward differentiation methods and Jackiewicz [48] and Calvo and Grande [20] determined stability regions for θ -methods. Similar results with respect to the test equation (4.1) were obtained by Cryer [23] and Barwell [9]. Cryer proved that the θ -methods are DA_0 -stable if and only if $\theta \in [\frac{1}{2}, 1]$ and that the Backward Euler method and the trapeizodal method are GDA_0 -stable. Barwell proved that the Backward Euler method is Q-stable and conjectured that it is GQ-stable. For more general methods some stability results were established by Wiederholt [81], Al-Mutib [1] and Oppelstrup [66]. Wiederholt determined numerically (via boundary locus method) the set of all (ha, hb) such that y_h given by (4.4) tends to zero as $t \to \infty$ for second order Milne predictor-corrector method and third order Adams predictor-corrector method for m = 1, 2 and 3. Similar results were obtained by Al-Mutib for the Runge-Kutta-Merson method, the trapezium rule and the fourth order implicit Runge-Kutta method. Oppelstrup investigated stability properties of Runge-Kutta-Fehlberg method combined with Hermite-Birkhoff interpolation with respect to the test equation (4.1).

More general test equations for FDEs were considered by Bickart [15, 16], Brayton and Willoughby [18], Fox, Mayers, Ockendon and Tayler [34], Kato and McLeod [58], Bakke and Jackiewicz [5], and Torelli [77].

A breakthrough in the stability analysis of numerical methods for DDEs came with the paper by Roth and Watanabe [67] and, especially, by Zennaro [84]. Roth and Watanabe [67] introduced the technique based on argument principle which directly relates the region of absolute stability for DDEs corresponding to a y(t) term with the region corresponding to the delay term $by(t-\tau)$. Following [67] we will illustrate this technique for backward Euler method for (3.1). This method takes the form

$$(4.5) y_h(t_{i-1} + rh) = y_h(t_{i-1}) + rhf(t_i, y_h(t_i), y_h(\alpha(t_i))),$$

 $i = 1, 2, ..., r \in (0, 1]$. An application of this method to (4.2) with $h = \tau/m$, where m is a positive integer leads to the difference equation

$$(4.6) y_i = y_{i-1} + h(ay_i + by_{i-m}),$$

 $i=1,2,\ldots$, where $y_i:=y_h(t_i)$. The method (4.5) is said to be P-stable if the solution $\{y_i\}_{i=0}^{\infty}$ to (4.6) tends to zero as $i\to\infty$ for any (ha,hb) such that |b|<-Re(a). This condition means that the approximate solution $\{y_i\}_{i=0}^{\infty}$ tends to zero as $i\to\infty$ whenever the theoretical solution Y(t) to (4.2) tends to zero as $t\to\infty$.

The characteristic polynomial of (4.6) is $\xi^{i-m}\phi(\xi)$ where

$$\phi(\xi) = \xi^m - \xi^{m-1} - ha\xi^m - hb.$$

A necessary and sufficient condition for asymptotic stability of the solution to (4.6) is that all m roots of the polynomial ϕ lie within the unit circle.

To investigate the location of roots of this polynomial it is convenient to introduce the rational function

$$g(\xi) = -g_1(\xi) + g_2(\xi) = -\left(\left(\frac{1}{\xi} + 1\right) - ha\right) + hb\xi^{-m}$$

which has a pole of order m at the origin and m zeros at unknown locations. The loci of g_1 and g_2 for ξ on the unit circle are circles with centres at 1-ha and 0 and radii 1 and h|b|. The locus of the function g_1 is the boundary of the region of absolute stability of the backward Euler method for ODEs displaced by -ha. Thus this approach relates directly the stability region for ODEs with the region corresponding to the delay term. It can be checked that if |b| < -Re(a) then the loci of g_1 and g_2 are disjoint and, as a consequence, the change of argument of $g(\xi)$ as ξ traces the unit circle is zero. Hence, by the argument principle, all zeros of g lie within the unit circle, which proves that the method (4.5) is P-stable.

This technique was used in [67] to show that for every A-stable, $A(\alpha)$ -stable, or stiffly stable linear multistep formula for ODEs there is a corresponding formula for DDEs with analogous stability properties.

Zennaro [84] investigated stability properties of Runge-Kutta methods for DDEs (3.1) with delay function $\alpha(t)=t-\tau,\tau>0$. These are the methods of the form

$$\begin{cases} y_{i+1} = y_i + h \sum_{r=1}^{\nu} w_r k_{i+1}^{(r)}, \\ k_{i+1}^{(r)} = f(t_i + c_r h, y_i + h \sum_{s=1}^{\nu} a_{rs} k_{i+1}^{(s)}, y_{i-m} + h \sum_{s=1}^{\nu} b_{rs} k_{i-m+1}^{(s)}), \end{cases}$$

 $r=1,2,\ldots,\nu, i=0,1,\ldots$, where $w_r,a_{r,s},b_{r,s}$ are real coefficients and $c_r=\sum_{s=1}^{\nu}a_{r,s}$. Put $w=[w_1,\ldots,w_{\nu}]^T, A=[a_{r,s}]_{r,s=1}^{\nu}, B=[b_{r,s}]_{r,s=1}^{\nu}$. We refer to (4.7) as $\{w,A,B\}$ method. Zennaro showed that the application of (4.7) to the test equation (4.2) leads to the vector recurrence relation

$$(4.8) Y_{i+1} = LY_i + MY_{i-m+1} + NY_{i-m},$$

 $i=m,m+1,\ldots$, where $Y_i:=[y_i,hk_i^T]^T,k_i:=[k_i^{(1)},\ldots,k_i^{(\nu)}]^T$, and where L,M and N are the following $(\nu+1)\times(\nu+1)$ matrices:

$$L := \begin{bmatrix} 1 + \alpha \eta & 0 \dots 0 \\ \alpha (I - \alpha A)^{-1} u & 0 \end{bmatrix},$$

$$M := \begin{bmatrix} 0 & \beta w^T (I - \alpha A)^{-1} B \\ 0 \\ \vdots & \beta (I - \alpha A)^{-1} B \\ 0 & \vdots \end{bmatrix},$$

$$N := \begin{bmatrix} \beta \eta & 0 \dots 0 \\ \beta (I - \alpha A)^{-1} u & 0 \end{bmatrix}.$$

Here, $\alpha = ha, \beta = hb, u = [1, 1, ..., 1]^T$ and $\eta := w^T (I - \alpha A)^{-1} u$ provided $I - \alpha A$ is nonsingular. The characteristic equation of (4.8) is

$$\det(\lambda^{m+1}I - \lambda^m L - \lambda M - N) = 0$$

To investigate the location of roots to this equation Zennaro [84] introduced the rational function

$$r_{\alpha}(z) := 1 + (\alpha + z)w^{T}(I - \alpha A - zB)^{-1}u,$$

which depends on α . This function is a generalization of stability function $R(\alpha) = r_{\alpha}(0) = 1 + \alpha w^{T}(1 - \alpha A)^{-1}u$ of Runge-Kutta method $\{w, A\}$ for ODEs. Zennaro's technique is based on the nontrivial observation that under some technical conditions the nonzero roots to (4.8) are the same as the roots to the equation $\lambda = r_{\alpha}(\beta/\lambda^{m})$ which is easier to investigate.

Put $\Gamma_{\alpha} := \{z : |r_{\alpha}(z)| = 1\}$ and define $\sigma_{\alpha} := \inf\{|z| : z \in \Gamma_{\alpha}\}$. The main result of [84] is the following.

THEOREM 4.1. Assume that the matrix $I-\alpha A-zB$ is singular if and only if z is a pole of r_{α} . Then the interior of the region of stability of the method $\{w,A,B\}$ with respect to (4.2) (i.e the set of all points $(\alpha,\beta)=(ha,hb)$ for which the roots to the equation (4.8) or, equivalently, to the equation $\lambda = r_{\alpha}(\frac{\beta}{\lambda m})$ are inside of the unit circle) is given by

$$\{(\alpha,\beta): \alpha \in S_A \quad and \quad |\beta| < \sigma_{\alpha}\},\$$

where S_A is the region of absolute stability of the Runge-Kutta method $\{w,A\}$ for ODEs.

The following important result can be concluded from this theorem.

THEOREM 4.2 (Zennaro [84]). Assume that the condition given in Theorem 4.1 hold and that $\{w, A\}$ method for ODEs is A-stable. Then the corresponding $\{w, A, A\}$ method for DDEs is P-stable.

Zennaro's technique has been extended by Bellen, Jackiewicz and Zennaro [12] to Runge-Kutta methods for neutral DDEsof the form

(4.9)
$$\begin{cases} y'(t) = f(t, y(t), y(t-\tau), y'(t-\tau)), & t \ge 0, \\ y(t) = g(t), & t \in [-\tau, 0], \end{cases}$$

 $\tau > 0$. The stability analysis is based on the test equation

(4.10)
$$\begin{cases} y'(t) = ay(t) + by(t - \tau) + cy'(t - \tau), & t \ge 0, \\ y(t) = g(t), & t \in [-\tau, 0], \end{cases}$$

where a, b and c are complex parameters. The following result was proved in [12] about the asymptotic behaviour of solutions to (4.10).

THEOREM 4.3. Assume that $|a\overline{c} - \overline{b}| + |ac + b| < -2 \operatorname{Re}(a)$. Then every solution to (4.10) tends to zero as $t \to \infty$.

If a, b and c are real then the condition $|a\overline{c}-\overline{b}|+|ac+b|<-2\operatorname{Re}(a)$, is equivalent to the conditions |b|<-a and |c|<1. This is the essence of the result by Brayton and Willoughby [18]. If a, b are complex and c=0 then the hypothesis of the Theorem 4.3 reduces to $|b|<-\operatorname{Re}(a)$ which gives a sufficient condition for the stability of the test equation (4.2), compare Barwell [8].

Consider the following p-stage Runge-Kutta method for the problem (4.9)

(4.11)
$$\begin{cases} y_{i+1} = y_i + h \sum_{j=1}^p w_j z_{i+1}^{(j)}, \\ z_{i+1}^{(j)} = f(t_i + c_j h, y_i + h \sum_{s=1}^p a_{js} z_{i+1}^{(s)}, \\ y_{i-m} + h \sum_{s=1}^p b_{js} z_{i-m+1}^{(s)}, \sum_{s=1}^p c_{js} z_{i-m+1}^{(s)}), \end{cases}$$

 $j=1,2,\ldots,p$, where $c_j=\sum_{s=1}^p a_{js}$. Here, the vector $w=[w_1,\ldots,w_p]^T$, and the matrix $A=[a_{js}]_{j,s=1}^p$ define a Runge-Kutta method for ODEs. Put $B=[b_{js}]_{j,s=1}^p, C=[c_{js}]_{j,s=1}^p$. Then the Runge-Kutta method (4.11) for (4.9) can be described by the quadruple $\{w,A,B,C\}$.

Denote by $\{y_i(m,ha,hb,c)\}_{i=0}^{\infty}$ the sequence obtained from applying the method (4.11) to (4.10) for a given value of positive integer m and $h=\tau/m$. The method (4.11) is said to be stable for given (ha,hb,c) if the sequence $\{y_i(m,ha,hb,c)\}_{i=0}^{\infty}$ tends to zero as $i\to\infty$ for any integer $m\geq 1$. The region of stability of (4.11) is the set of all values (ha,hb,c) for which (4.11) is stable. This method is said to be NP-stable if the region of stability contains the set $\{(ha,hb,c): |a\overline{c}-\overline{b}|+|ac+b|<-2\mathrm{Re}(a)\}$. This condition means that the approximate solution $\{y_i(m,ha,hb,c)\}_{i=0}^{\infty}$ tends to zero as $i\to\infty$ whenever the theoretical solution Y(t) to (4.10) tends to zero as $t\to\infty$.

Put $\alpha = ha, \beta = hb, q = \frac{\beta}{c}$, and consider the rational function

$$r_{\alpha,q}(z) := 1 + (\alpha + qz)w^T(I - \alpha A - z(qB + C))^{-1}u,$$

where $u = [1, 1, ..., 1]^T$. This function is generalization of stability function $r_{\alpha}(z)$ of Runge-Kutta method (4.7) for DDEs. Define the curve

$$\Gamma_{\alpha,q} := \{ z \in C : |r_{\alpha,q}(z)| = 1 \}$$

and put

$$\sigma_{\alpha,q} := inf\{|z| : z \in \Gamma_{\alpha,q}\}.$$

We have the following characterization of stability region of Runge-Kutta method (4.11).

Theorem 4.4 ([12]). Assume that the matrix $I - \alpha A - z(qB + C)$ is singular if and only if z is a pole of $r_{\alpha,q}$. Denote by S_A the (open) region of absolute stability of the Runge-Kutta method $\{w,A\}$ for ODEs. Then the interior of the region of stability of the Runge-Kutta method $\{w,A,B,C\}$

for (4.9) is given by

$$\{(\alpha, \beta, c) : \alpha \in S_A \text{ and } |c| < \sigma_{\alpha, g}\}.$$

The next theorem deals with the special case of the method (4.11) for which B = A and C = I, where I is the identity matrix.

THEOREM 4.5 ([12]). Assume that the condition given in Theorem 4.4 holds. Then the interior of the region of stability of the Runge-Kutta method $\{w, A, A, I\}$ for (4.9) is given by

$$\{(\alpha, \beta, c) : \alpha \in S_A \text{ and } |c| < \inf\{|z| : \frac{\alpha + qz}{1 - z} \in \partial S_A\}\},$$

where ∂S_A stands for the boundary of the region S_A .

The following important result can be concluded from Theorem 4.5.

THEOREM 4.6 ([12]). Assume that the Runge-Kutta method $\{w, A\}$ for ODEs is A-stable. Then the corresponding method $\{w, A, A, I\}$ for (4.9) is NP-stable.

The technique presented in [12] was also used to investigate stability properties of fully implicit one-step methods for NFDEs (1.2) introduced in [47]. These are the methods of the form

$$(4.12) \begin{cases} y_h(t_i+rh) = y_h(t_i) + h \sum_{j=0}^p a_j^p(r) z_h(t_i+b_j^p h), & r \in (0,1], \\ z_h(t_i+rh) = \sum_{j=0}^{p+1} l_j^{p+1}(r) z_h(t_i+b_j^{p+1} h), & r \in (0,1], \\ z_h(t_i+rh) = f_h(t_i+b_j^{p+1} h, y_h(\cdot), z_h(\cdot), \end{cases}$$

 $i=0,1,\ldots,N-1,Nh=b-a,y_h(t)=g_h(t),z_h(t)=g_h'(t),t\in[\overline{a},a].$ Here, f_h is a discrete approximation to f,g_h and g_h' are approximation to g and g_h' and b_i^{p+1} are distinct points from the interval [0,1], and

$$a_j^q(r) = \int\limits_0^r l_j^q(s)ds,$$

where l_j^q are Lagrange's fundamental polynomials

$$l_j^q(r) = \prod_{\substack{i=0\\i\neq j}}^q \frac{r - b_i^q}{b_j^q - b_i^q}.$$

We have the following theorem.

THEOREM 4.7 (compare [12]). Assume that the method (4.12) applied to ODEs is A-stable. Then this method is NP-stable.

It is known that if b_j^q are chosen to be, for example, the Lobatto points for [0,1] then the method (4.12) applied to ODEs is A-stable. Therefore, it fol-

lows from Theorem 4.7 that in such a case this method is NP-stable. As discussed in [12] the choice of b_j^{p+1} does not affect stability properties of (4.12).

5. Concluding remarks. In our review we concentrated mainly on the methods for FDEs and NFDEs which are analogues of discrete variable methods for ODEs. Moreover, while discussing specific problems of implementation of these methods and their stability properties we considered mainly methods for special cases of (1.1) and (1.2), such as DDEs, neutral DDEs and DDEs with state dependent delays. Other approaches to the numerical solution of these equations have been considered in the literature. De Gee [27] discussed extrapolation methods for DDEs. Amillo-Gil [3], Banks and Burns [6], Banks and Kappel [7], and Kappel and Kunish [57] considered approximation techniques for DDEs based on Kato-Trotter theorem for semigroups of operators. Fox, Mayers, Ockendon and Tayler [34] and Ito and Teglas [42] examined some numerical techniques for DDEs based on the Lanczos-Tau method. To make this paper of reasonable length we have decided not to address these developments here in more detail.

Another important special case of (1.1) and (1.2) are VIDEs. The recent book by Brunner and van der Houwen [19] presents the state-of-the-art in the numerical solution of Volterra equations up to the year 1986 and for this reason we did not address here specific implementation and stability problems in this area.

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