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Convergence of one-leg multistep methods for stiff nonlinear initial value problems

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For proving convergence of numerical methods for stiff initial value problems, not only stability is needed, but also bounds for the local errors which are not affected by stiffness. In this paper global error bounds are derived for multistep schemes applied to classes of arbitrarily stiff, nonlinear initial value problems. It will be shown that stable one-leg methods are convergent for stiff problems with the same order as for nonstiff problems, provided that the stepsize variation is sufficiently regular. Using a well known equivalence relation between one-leg and linear multistep methods, convergence results for linear multistep methods on uniform grids will also be obtained.

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1. Introduction

In this paper we shall discuss convergence of multistep methods applied to stiff nonlinear initial value problems

$$u'(t) = f(t,u(t)) \ (0<t\leqslant T), \ u(0) \text{ given}, \tag{1.1}$$

with $u(0)\in\mathbb{R}^m$ and $f:[0,T]\times\mathbb{R}^m\rightarrow\mathbb{R}^m$. Most attention will be given to k-step *one-leg methods,* where successive approximations u_{n+k} to the exact solution $u(t)$ at gridpoints $t_{n+k}=t_{n+k-1}+h$ are computed from

$$\sum_{j=0}^{k}\alpha_j u_{n+j} = hf\Big(\sum_{j=0}^{k}\beta_j t_{n+j}, \sum_{j=0}^{k}\beta_j u_{n+j}\Big) \ \ (n=0,1,2,...). \tag{1.2}$$

Compared with the corresponding *linear multistep method*

$$\sum_{j=0}^{k}\alpha_j u_{n+j} = h\sum_{j=0}^{k}\beta_j f(t_{n+j},u_{n+j}) \quad (n=0,1,2,...), \tag{1.3}$$

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the one-leg method (1.2) may have stronger nonlinear stability properties, such as G-stability, and a more robust behaviour on nonuniform grids, see [4], [13]. On the other hand, it is known [5] that to obtain a one-leg method of high *order* (i.e. order of consistency for nonstiff problems) the parameters α_j, β_j have to satisfy more constraints than for linear multistep methods (see also Section 3).

We shall be concerned with bounds for the global errors $u(t_n) - u_n$ that are not affected by stiffness. Such bounds have been studied quite extensively for Runge-Kutta methods, see for example [8], [9] and [10]. Most Runge-Kutta methods suffer from an *order reduction* in the presence of stiffness, i.e., the order of convergence for stiff problems may be considerably lower than for nonstiff problems, even if the solution $u(t)$ is very smooth. As we shall see, such order reduction will not occur with one-leg methods, provided that the grid is sufficiently regular.

Stiffness independent error bounds can be obtained for various classes of initial value problems. The most general class that will be considered in this paper consists of the problems (1.1) where the function f satisfies the monotonicity condition

$$(f(t,v) - f(t,\tilde{v}),\ v - \tilde{v}) \leq 0 \quad (\text{for all } t \in [0,T] \text{ and } v, \tilde{v} \in \mathbb{R}^m) \tag{1.4}$$

with respect to some inner product $(\cdot,\cdot)$ on $\mathbb{R}^m$. Although sufficient stability conditions for one-leg methods are known, this does not lead to convergence results in a straightforward way, since the local errors will depend on the stiffness (except for methods like BDF, which are at the same time one-leg and linear multistep methods). A complete convergence analysis for the implicit midpoint rule and the trapezoidal rule applied to problems of the above type can be found in [11]. Our approach is closely related to this analysis. One of the main results in this paper is that A-stable multistep methods (1.2) or (1.3) applied with constant stepsizes to a problem satisfying (1.4) will be convergent, independently of the stiffness, with the same order as for nonstiff problems.

For the sake of simplicity we shall confine ourselves until Section 5 to uniform grids $t_n = nh$ $(n = 0, 1, 2, \ldots)$. After some preliminaries in Section 2, convergence of one-leg methods is discussed in Section 3. It will be shown that the local error, defined as the discretization error which is introduced in one single step of the integration process, may slightly suffer from an order reduction: its order will be in general one lower for stiff problems than for nonstiff problems. For stable methods, however, this reduction will not be present in the global discretization errors, due to damping and cancellation effects. In Section 4 convergence results for linear multistep methods are derived, by using the equivalence relation of [3] between the linear multistep method (1.3) and its one-leg twin (1.2). Finally, in Section 5 it is indicated to what extent the results for one-leg methods will carry over to variable stepsizes.

2. Preliminaries

Consider the polynomials ρ and σ containing the coefficients of the method

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j, \quad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j.$$

Let E stand for the forward shift operator and $\bar{t}_n = \sigma(E)t_n$ for $n = 0, 1, ..., N$, with N being the number of steps needed to cover the interval $[0, T]$ at a given stepsize h. It will be assumed that $\alpha_k \neq 0$ and the polynomials ρ, σ have no common zeros (irreducibility), and that $\rho(1) = 0, \sigma(1) = \rho'(1) = 1$ (consistency). Further it will be assumed, for the one-leg methods, that $t_n \leqslant \bar{t}_n \leqslant t_{n+k}$; otherwise some $\bar{t}_n$-values would be outside $[0, T]$ and this would require certain modifications. The initial value problem (1.1) under consideration is assumed to be such that all derivatives $u^{(j)}(t)$ of the exact solution that are needed in the analysis do exist, and $f : [0, T] \times \mathbb{R}^m \to \mathbb{R}^m$ is continuously differentiable. On the space $\mathbb{R}^m$ we shall deal with a norm $|v| = (v, v)^{1/2}$ generated by some inner product (v, w).

The one-leg scheme (1.2) can be written as

$$\rho(E)u_n = hf(\bar{t}_n, \bar{u}_n), \quad \bar{u}_n = \sigma(E)u_n. \tag{2.1}$$

For the exact solution u of (1.1) we have

$$\rho(E)u(t_n) = hf(\bar{t}_n, u(\bar{t}_n)) + r_n, \quad u(\bar{t}_n) = \sigma(E)u(t_n) + q_n \tag{2.2}$$

where r_n, q_n are discretization errors due to differentiation and interpolation, respectively. These errors, which only depend on the smoothness of u, will be considered more closely in Section 3 (cf. also [5], [6]).

Let $\epsilon_n = u(t_n) - u_n$ denote the global discretization errors of the one-leg scheme, and put $\bar{\epsilon}_n = u(\bar{t}_n) - \bar{u}_n$. By subtraction of (2.1) from (2.2) it follows that

$$\rho(E)\epsilon_n = Z_n \bar{\epsilon}_n + r_n, \quad \bar{\epsilon}_n = \sigma(E)\epsilon_n + q_n \tag{2.3}$$

where the $m \times m$ matrix Z_n is given by

$$Z_n = h\int_0^1 J(\bar{t}_n, \theta u(\bar{t}_n) + (1-\theta)\bar{u}_n) d\theta \tag{2.4}$$

with $J(t, v)$ standing for the Jacobian $[\partial f(t, v)/\partial v]$. Elimination of $\bar{\epsilon}_n$ in (2.3) leads to

$$\rho(E)\epsilon_n = Z_n \sigma(E)\epsilon_n + r_n + Z_n q_n. \tag{2.5}$$

This recursion for the global errors can be written in the somewhat more transparant form

$$\epsilon_{n+k} = \sum_{j=1}^{k} \psi_j(Z_n)\epsilon_{n+k-j} + \delta_n \tag{2.6}$$

where $\delta_n = (\alpha_k I - \beta_k Z_n)^{-1}(r_n + Z_n q_n)$ and $\psi_j(Z_n) = -(\alpha_k I - \beta_k Z_n)^{-1}(\alpha_{k-j} I - \beta_{k-j} Z_n)$ with I the $m \times m$ identity matrix. Note that, due to $\rho(1)=0, \sigma(1)=1$, we have

$$\sum_{j=1}^{k} \psi_j(Z_n) - I = (\alpha_k I - \beta_k Z_n)^{-1} Z_n, \tag{2.7}$$

a relation which will be useful in the next section.

In order to facilitate the analysis, (2.6) will be formulated as a one-step recursion in $e_n = (\epsilon_{n+k-1}^T, \epsilon_{n+k-2}^T, \ldots, \epsilon_n^T)^T \in \mathbb{R}^{km}$,

$$e_{n+1} = R(Z_n)e_n + d_n \quad (n=0,1,\ldots,N) \tag{2.8}$$

where

$$R(Z_n) = \begin{bmatrix} \psi_1(Z_n) & \cdots & & \psi_k(Z_n) \\ I & 0 & & \\ & \ddots & \ddots & \\ & & I & 0 \end{bmatrix}, \quad d_n = \begin{bmatrix} \delta_n \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

To ensure stability of the one-leg scheme - which is, as we see from the above, governed by the matrices $R(Z_n)$ - appropriate assumptions on the method and the class of stiff initial value problems are needed. Using the given norm $|\cdot|$ on $\mathbb{R}^m$ we can define the norm $\|\cdot\|$ on $\mathbb{R}^{km}$ as

$$\|w\| = \max_{1 \leq j \leq k} |w_j| \quad \text{for } w = (w_1^T, w_2^T, \ldots, w_k^T)^T \in \mathbb{R}^{km}.$$

We shall use $|\cdot|$ and $\|\cdot\|$ also to denote the induced matrix norms for $m \times m$ and $km \times km$ matrices, respectively. It will be assumed in the following sections that there exists a constant $S > 0$ such that

$$\|R(Z_n)R(Z_{n-1})\ldots R(Z_l)\| \leq S \tag{2.9}$$

for all possible $Z_n, \ldots, Z_l$ given by (2.4) and $0 \leq l \leq n \leq N$. This stability assumption does not depend on our special choice of norm $\|\cdot\|$ which is merely taken for convenience; since k is fixed, all norms on $\mathbb{R}^{km}$ of the form

$$\|w\|' = |(|w_1|, |w_2|, \ldots, |w_k|)^T|', \quad |\cdot|' \text{ an absolute norm on } \mathbb{R}^k,$$

are equivalent, so that using $\|\cdot\|'$ in (2.9) would only alter the constant S. Sufficient conditions for (2.9) have been extensively studied, see [5], [13] and [15] (cf. also [12] for results with norms $|\cdot|$ on $\mathbb{R}^m$

not generated by an inner product). Here we shall give two examples for implicit methods where $h>0$ is allowed to be arbitrary.

First, assume f satisfies the monotonicity condition (1.4). As this condition implies that the difference $|\tilde{u}(t)-u(t)|$ between any two solutions $\tilde{u}, u$ of the differential equation in (1.1) is nonincreasing with t, the initial value problem (1.1) itself is stable. In [5] it was shown that for any A-stable one-leg method (1.2) a norm $|\cdot|'$ on $\mathbb{R}^k$ can be found such that $\|R(Z_n)\|'\leq 1$ whenever Z_n is given by (2.4) with $h>0$. This norm $|\cdot|'$ (the G-norm [5]) is determined by the coefficients α_j, β_j. So, A-stability and (1.4) are sufficient for (2.9) with a stability constant S determined by the method (and thus independent of the specific problem and its dimension).

Under more restrictive assumptions on f stability can also be guaranteed for methods which are not necessarily A-stable. We consider, as an example, one-leg methods which are A_0-contractive (in the maximum norm). This concept was introduced in [13]. For such methods we have, by definition, $\|R(z)\|\leq 1$ if $z\in\mathbb{R}(m=1), z\leq 0$. By a spectral decomposition of Z_n it is then easy to show that $\|R(Z_n)\|\leq 1$ whenever Z_n is given by (2.4) with $h>0$ and the Jacobian J of f is such that

$$J(t,v) \text{ is self-adjoint (w.r.t.}(\cdot,\cdot)) \text{ and all eigenvalues are nonpositive,} \tag{2.10}$$

for any $t\in[0,T]$, $v\in\mathbb{R}^m$. In case we are dealing with the Euclidian inner product v^Tw on $\mathbb{R}^m$, condition (2.10) means that f is a gradient mapping, $f(t,v)=-[\partial g(t,v)/\partial v]^T$, for some convex functional $g:\mathbb{R}\times\mathbb{R}^m\rightarrow\mathbb{R}^m$, see [14].

3. Convergence of one-leg methods

3.1. *Local error bounds*

Considering (2.6) we see that $\delta_n=(\alpha_k I-\beta_k Z_n)^{-1}\,(r_n+Z_n q_n)$ is a local discretization error, in the sense that if $\epsilon_n=\epsilon_{n+1}=\cdots=\epsilon_{n+k-1}=0$ then $\epsilon_{n+k}=\delta_n$. (In other words, δ_n is the error, due to discretization, which is introduced in one single step of the integration process.) For a p-th order method we expect that $|\delta_n|=O(h^{p+1})$.

Note that δ_n is different from the usual discretization error that is obtained by substituting the exact solution directly into (1.2). This error, which is approximately given by $r_n+Z_n q_n$, is not bounded uniformly in the stiffness and therefore inappropriate for stiff systems. This was observed already in [6], where also an alternative error was proposed for stepsize control (for our purpose, proving convergence for stiff problems, the δ_n seem more suitable).

Let γ_j be such that $t_{n+j}=\bar{t}_n+\gamma_j h$ $(j=0,1,...,k)$. By a Taylor series expansion of u, and the consistency conditions $\rho(1)=0$, $\sigma(1)=\rho'(1)=1$, it follows that

$$r_n = a_2 h^2 u''(\bar{t}_n) + a_3 h^3 u'''(\bar{t}_n) + \cdots \quad , a_i = \frac{1}{i!} \sum_{j=0}^{k} \alpha_j \gamma_j^i, \tag{3.1a}$$

$$q_n = b_2 h^2 u''(\bar{t}_n) + b_3 h^3 u'''(\bar{t}_n) + \cdots \quad , b_i = -\frac{1}{i!} \sum_{j=0}^{k} \beta_j \gamma_j^i. \tag{3.1b}$$

Now, for *nonstiff problems*, where f satisfies a Lipschitz condition with a moderate constant, we have $|Z_n| = O(h)$, and consequently

$$\delta_n = (\alpha_k^{-1} + O(h))(r_n + O(h) q_n).$$

In order to have $|\delta_n| = O(h^{p+1})$ it is then necessary and sufficient that

$$a_i = 0 \ (2 \leqslant i \leqslant p) \text{ and } b_i = 0 \ (2 \leqslant i \leqslant p-1), \tag{3.2}$$

which are the usual order conditions for one-leg methods (cf. [5], [6]). The order conditions for the linear multistep method (1.3), which read $a_i + b_{i-1} = 0 \, (2 \leqslant i \leqslant p)$, are the same if $p = 2$, but for $p \geqslant 3$ the one-leg method has to satisfy more constraints.

For *stiff problems* the order conditions (3.2) are not sufficient to have $|\delta_n| \leqslant C h^{p+1}$ for some moderately seized $C > 0$. From (2.7), (2.9) it can be concluded that there are constants $S_1, S_2 > 0$, only depending on S and the coefficients α_k, β_k, such that

$$|(\alpha_k I - \beta_k Z_n)^{-1} Z_n| \leqslant S_1 \ , \ \ |(\alpha_k I - \beta_k Z_n)^{-1}| \leqslant S_2,$$

but $S_1 \neq O(h)$ (for example if $Z_n = h\lambda, \lambda \to -\infty$). Consequently, (3.2) implies for stiff problems only $|\delta_n| = O(h^p)$. This local order reduction occurs with the implicit midpoint rule [11] and most other one-leg methods.

EXAMPLE 3.1. Consider the second order method CA2, introduced in [13],

$$u_{n+2} - u_{n+1} = hf(t_n + \tfrac{3}{2}h, \ \tfrac{3}{4}u_{n+2} + \tfrac{1}{4}u_n).$$

This method is A-stable and A_0-contractive (in the maximum norm). Consider further the model problem

$$u'(t) = \lambda[u(t) - g(t)] + g'(t), \ \ u(0) = g(0), \tag{3.3}$$

with solution $u(t) = g(t)$ for any $\lambda \leqslant 0$. Take $g(t) = \frac{1}{2}t^2$. Application of the above method with exact starting values $u_0 = u(0)$, $u_1 = u(t_1)$, gives

$$u(t_2) - u_2 = -\tfrac{3}{8}h^2(1 - \tfrac{3}{4}z)^{-1} z \ , \ \ z = h\lambda.$$

If the problem is nonstiff, $|\lambda| \leq 1$ say, then $|u(t_2)-u_2| \leq \frac{3}{8}h^3 + O(h^4)$, as we would expect after one step with a second order method. For $\lambda \to -\infty$, however, we only have $|u(t_2)-u_2| = \frac{1}{2}h^2$. Thus, due to stiffness one order of h is lost. □

The local order reduction is absent with methods that satisfy, in addition to (3.2), the extra order condition

$$b_p = 0. \tag{3.4}$$

This is satisfied, for instance, by the BDF methods (where all b_j are zero). It can also be shown that the local order reduction will not occur in case the initial value problem (1.1) is such that all partial derivatives $[\partial^{i+j} f(t,v)/\partial t^i \partial v^j]$ with $i, j \geq 0$, $(i,j) \neq (0,1)$ are bounded by a moderate constant (cf. [9] for a related result with Runge-Kutta methods). Note that the partial derivative with $(i,j)=(0,1)$, the Jacobian, is always large for stiff systems since its norm is proportional to the Lipschitz constant. For general stiff systems where other partial derivatives may also be large there will be a local order reduction if (3.4) is not satisfied, as can be seen by considering problems of the type (3.3) with $\lambda << 0$ and g a smooth function.

3.2. *Global error bounds*

For nonstiff problems the local condition $|\delta_n| = O(h^{p+1})$ is necessary to have $|\epsilon_n| = 0(h^p)$, global convergence of order p. For stiff problems there may be damping or cancellation of local errors, as a result of which there can be convergence of order p while $|\delta_n| = O(h^p)$ only. This was shown in [11] to be the case for the implicit midpoint rule. Related results for Runge-Kutta methods can be found in [1] and [2].

LEMMA 3.2. *Consider recursion (2.8). Assume the stability condition (2.9) holds with a constant $S>0$. Assume further that there exists a constant $D>0$ and vectors $x_n, y_n \in \mathbb{R}^{km}$ such that*

$$d_n = (I-R(Z_n))x_n + y_n, \tag{3.5a}$$

$$\|x_n\| \leq Dh^p, \quad \sum_{j=0}^{n-1} \|x_{j+1}-x_j\| \leq Dh^p, \quad \sum_{j=0}^{n-1} \|y_j\| \leq Dh^p \tag{3.5b}$$

for all $n=0,1,...,N$. Then, for all n,

$$\|e_n\| \leq S\,\|e_0\| + (3S+1)Dh^p.$$

Proof. Let $\hat{e}_n = e_n - x_n$. These perturbed errors satisfy

$$\hat{e}_n = R(Z_{n-1})\hat{e}_{n-1} + \hat{d}_{n-1}, \quad \hat{d}_{n-1} = y_{n-1} + x_{n-1} - x_n \quad (n=1,2,...,N).$$

By writing out $\hat{e}_n$ fully in terms of $R(Z_j)$, $\hat{d}_j$ $(0 \leqslant j \leqslant n-1)$ and $\hat{e}_0$, it easily follows from (2.9) that

$$\|\hat{e}_n\| \leqslant S\ \|\hat{e}_0\| + S \sum_{j=0}^{n-1} \|\hat{d}_j\|.$$

Hence

$$\|e_n\| \leqslant S\ \|e_0\| + S \sum_{j=0}^{n-1} \|y_j\| + S \sum_{j=0}^{n-1} \|x_j - x_{j+1}\| + S\ \|x_0\| + \|x_n\|,$$

which yields the proof of the lemma. □

Theorem 3.3. *Consider a one-leg method (1.2) satisfying the order conditions (3.2) with $p \geqslant 1$. Assume (2.9) holds with stability constant $S>0$. Then there is a constant $C>0$, only depending on S,T and bounds for derivatives of $u(t)$, such that*

$$|u(t_n) - u_n| \leqslant S \max_{0 \leqslant j \leqslant k-1} |u(t_j) - u_j| + Ch^p \qquad \textit{for all } n \geqslant k,\ nh \leqslant T.$$

Proof. In order to apply Lemma 3.2 it has to be determined whether the vector d_n in (2.8) can be decomposed as indicated. Let $x_n = (x_{1n}^T, \ldots, x_{kn}^T)^T$ and $y_n = (y_{1n}^T, \ldots, y_{kn}^T)^T$ with $x_{jn}, y_{jn} \in \mathbb{R}^m$. These vectors should satisfy

$$\delta_n = (I - \psi_1(Z_n))x_{1n} - \psi_2(Z_n)x_{2n} - \cdots - \psi_k(Z_n)x_{kn} + y_{1n},$$

$$0 = -x_{j-1,n} + x_{jn} + y_{jn} \quad (j=2,3,...,k).$$

Taking $x_{1n} = x_{2n} = \cdots = x_{kn} = q_n$, $y_{1n} = (\alpha_k I - \beta_k Z_n)^{-1} r_n$ and $y_{2n} = \cdots = y_{kn} = 0$, it is easily seen from (2.7) that (3.5a) is fulfilled and

$$\|x_n\| \leqslant D_1 h^p,\ \|x_{n+1} - x_n\| \leqslant D_2 h^{p+1},\ \|y_n\| \leqslant D_3 h^{p+1}$$

for all n, with D_1, D_2, D_3 determined by S and the solution u (see Section 3.1). Hence, Lemma 3.2 can be applied with $D = max\{D_1, D_2 T, D_3 T\}$ which leads to the error bound of the theorem. □

This convergence result shows that the order reduction is annihilated in the transition from local to global error. For stable one-leg schemes the order of convergence for stiff problems will be the same as in the nonstiff case.

4. Convergence of linear multistep methods

By using the equivalence relation, given in [3], between one-leg and linear multistep methods on uniform grids, the convergence result for one-leg methods can be used to prove convergence of linear multistep methods applied to stiff nonlinear initial value problems.

Consider the linear multistep method (1.3), which can be written with the generating polynomials ρ and σ as

$$\rho(E)u_n = h\sigma(E)f(t_n,u_n) \quad (n=0,1,...). \tag{4.1}$$

Let s_n be shifted gridpoints such that $\sigma(E)s_n = t_n$. Usually, some of the first shifted gridpoints $s_0, s_1,..,s_{n_0-1}$, say, will be negative. Assume for the moment that the solution $u(t)$ of (1.1) can be continued in a smooth way for $t<0$. On the shifted grid we then consider one-leg approximations $v_n \approx u(s_n)$,

$$\rho(E)v_n = hf(t_n,\sigma(E)v_n) \quad (n=0,1,...). \tag{4.2}$$

Since $\rho(E)$ and $\sigma(E)$ commute, premultiplication of (4.2) with $\sigma(E)$ shows that the interpolated values $\overline{v}_n = \sigma(E)v_n$ satisfy the same recursion as the u_n. Therefore, if $\overline{v}_j = u_j$ $(0 \leqslant j \leqslant k-1)$ then $\overline{v}_n = u_n$ for all n.

The condition $\overline{v}_j = u_j$ $(0 \leqslant j \leqslant k-1)$ will hold iff $v_0, v_1, \ldots, v_{2k-1}$ satisfy

$$\sigma(E)v_j = u_j\,, \quad \rho(E)v_j = hf(t_j, u_j) \quad (0 \leqslant j \leqslant k-1). \tag{4.3}$$

Note that the fact that ρ and σ have no common factors implies that this system of linear algebraic equations has a unique solution (as can be seen from relation (1.11) in [3]). Now, let p be the order of the one-leg scheme, and assume that the starting values for the linear multistep method are such that

$$|u(t_j)-u_j| \leqslant C_0h^p\,, \quad |u'(t_j)-f(t_j, u_j)| \leqslant C_0h^{p-1} \quad (0 \leqslant j \leqslant k-1) \tag{4.4}$$

for some $C_0>0$. The order conditions (3.2) imply that

$$|u(t_n)-\sigma(E)u(s_n)| \leqslant C_1h^p\,, \quad |u'(t_n)-h^{-1}\rho(E)u(s_n)| \leqslant C_1h^p$$

for all n, with $C_1>0$ only depending on derivatives of u. Hence,

$$|\rho(E)[v_j-u(s_j)]| \leqslant (C_0+C_1h)h^p, \quad |\sigma(E)[v_j-u(s_j)]| \leqslant (C_0+C_1)h^p \quad (0 \leqslant j \leqslant k-1).$$

It follows that there is a $C_0'>0$, determined by C_0 and the smoothness of u, such that the starting values for the one-leg scheme (4.2) satisfy

$$|v_j - u(s_j)| \leq C_0' h^p \quad (0 \leq j \leq k-1). \tag{4.5}$$

Assuming the one-leg method to be stable, in the sense of (2.9), Theorem 3.3 shows that $|v_n - u(s_n)|$ can be bounded by $(SC_0' + C)h^p$ for all n. Since

$$u(t_n) - u_n \;=\; u(t_n) - \bar{v}_n \;=\; [u(t_n) - \sigma(E)u(s_n)] \;+\; \sigma(E)[u(s_n) - v_n]$$

we see that there is a $C'>0$, only depending on S, C_0, T and smoothness of u, such that

$$|u(t_n) - u_n| \leq C' h^p \qquad \text{for all } n \geq 0,\ nh \leq T. \tag{4.6}$$

There are situations where the assumption that u can be continued in a smooth way on a small interval to the left of the origin is not realistic, for instance if (1.1) originates from discretization in space of a parabolic partial differential equation with nonsmooth initial data. In such a situation the above convergence proof can be modified. If $\epsilon_n = u(t_n) - u_n$ are global errors of the linear multistep scheme and Z_n is defined, similarly as (2.4), such that $Z_n \epsilon_n = hf(t_n,\ u(t_n)) - hf(t_n, u_n)$, then it follows that

$$\rho(E)\epsilon_n \;=\; \sigma(E) Z_n \epsilon_n \;+\; p_n\,, \quad p_n \;=\; \rho(E)u(t_n) - h\sigma(E)u'(t_n). \tag{4.7}$$

This local error p_n is bounded in norm by $C_2 h^{q+1}$, where $C_2>0$ and q is the order of the linear multistep method (which is at least equal to p). Defining $\hat{\epsilon}_n = (\alpha_k I - \beta_k Z_n)\epsilon_n$, we obtain

$$\hat{\epsilon}_{n+k} \;=\; \sum_{j=1}^{k} \psi_j(Z_{n+k-j})\hat{\epsilon}_{n+k-j} \;+\; p_n. \tag{4.8}$$

In view of (2.9) we have $|\psi_j(Z_{n+k-j})| \leq S$, which shows that

$$|\hat{\epsilon}_{n+k}| \;\leq\; kS \max_{0 \leq j \leq k-1} |\hat{\epsilon}_{n+j}| \;+\; |p_n|. \tag{4.9}$$

The condition (4.4) implies $|\hat{\epsilon}_j| \leq (|\alpha_k| + |\beta_k|)C_0 h^p$ $(0 \leq j \leq k-1)$. Although $kS>1$, in general, it can be shown from (4.9) that after a fixed, finite number of steps, say n_0, we still have

$$|u(t_{n_0+j}) - u_{n_0+j}| \leq C_0'' h^p,\ |u'(t_{n_0+j}) - f(t_{n_0+j},\ u_{n_0+j})| \leq C_0'' h^{p-1} \quad (0 \leq j \leq k-1) \tag{4.10}$$

where $C_0''>0$ depends on n_0, C_0, S and smoothness of u. Taking n_0 such that $s_{n_0} \geq 0$ we can now proceed as before, using the equivalence relation between (4.1) and (4.2) for $n \geq n_0$.

Summarizing, we have obtained the following result.

THEOREM 4.1. *Consider the linear multistep method (1.3) and let p be the order of the corresponding one-leg method (1.2). Assume (2.9) and (4.4) hold. Then there is a constant $C'>0$, only depending on C_0, S, T and bounds for derivatives of u, such that*

$$|u(t_n)-u_n| \leq C'h^p \quad \text{for all } n\geq 0,\ nh\leq T. \quad \square$$

For stiff problems the condition (4.4) is more difficult to fulfil than only $|u(t_j)-u_j| \leq C_0 h^p$ $(0\leq j\leq k-1)$. By considering the model problems

$$u'(t) = \lambda(t)[u(t)-g(t)] + g'(t), \quad u(0) = g(0)$$

with strongly varying $\lambda(t)<0$ and smooth g, it can be seen that (4.4) is necessary for Theorem 4.1.

The convergence result in Theorem 4.1 is completely satisfactory for linear multistep methods whose order q is equal to the order p of their one-leg twin. As noted before, if $q\leq 2$ (A-stable methods, for example) then $q=p$. In general, however, we may have $q>p$. The A_0-contractive Adams type methods CAl of [13] all have $p=2$ while $q=l$. For such methods Theorem 4.1 does not seem to be optimal. In situations where the linear multistep scheme itself is known to be stable (Z_n is constant) the detour along the one-leg methods is unnecessary and convergence with order q follows in a straightforward way. It should be noted that in such a situation the results in Section 3 for the one-leg methods are not optimal either, if we consider instead of $\epsilon_n = u(t_n)-u_n$ the errors $\bar{\epsilon}_n = u(\bar{t}_n) - \sigma(E)u_n$ at the collocation points $\bar{t}_n = \sigma(E)t_n$ (cf. [6]).

5. VARIABLE STEPSIZES

Convergence results for one-leg methods applied to stiff systems on non-uniform grids can be derived in a similar way as in Section 3. We shall indicate here how the convergence will be affected by variable stepsizes. The result for linear multistep methods cannot be easily extended since there is, in general, no equivalence between one-leg and linear multistep methods on non-uniform grids, see [5]. Convergence results for the trapezoidal rule can be found in [11], where it was shown that in order to have convergence, more restrictive assumptions on the stepsize variations are needed than for its one-leg twin the implicit midpoint rule (cf. Example 5.1 below).

In the variable stepsize formulation of the one-leg scheme (1.2), h is replaced by $h_{n+k} = t_{n+k} - t_{n+k-1}$ and the coefficients α_j, β_j are allowed to vary with n,

$$\alpha_{jn} = \alpha_j(\omega_{n+2}, \ldots, \omega_{n+k}), \quad \beta_{jn} = \beta_j(\omega_{n+2}, \ldots, \omega_{n+k}) \tag{5.1}$$

where $\omega_n = h_n/h_{n-1}$. Let h be the maximal stepsize and assume that $|\omega_n| \leq \Omega$, $|\alpha_{jn}|, |\beta_{jn}| \leq \Omega'$ for certain Ω, $\Omega'>0$. Assume further that the scheme is stable in a similar way as in (2.9) (see [7], [13] for some sufficient conditions).

As before, the global errors $\epsilon_n = u(t_n) - u_n$ satisfy a recursion (2.6) with local errors

$$\delta_n = (\alpha_{kn} I - \beta_{kn} Z_n)^{-1} (r_n + Z_n q_n)$$

where r_n, q_n can be written as

$$r_n = \rho_n(E)u(t_n) - h_{n+k}u'(\sigma_n(E)t_n), \quad q_n = u(\sigma_n(E)t_n) - \sigma_n(E)u(t_n)$$

with generating polynomials ρ_n, σ_n containing the coefficients α_{jn} and β_{jn}, respectively. If p is the order of the method for variable stepsizes, we have

$$r_n = O(h_n^{p+1}), \quad q_n = \theta_n u^{(p)}(t_n) + O(h_n^{p+1})$$

with

$$\theta_n = \frac{1}{p!}\{(\sum_{j=0}^{k} \beta_{jn}(t_{n+j} - t_n))^p - \sum_{j=0}^{k} \beta_{jn}(t_{n+j} - t_n)^p\}. \tag{5.2}$$

Note that $t_{n+j} - t_n = h_n(\omega_{n+1} + \omega_{n+1}\omega_{n+2} + ... + [\omega_{n+1}...\omega_{n+j}])$ and $\theta_n = O(h_n^p)$. Stability thus implies $|\epsilon_n| = O(h^{p-1})$ for all n.

If the grid is sufficiently regular, convergence with order p can also be proved. Proceeding as in the proof of Theorem 3.3 we get $|\epsilon_n| = O(h^p)$ (independently of the stiffness) under the assumption that there is a $D>0$ such that

$$\sum_{n=0}^{N-1} |q_{n+1} - q_n| \leqslant Dh^p.$$

This will hold for arbitrary, smooth solutions u iff

$$\sum_{n=0}^{N-1} |\theta_{n+1} - \theta_n| \leqslant D'h^p \tag{5.3}$$

for some $D'>0$. If the functions β_j in (5.1) are Lipschitz continuous in a neighbourhood of $(\omega_{n+2}, \ldots, \omega_{n+k}) = (1,1,...,1)$ and

$$\omega_n = 1 + O(h) \tag{5.4}$$

for all n, it easily follows that $|\theta_{n+1} - \theta_n| = h_n^p O(h)$. Consequently, (5.3) is then satisfied and we have order p convergence. For specific methods this can be proved under assumptions on the stepsizes less restrictive than (5.4).

EXAMPLE 5.1. For the implicit midpoint rule

$$u_{n+1}-u_n = h_{n+1}f(t_n+\frac{1}{2}h_{n+1}, \frac{1}{2}u_{n+1}+\frac{1}{2}u_n),$$

we have $p=2$ and $\theta_n=-\frac{1}{8}h_{n+1}^2$. This method is stable for arbitrary problems (1.1) where f satisfies (1.4). From (5.3) a result of [11] is reobtained: the method is convergent of order 2, independently of the stiffness, provided that

$$\sum_{n=0}^{N-1} |h_{n+1}^2-h_n^2| = O(h^2). \tag{5.5}$$

This condition is satisfied if the number of sign changes in the sequence $\{h_{n+1}-h_n\}$ is bounded by a fixed, finite number. This seems a reasonable assumption for numerical codes, where h_n will be somehow related to the smoothness of solutions near t_n. It was also shown in [11] that (5.5) is necessary to guarantee second order convergence; for stepsize sequences like $h_n=\frac{1}{2}h$ (for n odd), $h_n=h$ (for n even) the order will reduce to 1. □

EXAMPLE 5.2. The variable stepsize formulation of the Adams-type method CA2 of [13] (cf. Example 3.1) reads

$$u_{n+2}-u_{n+1} = h_{n+2}f(t_{n+1}+\frac{1}{2}h_{n+2}, \frac{1}{2}\frac{2+\omega_{n+2}}{1+\omega_{n+2}}u_{n+2}+\frac{1}{2}\frac{\omega_{n+2}}{1+\omega_{n+2}}u_n).$$

This method is A_0-contractive (in the maximum norm) for arbitrary stepsize sequences, and we have order $p=2$ and $\theta_n=-\frac{1}{8}h_{n+2}^2-\frac{1}{4}h_{n+1}h_{n+2}$. Hence

$$|\theta_n-\theta_{n-1}| \leqslant \frac{1}{8}|h_{n+2}^2-h_{n+1}^2| + \frac{1}{4}h_{n+1}|h_{n+2}-h_n| \leqslant$$

$$\leqslant \frac{3}{8}|h_{n+2}^2-h_{n+1}^2| + \frac{1}{4}|h_{n+1}^2-h_n^2|.$$

Thus we see that this method is also convergent of order 2, independently of the stiffness, if the grid refinement is such that (5.5) is satisfied. □

REFERENCES

1. K. BURRAGE and W.H. HUNDSDORFER, *The order of B-convergence of algebraically stable Runge-Kutta methods,* BIT 27 (1987), 62-71.
2. K. BURRAGE, W.H. HUNDSDORFER and J.G. VERWER, *A study of B-convergence of Runge-Kutta methods,* Computing 36 (1986), 17-34.

3. G. Dahlquist, *Error analysis for a class of methods for stiff nonlinear initial value problems,* Proc. Num. Anal. Dundee 1975, G.A. Watson (ed.), Lecture Notes in Mathematics 506, Springer Verlag, Berlin, 1976.
4. G. Dahlquist, *G-stability is equivalent to A-stability,* BIT 18 (1978), 384-401.
5. G. Dahlquist, *Some properties of linear multistep and one-leg methods for ODEs,* Proc. 1979 SIGNUM meeting on numerical ODEs, R.D. Skeel (ed.), Report R79/963, Dept. of Comp. Sc., Univ. of Illinois at Urbana-Champaign (1979).
6. G. Dahlquist, *On one-leg multistep methods,* SIAM J. Numer. Anal. 20 (1983), 1130-1138.
7. G. Dahlquist, W. Lininger and O. Nevanlinna, *Stability of two-step methods for variable integration steps,* SIAM J. Numer. Anal. 20 (1983), 1071-1085.
8. K. Dekker and J.G. Verwer, *Stability of Runge-Kutta methods for stiff nonlinear differential equations,* North-Holland, Amsterdam, 1984.
9. R. Frank, J. Schneid and C.W. Ueberhuber, *Order results for implicit Runge-Kutta methods,* SIAM J. Numer. Anal. 22 (1985), 497-514.
10. E. Hairer, Ch. Lubich and M. Roche, *Error of Runge-Kutta methods for stiff problems studied via differential algebraic equations,* Report, Dept. de Math., Univ. de Genève (1987).
11. J.F.B.M. Kraaijevanger, *B-convergence of the implicit midpoint rule and the trapezoidal rule,* BIT 25 (1985), 652-666.
12. H.W.J. Lenferink, *Contractivity preserving implicit linear multistep methods,* Report TW-88-03, Dept. of Math. and Comp. Sc., Leiden Univ. (1988).
13. O. Nevanlinna and W. Lininger, *Contractive methods for stiff differential equations,* Part I, BIT 18 (1978), 457-474; Part II, BIT 19 (1979), 53-72.
14. J.M. Ortega and W.C. Rheinboldt, *Iterative solution of nonlinear equations in several variables,* Acadamic Press, New York, 1970.
15 J. Sand, *On contractive one-leg methods,* Report TRITA-NA-8218,Dept. of Num. Anal. and Comp. Sc., Royal Inst. of Techn., Stockholm (1982).