Milan Práger; Jiří Taufer; Emil Vitásek

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SOME NEW METHODS FOR NUMERICAL SOLUTION OF INITIAL VALUE PROBLEMS

by MILAN PRÁGER, JIŘÍ TAUFER and EMIL VITÁSEK

§ 1. INTRODUCTION

When solving many technical problems leading to initial-value problems for ordinary differential equations (typical examples are stiff problems) by finite-difference methods it is important not to aim only at high asymptotic accuracy but also to satisfy other requirements. One of such requirements is Dahlquist's A-stability which has often proved very useful. It is well known, however, that in the class of basic methods for numerical solution of initial-value problems (as the linear multistep methods, the Runge-Kutta-type methods) there exist no A-stable methods of order higher than 2 (cf. DAHLQUIST [1963]). This to a great extent negative result made us to be concerned with a larger class of methods that would contain A-stable methods of arbitrarily high order. Because it is also well known that the A-stable linear multistep methods are necessarily implicit (cf. again DAHLQUIST [1963]), our methods will bear more implicit character in the sense that instead of computing the approximate solution in one point from the (known) approximate solutions in l preceding points (as it is in the case of linear l-step method) we will compute the approximate solutions in k successive points simultaneously from some (generaly nonlinear) system of equations supposing the solution is known in l successive points. From this reason these methods will be called *overimplicit* methods.

In the lecture, the necessary and sufficient conditions for the convergence of overimplicit methods will be given and the existence of A-stable methods of arbitrarily high order will be studied. Before passing to the main subject of this lecture we would like to note that the overimplicit methods can be used not only for the solution of stiff problems but also for construction of numerical methods for solving partial differential equations of parabolic type which are of arbitrarily high order of accuracy with respect to the time mesh-size. This fact can be most easily comprehended assuming that the parabolic equation is solved by transformation on the system of ordinary differential equations (discretizating only the space variables) and observing that the resulting system of ordinary differential equations is the more stiff the more fine is the space mesh.

§ 2. OVERIMPLICIT MULTISTEP METHODS

For the sake of simplicity, we will deal only with one differential equation of the first order

$$y' = f(x, y) \quad \text{in} \quad \langle a, b \rangle \tag{2.1}$$

with the initial condition

$$y(a) = \eta\,. \tag{2.2}$$

Let us note, however, that all what follows is true also for systems of ordinary differential equations. The right-hand term of the given differential equation is assumed to be defined, continuous and satisfying the Lipschitz condition with respect to y (with a constant independent of x) in the strip $a \leqq x \leqq b$, $-\infty < y < \infty$ so that the solution of the problem (2.1) and (2.2) exists and is unique in the whole interval $\langle a, b\rangle$. The approximate solution will be sought in points $x_i = a + ih$, $i = 0, 1, \ldots$, (or in some of them) where $h > 0$ is the mesh-size. One step of the method under consideration consists—as it was already mentioned—in computing the approximate solutions $y_{n+1}, \ldots, y_{n+k}$ in the points $x_{n+1}, \ldots, x_{n+k}$ (assuming the approximate solutions $y_{n-l+1}, \ldots, y_n$ in the points $x_{n-l+1}, \ldots, x_n$ to be known) simultaneously from the system

$$\begin{bmatrix} y_{n+1} \\ \vdots \\ y_{n+k} \end{bmatrix} + \mathbf{B} \begin{bmatrix} y_{n-l+1} \\ \vdots \\ y_n \end{bmatrix} = h\mathbf{C} \begin{bmatrix} f_{n+1} \\ \vdots \\ f_{n+k} \end{bmatrix} + h\mathbf{D} \begin{bmatrix} f_{n-l+1} \\ \vdots \\ f_n \end{bmatrix} \tag{2.3}$$

where $f_j = f(x_j, y_j)$, $\mathbf{C}$ is a square matrix of order k and $\mathbf{B}$, $\mathbf{D}$ are $k \times l$ matrices.

The fact that the function $f(x, y)$ satisfies the Lipschitz condition guarantees the existence and the uniqueness of the solution of (2.3) for any sufficiently small h so that one step of our method is really defined. In order to describe the whole method it is necessary, moreover, to indicate how to continue in the following step i.e. to indicate how to choose the new l initial values. The method will proceed in advance obviously only in that case when the new initial values will be chosen from the values $y_{n-l+2}, \ldots, y_{n+k}$. Because this may be obviously done in different ways, specify the new initial values as $y_{n-l+1+s}, \ldots, y_{n+s}$ where s is an integer, $1 \leqq s \leqq k$. Hence, our method is characterized not only by the matrices $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$ but also by the parameter s. Let us note that if $s < k$ it is necessary to forget the values $y_{n+s+1}, \ldots, y_{n+k}$ computed in one step of the method and to recompute them in the following step. For the sake of simplicity of the notation, we will always denote the approximate solution in the point x_j by only one symbol y_j even though this value need not be the same in different phases of the computation. This licence cannot cause any misunderstanding.

§ 3. CONVERGENCE OF OVERIMPLICIT METHODS

Before formulating the main result of this section it is necessary to introduce some concepts and notations.

Definition 3.1. *The method* (2.3) *given by matrices* $\mathbf{B} = \{b_{ij}\}$, $\mathbf{C} = \{c_{ij}\}$, $\mathbf{D} =$

$= \{d_{ij}\}$ *will be said to be of order* p (p *positive integer*) *if the following* $k(p+1)$ *conditions are satisfied*:

$$1 + \sum_{j=1}^{l} b_{ij} = 0, \qquad 1 - \sum_{j=1}^{l} b_{ij}(l-j) = \sum_{j=1}^{k} c_{ij} + \sum_{j=1}^{l} d_{ij}, \tag{3.1}$$

$$i^{\nu} + (-1)^{\nu} \sum_{j=1}^{l} b_{ij}(l-j)^{\nu} = \nu\Big[\sum_{j=1}^{k} c_{ij} j^{\nu-1} + (-1)^{\nu-1} \sum_{j=1}^{l} d_{ij}(l-j)^{\nu-1}\Big],$$

$$\nu = 2, \ldots, p; \; i = 1, \ldots, k.$$

Definition 3.2. *The method* (2.3) *will be said consistent if it is of order at least one.*

Remark 3.1. Let us draw the reader's attention to the fact that both the consistence and the order of the method depend only on the matrices $\boldsymbol{B}$, $\boldsymbol{C}$, $\boldsymbol{D}$ and do not depend on the parameter s.

Definition 3.3. *Let* $y \in C^1$ *and let*

$$\begin{bmatrix} y(x+h) \\ \vdots \\ y(x+kh) \end{bmatrix} + \boldsymbol{B} \begin{bmatrix} y(x-(l-1)h) \\ \vdots \\ y(x) \end{bmatrix} - h\boldsymbol{C} \begin{bmatrix} y'(x+h) \\ \vdots \\ y'(x+kh) \end{bmatrix} - h\boldsymbol{D} \begin{bmatrix} y'(x-(l-1)h) \\ \vdots \\ y'(x) \end{bmatrix} = \boldsymbol{L}(y(x); h). \tag{3.2}$$

The vector $\boldsymbol{L}(y(x); h)$ *with components* $L_i(y(x); h)$ *will be called the local error of the method.*

The conditions (3.1) express that the local error of the method (2.3) is of the order h^{p+1}. More precisely, it holds

Lemma 3.1. *Let there be given the method* (2.3) *of order* p; *let* $y(x) \in C^{p+1}(\langle a, b\rangle)$ *and let* $Y = \max |y^{(p+1)}(x)|$. *Then there exists a constant* K *such that*

$$|L_i(y(x); h)| \leqq KYh^{p+1} \tag{3.3}$$

for $i = 1, \ldots, k$ *and for any* $x \in (a, b)$ *for which the expression* $\boldsymbol{L}(y(x); h)$ *has sense.*

Because we are dealing with the multistep method it can be expected that the convergence will be guaranteed not only by the assumption that the local error is small but that some other conditions similar to Dahlquist's stability conditions will have to be fulfilled (cf., for example, HENRICI [1962]). In order to be able to formulate them, let us introduce some further notation.

Thus, let the method (2.3) be given and let firstly $l \leqq s$. Let us define in this case the matrix $\boldsymbol{R}$ by the equation

$$\boldsymbol{R} = [\boldsymbol{O}_{l,s-l}, \boldsymbol{I}_l, \boldsymbol{O}_{l,k-s}] \tag{3.4}$$

where $\mathbf{O}_{m,n}$ is $m \times n$ null matrix[1]) and $\mathbf{I}_l$ is the unit matrix of order l. Further, define the matrix $\mathbf{E}$ by the equation

$$\mathbf{E} = -\mathbf{RB}. \tag{3.5}$$

Secondly, let $l > s$ and define the matrix $\mathbf{S}$ by the equation

$$\mathbf{S} = [\mathbf{I}_s, \mathbf{O}_{s,k-s}]. \tag{3.6}$$

Further, let

$$i = \left[\frac{l-1}{s}\right].^{2}) \tag{3.7}$$

Construct the matrix

$$\mathbf{B}^{(1)} = [\mathbf{O}_{k,(i+1)s-l}, \mathbf{B}] \tag{3.8}$$

and divide the matrix $\mathbf{SB}^{(1)}$ into $i + 1$ square blocks $\mathbf{B}_j$ in such a way that

$$\mathbf{SB}^{(1)} = [\mathbf{B}_0, \ldots, \mathbf{B}_i]. \tag{3.9}$$

Finaly, construct the matrix

$$\mathbf{E} = \begin{bmatrix} \mathbf{O}_{s,s} & \mathbf{I}_s & \mathbf{O}_{s,s} & \cdots & \mathbf{O}_{s,s} \\ \vdots & & & & \vdots \\ & & & & \mathbf{O}_{s,s} \\ \mathbf{O}_{s,s} & \cdots & \mathbf{O}_{s,s} & & \mathbf{I}_s \\ -\mathbf{B}_0 & \cdots & & & -\mathbf{B}_i \end{bmatrix} \tag{3.10}$$

After introd ucing these matrices we are able to define the stability of the overimplicit method (2.3).

Definition 3.4. *The overimplicit method* (2.3) *will be said to be stable if it exists a constant* Γ *su ch that for any* n

$$\| \mathbf{E}^n \| \leqq \Gamma^{3}) \tag{3.11}$$

where $\mathbf{E}$ *is defined by* (3.5) *or* (3.10).

Remark 3.2. The condition (3.11) can be alternatively expressed in such a way that the matrix $\mathbf{E}$ has eigenvalues smaller or equal to 1 in magnitude and that only linear elementary divisors correspond to eigenvalues of magnitude equal to 1.

Remark 3.3. Let us draw the reader's attention to the fact that only the matrix $\mathbf{B}$ and the parameter s are concerned in Definition 3.4.

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[1]) If some index of the matrix $\mathbf{O}_{m,n}$ is zero then this matrix does not occur in (3.4) at all.

[2]) The symbol $[a]$ denotes the integral part of the number a.

[3]) Here one can take an arbitrary norm of a matrix as a linear mapping; let us consider for the definiteness the spectral norm.

Now we can formulate the basic theorems concerning the convergence of the overimplicit method.

Theorem 3.1. *A stable and consistent overimplicit method is convergent.*

Remark 3.4. Using the standard procedure consisting in the investigation of special differential equations, it could be proved that the conditions of Theorem 3.1 are also necessary.

Theorem 3.2. *Let there be given a stable overimplicit method of order* $p \geqq 1$. *Let the solution of the given differential equation* (2.1) *have continuous derivatives up to order* $p+1$. *Finally, let the initial conditions by which the approximate solution is determined be given with the accuracy of order* $O(h^p)$. *Then the discretization error is also of order* $O(h^p)$.

§ 4. A-STABILITY OF OVERIMPLICIT METHODS

In order to be able to speak precisely, let us remind the definition of Dahlquist's A-stability.

Definition 4.1. *A numerical method for solving initial-value problems for ordinary differential equations is said to be A-stable if any solution of the difference equation which arises by application of the given method on the differential equation* $y' = Ay$ *where* A *is a complex constant with negative real part converges to zero for* $n \to \infty$.

Now it can be proved

Theorem 4.1. *In the class of overimplicit methods there exist A-stable methods of arbitrarily high order.*

This theorem can be simplest proved in such a way that one shows that the class of overimplicit methods is large enough to contain methods which, having been applied on a linear differential equation with constant coefficients, lead to arbitrary rational approximation of the corresponding exponential function. Then one uses the well-known fact that for the Padé approximation $P(z)$ of e^z where z is an arbitrary complex number with negative real part it holds $|P(z)| < 1$. The proof of Theorem 4.1 is, however, not constructive and from that reason we turn now our attention to construction of concrete methods which are in some sense natural and we will study their A-stability. If we recall the basic idea of the multistep methods of Adams type we are led naturally to the subset of the class of overimplicit methods of the form:

$$y_{n+i} - y_n = \int_{x_n}^{x_{n+i}} P(x)\,\mathrm{d}x, \quad i = 1, \ldots, k \tag{4.1}$$

where $P(x)$ is the interpolation polynomial of degree k which has the values f_{n+i} in the points x_{n+i}, $i = 0, \ldots, k$.

In these methods $l = 1$ and, consequently, these methods do not need any starting procedures. We will call them *overimplicit methods of Adams type.* The formula (4.1) can be rewritten in the form

$$y_{n+i} - y_n = h \sum_{j=0}^{k} \gamma_{ij} f(x_{n+j}, y_{n+j}), \qquad i = 1, \ldots, k, \tag{4.2}$$

where

$$\gamma_{ij} = \int_0^i l_j(t)\, \mathrm{d}t \tag{4.3}$$

and $l_j(t)$ is the elementary Lagrange interpolation polynomial for the points $t = 0, \ldots, k$ i.e. the polynomial of degree k which has in the points $t = 0, \ldots, k$, $t \neq j$ the values 0 and in the point $t = j$ the value 1. It is seen immediately that an overimplicit method of Adams type is of order $k + 1$ and that it is stable for any s. As far as the convergence is concerned, Theorems 3.1 and 3.2 can be applied.

In what follows we shall study the A-stability of the method (4.2) in the case $s = k$. In this case, the course of computation will be such that from given y_0 one computes $y_1, \ldots, y_k$, in the further step from y_k it will be computed $y_{k+1}, \ldots, y_{2k}$ etc. Thus, only $y_{rk}, r = 1, 2, \ldots$, will play the essential role and the other values of the approximate solution will be only auxiliary. It can be expected that when applying this method on a linear differential equation (so that the system (4.2) will be also linear) it will be possible to eliminate these auxiliary values and to derive some one-step method in which $y_{(r+1)k}$ will be computed from y_{rk}.

Thus, let the linear differential equation

$$y' = Ay \tag{4.4}$$

where A is a (complex) constant be given. After elementary using of Cramer rule the above mentioned method for solving the equation (4.4) can be written in the form

$$y_{(r+1)k} = \frac{Q(-z)}{Q(z)}\, y_{rk}, \qquad r = 0, 1, \ldots, \tag{4.5}$$

where $z = Ah$ and

$$Q(z) = \det (\boldsymbol{I} - z\boldsymbol{C}) \tag{4.6}$$

with

$$\boldsymbol{C} = \begin{bmatrix} \gamma_{11} & \cdots & \gamma_{1k} \\ \vdots & & \vdots \\ \gamma_{k1} & \cdots & \gamma_{kk} \end{bmatrix}.$$

From the formula (4.5) it follows immediately

Theorem 4.2. *An overimplicit method of Adams type with $s = k$ is A-stable if and only if all roots of the polynomial $Q(z)$ given by (4.6) lie in the right-hand halfplane.*

Further, it can be easily shown that the coefficients of the polynomial $Q(z)$ can be computed explicitely. Namely, if we denote the coefficients of $Q(z)$ by q_j,

$$q_j = K(k - j + 1)\,!\,p_{k-j+1} \tag{4.8}$$

where K is a constant depending only on k and p_j are the coefficients of the polynomial which has the roots in the points $1, \ldots, k$. Consequently, Theorem 4.2 and the formula (4.8) enable us to determine if the method under consideration is A-stable or not. It has been shown in such a way that the above methods up to $k = 8$ are A-stable, for $k = 9, 10$, they are not A-stable, but we have no definite results for general k yet.

Finally, we would like to mention that the problems presented above do not exhaust by far all aspects of the overimplicit methods. Many problems continue to be open, for example, the properties of the overimplicit methods the local errors of which are in different lines different, the exact description of the connection of overimplicit methods with Padé approximations etc.

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Authors' address:

Milan Práger, Jiří Taufer, Emil Vitásek
Mathematical Institute, Czechoslovak Academy of Sciences
Opletalova 45, 110 00 Praha 1
Czechoslovakia