Implicit Taylor series methods and stiff semi-linear initial value problems

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Abstract

In this paper we study solvability of the algebraic equations, stability, contractivity and convergence properties of the implicit Taylor series method applied to two classes of stiff semi-linear systems of ordinary differential equations. All results presented are independent of the stiffness of the systems.

Key words. Implicit Taylor series methods, stiff semi-linear initial value problems, solvability of the algebraic equations, C-stability, contractivity, B-convergence, asymptotic error estimates.

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1 Introduction

Let $[x_0, x_e]$ be a compact interval of $\mathbb{R}$. For every $x \in [x_0, x_e]$ let $G_x \subseteq \mathbb{R}^m$ be an open set, $G := \{\bigcup(\{x\} \times G_x) : x \in [x_0, x_e]\}$, and $f : G \to \mathbb{R}^m$.

We shall be concerned with the numerical solution of stiff initial value problems (IVPs) for systems of ordinary differential equations (ODEs)

$$y'(x) = f(x, y(x)), \quad x \in [x_0, x_e], \tag{1.1a}$$

$$y(x_0) = y_0 \,. \tag{1.1b}$$

Let y_n be a known approximation for the solution of (**??**) at the point x_n and we are looking for an approximate y_{n+1} for $y(x_{n+1})$ with $x_{n+1} = x_n + h_n$.

If f is sufficiently often differentiable and is then, as for example in [**?**], for functions $\varphi\colon G \to \mathbb{R}^m$ the differential operator D defined by

$$(D\varphi)(x, y) = \frac{\partial\varphi}{\partial x}(x, y) + \frac{\partial\varphi}{\partial y}(x, y) \cdot f(x, y), \tag{1.2}$$

then for the solution of (**??**) we have

$$y^{(i)}(x) = (D^i y)(x, y(x)), \qquad i = 0, 1, 2, \ldots$$

and the here examined Taylor series method can be written as

$$\sum_{j=0}^{q} (-1)^j \left(D^j y\right)(x_{n+1}, y_{n+1}) \frac{h_n^j}{j!} \frac{\binom{q}{j}}{\binom{p+q}{j}} = \sum_{i=0}^{p} \left(D^i y\right)(x_n, y_n) \frac{h_n^i}{i!} \frac{\binom{p}{i}}{\binom{p+q}{i}} \tag{1.3}$$

(cf., e.g. [**?**], [**?**], [**?**] or [**?**]). Other names of this method are Obreschkoff, Hermite-Obreschkoff, Hermite-Taylor, or HOP method. This formula also is the basis for an interval method for IVPs, cf., e.g. [**?**], [**?**]. In this paper we are concerned only with the "point" method (**??**).

For $q = 0$, (**??**) is the well known (explicit) Taylor series method. For $q > 0$, (**??**) is an implicit equation for y_{n+1}. In [**?**] the solvability of this equation is derived from the implicit function theorem. This theorem guarantees the existence of a unique solution of (**??**) for sufficiently small $|h_n|$. In [**?**] a constructive proof and a bound for the step size is given. In general, the restriction on the step size depends on the Lipschitz constants of the functions $(D^j y)(x, \cdot)$ $(j = 1, \ldots, q)$.

Method (**??**) has the order of consistency $p + q$. In [**?**] a continuous approximation of the solution trajectory, which is uniformly of the same order, is given. The method is A-stable for $q - 2 \leq p \leq q$ and L-stable for $q - 2 \leq p \leq q - 1$.

Special cases of this method are:

$p = 1$,	$q = 0$:	explicit Euler method
$p = 0$,	$q = 1$:	implicit Euler method

$$p = 1, \quad q = 1 \;: \qquad \text{trapezoidal rule}$$

The implicit Euler method is BN-stable and hence also AN-stable. But in [?] it was shown that, except for the implicit Euler method, implicit Taylor series methods are not AN- or B-stable.

If a numerical method has good linear but in general no nonlinear stability properties then it lies at hand that one analyses the properties and the suitability of the method when solving ODEs with only small nonlinear perturbations, so-called semi-linear problems. For linearly implicit Runge-Kutta methods for instance, similar investigations are made in [?], [?], [?] or [?].

The analysis in this paper will be restricted to two classes of semi-linear problems with

$$f(x, y) = A\, y + g(x, y), \quad A \in \mathbb{R}^{m\times m}. \tag{1.4}$$

For differential equations (**??**), (**??**) and integers $i \geq 0$ let the functions $(D_i\, y) : G \to \mathbb{R}^m$ be defined by

$$(D_i\, y)(x, z) := (D^i y)(x, z) - A^i\, z, \qquad i = 0, 1, \ldots \tag{1.5}$$

In particular we have

$$(D_0\, y)(x, z) \equiv 0 \quad \text{and} \quad (D_1\, y)(x, z) = g(x, z) \quad \text{for all} \quad (x, z) \in G. \tag{1.6}$$

The first class of equations consists of ODEs (**??**), (**??**) possessing the following properties:

1. It holds that

$$\langle A\, u, u\rangle \leq \mu\, \|u\|^2, \qquad \mu \leq 0 \qquad \text{for all} \qquad u \in \mathbb{R}^m. \tag{1.7}$$

2. For every $x \in [x_0, x_e]$ there is an open convex set $U_x \subseteq \mathbb{R}^m$, so that for

$$U := \left\{ \bigcup (\{x\} \times U_x) : x \in [x_0, x_e] \right\}$$

the relation

$$\{(x, y(x)) \in \mathbb{R}^{m+1} : x \in [x_0, x_e]\} \subset U \subseteq G$$

is valid, and there are constants $L_i \geq 0$ such that

$$\|(D_i\, y)(x, u) - (D_i\, y)(x, v)\| \leq L_i \|u - v\|$$
$$\text{for} \quad 1 \leq i \leq \max(p, q) \quad \text{and all} \quad (x, u), (x, v) \in U. \tag{1.8}$$

The second class consists of ODEs (**??**), (**??**) with

1.

$$A = \lambda B, \qquad \lambda > 0 \tag{1.9a}$$

and

$$\langle B u, u\rangle \le \mu \|u\|^2, \qquad \mu \le \mu_0 < 0 \qquad \text{for all} \qquad u \in \mathbb{R}^m. \tag{1.9b}$$

2. A set U, as defined above, exists, such that

$$\|(D_i\, y)(x,u) - (D_i\, y)(x,v)\| \le \lambda^{i-1} L_i \|u - v\|$$
$$\text{for} \quad 1 \le i \le \max(p,q) \quad \text{and all} \quad (x,u),\,(x,v) \in U. \tag{1.10}$$

$\langle\cdot,\cdot\rangle$ is an inner product on $\mathbb{R}^m$ and $\|\cdot\|$ stands for the corresponding norm on $\mathbb{R}^m$. The constants L_i should be of moderate size. For the second class of ODEs μ should also be of moderate size.

The class of functions f given by (**??**) and satisfying (**??**), (**??**) will be denoted by $\mathcal{F}_1$. The class of functions satisfying (**??**), (**??**) will be denoted by $\mathcal{F}_2$. Occasionally, the IVPs (**??**) with $f \in \mathcal{F}_i$ $(i = 1,2)$ will also be referred to as the class of problem $\mathcal{F}_i$. The problems in these classes may be of arbitrary stiffness since there is no bound on the Lipschitz constant of $f(x,\cdot)$. On the other hand these problems are properly posed because the $f(x,\cdot)$ do satisfy one-sided Lipschitz conditions with constants $\mu + L_1$ and $\lambda\mu + L_1$, respectively.

It is the object of this paper to derive stability and convergence results which hold uniformly on the classes $\mathcal{F}_1$ and $\mathcal{F}_2$. In particular, the results are independent of the stiffness of the problems under consideration and the dimension m.

Even if for all $x \in [x_0, x_e]$ the function $g(x,\cdot)$ is Lipschitz continuous on $\mathbb{R}^m$, the $(D_i\, y)(x,\cdot)$ (for $i > 1$) will generally not be Lipschitz on the whole $\mathbb{R}^m$. To make the investigations easier, in Section **??** we define an extension of method (**??**) which is defined and Lipschitz on $[x_0, x_e] \times \mathbb{R}^m$ and which corresponds to (**??**) on a set $W \subseteq U$.

In Section **??** we give a constructive proof for the existence of a unique solution of the algebraic equations of the implicit Taylor series method. If there is a restriction on the step sizes then this restriction does not depend on the stiffness of the problem.

Since the paper of Prothero and Robinson [**?**] it has become known that stiffness may not only affect the stability of a method but also its order of accuracy. To derive realistic bounds for the error in the smooth phase, Frank, Schneid and Überhuber (cf., e.g. [**?**]) developed the concept of B-consistency and B-convergence. Following this concept, see also [**?**], we put

$$\|y^{(r)}\| := \max\{\|y^{(r)}(x)\| : x \in [x_0, x_e]\}$$

and give the following definitions.

Definition 1.1. Method (**??**) is said to be *C-stable* on the set of functions $\mathcal{F} = \mathcal{F}_1$ or $\mathcal{F} = \mathcal{F}_2$ if there are constants $C_0, h_0' > 0$ such that for all $f \in \mathcal{F}$ for two numerical solutions

$$\|y_{n+1} - \hat{y}_{n+1}\| \le (1 + C_0\, h_n)\|y_n - \hat{y}_n\| \quad \text{for} \quad 0 < h_n \le \min(h_0', x_e - x_n)\,.$$

It is *B-consistent* of order r on $\mathcal{F}$ if there are constants $C_1, h_1' > 0$ such that for all $f \in \mathcal{F}$ and $y_n = y(x_n)$

$$\|y(x_{n+1}) - y_{n+1}\| \le C_1\, h_n^{r+1} \quad \text{for} \quad 0 < h_n \le \min(h_1', x_e - x_n)\,.$$

Method (**??**) is *B-convergent* of order r on $\mathcal{F}$ if there are constants $C_2, h_2' > 0$ such that for all $f \in \mathcal{F}$

$$\|y(x_n) - y_n\| \le C_2\, h_{max}^r \quad \text{for} \quad 0 < h_{max} \le \min(h_2', x_e - x_n), \quad h_{max} = \max h_i\,.$$

In the case $\mathcal{F} = \mathcal{F}_1$ the constants C_0, C_1, C_2, h_0', h_1' and h_2' may only depend on L_i $(i = 1, \ldots, q)$, $\|y^{(r_0)}\|$ for a $r_0 \in \mathbb{N}$, on $x_e - x_0$, the coefficients of the method and geometrical parameters related to the set U. For the class $\mathcal{F} = \mathcal{F}_2$ these constants may also depend on μ.

In Section **??** we show that the A-stable methods (**??**) are C-stable on $\mathcal{F}_1$ and $\mathcal{F}_2$ and the contractivity is investigated. In Section **??** it is shown that the A-stable methods are B-convergent of order $p + q$ on $\mathcal{F}_1$ and $\mathcal{F}_2$. In Section **??** some asymptotic error estimates are given.

2 Preliminaries

For $0 \le i \le p$ and $0 \le j \le q$ let

$$\alpha_i = \alpha_i(p,q) := \frac{1}{i!}\frac{\binom{p}{i}}{\binom{p+q}{i}}, \qquad \beta_j = \beta_j(p,q) := \frac{1}{j!}\frac{\binom{q}{j}}{\binom{p+q}{j}} \tag{2.1a}$$

and

$$P_{pq}(z) := \sum_{i=0}^{p} \alpha_i\, z^i, \qquad Q_{pq}(z) := \sum_{j=0}^{q} \beta_j (-z)^j, \qquad R_{pq}(z) := \frac{P_{pq}(z)}{Q_{pq}(z)}. \tag{2.1b}$$

$R_{pq}(z)$ is the stability function of method (**??**). With these abbreviations and with the functions $(D_i\, y)(\cdot,\cdot)$, defined by (**??**) and (**??**), method (**??**) for ODEs

(??), (??) can be written as

$$\sum_{j=0}^{q}(-1)^j\beta_j h_n^j A^j y_{n+1} + \sum_{j=0}^{q}(-1)^j\beta_j h_n^j (D_j\, y)\,(x_{n+1},y_{n+1})$$
$$= \sum_{i=0}^{p}\alpha_i h_n^i A^i y_n + \sum_{i=0}^{p}\alpha_i h_n^i (D_i\, y)\,(x_n,y_n)$$

and

$$Q_{pq}(h_nA)\,y_{n+1} + \sum_{j=0}^{q}(-1)^j\beta_j h_n^j (D_j\, y)\,(x_{n+1},y_{n+1})$$
$$= P_{pq}(h_nA)\,y_n + \sum_{i=0}^{p}\alpha_i h_n^i (D_i\, y)\,(x_n,y_n). \quad (2.2)$$

Because of (??) and (??), the inverse $Q_{pq}(h_nA)^{-1}$ exists for all $h_n > 0$. Therefore from (??) we get

$$y_{n+1} = R_{pq}(h_nA)\,y_n + Q_{pq}(h_nA)^{-1}\Bigg[\sum_{i=0}^{p}\alpha_i h_n^i (D_i\, y)\,(x_n,y_n) - \sum_{j=0}^{q}(-1)^j\beta_j h_n^j (D_j\, y)\,(x_{n+1},y_{n+1})\Bigg].$$

Because of (??) we write

$$y_{n+1} = R_{pq}(h_nA)\,y_n + Q_{pq}(h_nA)^{-1}\Bigg[\sum_{i=1}^{p}\alpha_i h_n^i (D_i\, y)\,(x_n,y_n) - \sum_{j=1}^{q}(-1)^j\beta_j h_n^j (D_j\, y)\,(x_{n+1},y_{n+1})\Bigg] \quad (2.3)$$

and suppose that the empty sum, for $p = 0$ or $q = 0$, has to be interpreted as zero. In all the following investigations we will always start from this form of method (??).

The functions $g(x,\cdot)$ may not be defined on the whole $\mathbb{R}^m$. Even if for all $x \in [x_0, x_e]$ the function $g(x,\cdot)$ is defined and Lipschitz continuous on $\mathbb{R}^m$, for $i > 1$ the $(D_i\, y)(x,\cdot)$ will generally not be Lipschitz on the whole $\mathbb{R}^m$. To get rid of these restrictions and to make the investigations easier we also will consider a modification of equation (??) which is defined and Lipschitz on the whole $[x_0, x_e] \times \mathbb{R}^m$. In the case $U \neq [x_0, x_e] \times \mathbb{R}^m$ let $0 < r_W < \infty$ so that

$$W := \{(x,z) \in \mathbb{R}^{m+1} : x \in [x_0, x_e], \|y(x) - z\| \leq r_W\} \subseteq U \quad (2.4)$$

holds ($y(x)$ is the solution of (**??**), (**??**)). If we have $U = G = [x_0, x_e] \times \mathbb{R}^m$ we put

$$W := [x_0, x_e] \times \mathbb{R}^m.$$

For $y \in \mathbb{R}^m$ let $S(y,r) := \{z \in \mathbb{R}^m : \|y - z\| = r\}$ and for all $(x,z) \in [x_0, x_e] \times \mathbb{R}^m \setminus W$ let z_W denote the point of intersection of the finite line connecting $y(x)$ and z with $S(y(x), r_W)$. For $1 \le i \le \max(p,q)$ and all $(x,z) \in [x_0, x_e] \times \mathbb{R}^m$ we define

$$(\widetilde{D}_i\, y)(x,z) := \begin{cases} (D_i\, y)(x,z), & \text{if} \quad (x,z) \in W \\ (D_i\, y)(x,z_W), & \text{if} \quad (x,z) \in [x_0, x_e] \times \mathbb{R}^m \setminus W\,. \end{cases} \tag{2.5}$$

If functions $(D_i\, y)(\cdot,\cdot)$ satisfy the conditions (**??**), then the $(\widetilde{D}_i\, y)(\cdot,\cdot)$ satisfy, with the same constants L_i, the global Lipschitz conditions

$$\|(\widetilde{D}_i\, y)(x,u) - (\widetilde{D}_i\, y)(x,v)\| \le L_i \|u - v\|$$
$$\text{for} \quad 1 \le i \le \max(p,q) \quad \text{and all} \quad (x,u), (x,v) \in [x_0, x_e] \times \mathbb{R}^m. \tag{2.6}$$

If functions $(D_i\, y)(\cdot,\cdot)$ satisfy the conditions (**??**), then the $(\widetilde{D}_i\, y)(\cdot,\cdot)$ satisfy, with the same constants L_i, the global Lipschitz conditions

$$\|(\widetilde{D}_i\, y)(x,u) - (\widetilde{D}_i\, y)(x,v)\| \le \lambda^{i-1} L_i \|u - v\|$$
$$\text{for} \quad 1 \le i \le \max(p,q) \quad \text{and all} \quad (x,u), (x,v) \in [x_0, x_e] \times \mathbb{R}^m \tag{2.7}$$

(cf., e.g. [**?**, p. 80] or [**?**, p. 120]). Beside equation (**??**), we also consider equation

$$y_{n+1} = R_{pq}(h_n A)\, y_n + Q_{pq}(h_n A)^{-1} \left[\sum_{i=1}^{p} \alpha_i h_n^i (\widetilde{D}_i\, y)\,(x_n, y_n) - \sum_{j=1}^{q} (-1)^j \beta_j h_n^j (\widetilde{D}_j\, y)\,(x_{n+1}, y_{n+1}) \right] \tag{2.8}$$

from now on. This equation is defined on the whole $[x_0, x_e] \times \mathbb{R}^m$. In the case of $(x_n, y_n), (x_{n+1}, y_{n+1}) \in W$, every solution y_{n+1} of equation (**??**) is also a solution of (**??**) and vice versa. If we have $U = G = [x_0, x_e] \times \mathbb{R}^m$ equations (**??**) and (**??**) coincide.

3 The solvability of the algebraic equations

Let us first consider equation (**??**). For this equation holds

Lemma 3.1. *Let $q > 0$, $q-2 \le p \le q \le 16$ and conditions (**??**) and (**??**) be valid. If in addition*

$$|\mu|^j \ge L_j \quad \textit{for all} \quad j = 1, \dots, q \tag{3.1}$$

*holds, then for all $(x_n, y_n) \in [x_0, x_e) \times \mathbb{R}^m$ and all $0 < h_n \le x_e - x_n$ equation (**??**) has a unique solution $y_{n+1} \in \mathbb{R}^m$.*
*If condition (**??**) is not valid, then there exists a constant $h_{11} > 0$, so that for all $(x_n, y_n) \in [x_0, x_e) \times \mathbb{R}^m$ and $0 < h_n \le \min(h_{11}, x_e - x_n)$ equation (**??**) has a unique solution $y_{n+1} \in \mathbb{R}^m$. In each case y_{n+1} can be obtained by iteration. h_{11} depends only on L_j and β_j $(j = 1, \dots, q)$.*

Proof. If we put

$$F(z) := R_{pq}(h_n A)\, y_n + Q_{pq}(h_n A)^{-1} \Bigg[\sum_{i=1}^{p} \alpha_i h_n^i (\widetilde{D}_i\, y)\,(x_n, y_n) - \sum_{j=1}^{q} (-1)^j \beta_j h_n^j (\widetilde{D}_j\, y)\,(x_{n+1}, z) \Bigg], \tag{3.2}$$

equation (**??**) can be written as

$$y_{n+1} = F(y_{n+1})\,. \tag{3.3}$$

From (**??**) and (**??**), it follows for $0 < h_n \le x_e - x_n$ that

$$\|F(u) - F(v)\| \le \|Q_{pq}(h_n A)^{-1}\| \sum_{j=1}^{q} \beta_j L_j h_n^j \|u - v\|. \tag{3.4}$$

Because of (**??**), for the here considered p, q and all $h_n > 0$ it follows from Corollary **??** that

$$\|Q_{pq}(h_n A)^{-1}\| \le Q_{pq}(h_n \mu)^{-1} \le 1 \tag{3.5}$$

holds. Therefore, from (**??**) we derive

$$\|F(u) - F(v)\| \le Q_{pq}(h_n \mu)^{-1} \sum_{j=1}^{q} \beta_j L_j h_n^j \, \|u - v\|. \tag{3.6}$$

From the definition of the function $Q_{pq}(z)$, from (**??**), (**??**) and (**??**) it follows that for $0 < h_n \le x_e - x_n$ function F is a contraction. The contraction mapping principle then ensures the existence and uniqueness of the solution and the convergence of the fixed-point iteration. If (**??**) is not valid, let x^* be the smallest positive root of $\sum_{j=1}^{q} \beta_j L_j x^j = 1$. Then for every

$$0 < h_{11} < x^* \tag{3.7}$$

and $0 < h_n \le \min(h_{11}, x_e - x_n)$ function F is a contraction. ■

Lemma 3.2. *Let $q > 0$, $q-2 \le p \le q \le 16$ and conditions (??) and (??) be valid. If in addition*

$$\lambda\,|\mu|^j \ge L_j \quad \textit{for all} \quad j = 1,\ldots,q \tag{3.8}$$

holds, then for all $(x_n, y_n) \in [x_0, x_e) \times \mathbb{R}^m$ and $0 < h_n \le x_e - x_n$ equation (??) has a unique solution $y_{n+1} \in \mathbb{R}^m$.
If condition (??) is not valid, then there exists a constant $h_{12} > 0$, so that for all $(x_n, y_n) \in [x_0, x_e) \times \mathbb{R}^m$ and $0 < h_n \le \min(h_{12}, x_e - x_n)$ equation (??) has a unique solution $y_{n+1} \in \mathbb{R}^m$. In each case y_{n+1} can be obtained by iteration. h_{12} depends only on L_j, β_j $(j = 1,\ldots,q)$ and on μ.

Proof. Again we look at (??) in the form of equation (??). From (??) and (??) it follows for $0 < h_n \le x_e - x_n$ that

$$\|F(u) - F(v)\| \le \|Q_{pq}(h_n A)^{-1}\| \sum_{j=1}^{q} \beta_j \lambda^{j-1} L_j\, h_n^j\, \|u - v\|,$$

and because of (??) we have

$$\|Q_{pq}(h_n A)^{-1}\| \le Q_{pq}(h_n \lambda \mu)^{-1} < 1 \tag{3.9}$$

and

$$\|F(u) - F(v)\| \le Q_{pq}(h_n \lambda \mu)^{-1} \sum_{j=1}^{q} \beta_j \lambda^{j-1} L_j\, h_n^j\, \|u - v\|. \tag{3.10}$$

From (??), (??) and (??) it follows that for $0 < h_n \le x_e - x_n$ function F is a contraction. If (??) is not valid, then define

$$G_1(x) := \frac{\sum_{j=1}^{q} \beta_j L_j x^{j-1}}{Q_{pq}(x\mu)}\,. \tag{3.11}$$

(??) then can be written as

$$\|F(u) - F(v)\| \le h_n\, G_1(h_n \lambda)\, \|u - v\|. \tag{3.12}$$

For the here considered p and q and $x \ge 0$ we have $0 \le G_1(x) < \infty$. Therefore, there exists a constant $M_1 > 0$, depending only on L_j, β_j $(j = 1,\ldots,q)$ and on μ, such that

$$0 \le G_1(x) \le M_1 < \infty \quad \text{for all} \quad x \ge 0 \tag{3.13}$$

holds. For every

$$0 < h_{12} < \frac{1}{M_1} \tag{3.14}$$

and $0 < h_n \le \min(h_{12}, x_e - x_n)$, F again is a contraction. ∎

Remark 3.1. The bounds h_{11} and h_{12}, defined by (**??**) and (**??**), and independent of μ and λ, respectively, are sufficient so that function F, defined by (**??**), is a contraction. Denote by h_{11}^* and h_{12}^* the upper bounds for the step sizes such that, under the suppositions as given in the Lemmas **??** and **??**, F is a contraction. Clearly, h_{11}^* and h_{12}^* depend on μ and λ, respectively. From (**??**) and (**??**) it follows that $\lim_{\mu\to-\infty} h_{11}^* = \infty$ and $\lim_{\lambda\to\infty} h_{12}^* = \infty$.

Remark 3.2. In the case $q > 1$ from $\mu \to 0$ it follows $M_1 \to \infty$ and $h_{12} \to 0$. This is the reason for the restriction $\mu \le \mu_0 < 0$ for the class $\mathcal{F}_2$.

Actually, we are interested in the solvability of equation (**??**). But only for $U = G = [x_0, x_e] \times \mathbb{R}^m$ equations (**??**) and (**??**), respectively (**??**), coincide. In the case

$$U \neq [x_0, x_e] \times \mathbb{R}^m \tag{3.15}$$

let $r_V \in \mathbb{R}$ with $0 < r_V < r_W$ and let

$$V := \{(x, z) \in \mathbb{R}^{m+1} : x \in [x_0, x_e), \|y(x) - z\| < r_V\}. \tag{3.16}$$

It then holds that

Theorem 3.1. *Suppose method* (**??**) *is A-stable and $p, q \le 16$. If* (**??**) *holds and V and W are defined by* (**??**) *and* (**??**)*, then there exists a constant $h_{21} > 0$, such that for all $f \in \mathcal{F}_1$, all $(x_n, y_n) \in V$ and $0 < h_n \le \min(h_{21}, x_e - x_n)$,* (**??**) *has a unique solution y_{n+1} with $(x_{n+1}, y_{n+1}) \in W$. h_{21} depends only on L_j $(j = 1, \dots, q)$, $\|y^{(p+q+1)}\|$, r_V, r_W and the coefficients of the method.*

Proof. If f is sufficiently often differentiable, then for the solution of (**??**) it holds that

$$\sum_{j=0}^{q} (-1)^j \beta_j\, h_n^j\, y^{(j)}(x_{n+1}) = \sum_{i=0}^{p} \alpha_i\, h_n^i\, y^{(i)}(x_n) + (-1)^q\, c_{pq}\, h_n^{p+q+1}\, y^{(p+q+1)}(\xi_n)$$

with

$$c_{pq} = \frac{p!\, q!}{(p+q)!\,(p+q+1)!}$$

and

$$y^{(p+q+1)}(\xi_n) := (y_1^{(p+q+1)}(\xi_{n1}), \dots, y_m^{(p+q+1)}(\xi_{nm}))^T, \quad \xi_{ni} \in (x_n, x_{n+1})$$

(cf., e.g. [**?**, p. 20]). For a solution of an ODE (**??**), (**??**), (**??**), and the p and q considered here, we therefore have for $0 < h_n \le x_e - x_n$

$$y(x_{n+1}) = R_{pq}(h_n A)\, y(x_n) + Q_{pq}(h_n A)^{-1} \left[\sum_{i=1}^{p} \alpha_i h_n^i (D_i\, y)\,(x_n, y(x_n)) \right.$$
$$\left. - \sum_{j=1}^{q} (-1)^j \beta_j h_n^j (D_j\, y)\,(x_{n+1}, y(x_{n+1})) + (-1)^q\, c_{pq}\, h_n^{p+q+1}\, y^{(p+q+1)}(\xi_n) \right]. \tag{3.17}$$

Before turning to the solution of method (**??**), we consider the related method (**??**). Because of the suppositions, as given in the Theorem, at least for $0 < h_n \leq \min(h_{11}, x_e - x_n)$ (with h_{11} defined by (**??**)), equation (**??**) has a unique solution y_{n+1}. Hence we get from (**??**) and (**??**)

$$
\begin{aligned}
\|y(x_{n+1}) - y_{n+1}\| &\leq \|R_{pq}(h_n A)\| \, \|y(x_n) - y_n\| \\
&\quad + \|Q_{pq}(h_n A)^{-1}\| \left[\sum_{i=1}^{p} \alpha_i h_n^i \|(D_i\, y)\,(x_n, y(x_n)) - (\widetilde{D}_i\, y)\,(x_n, y_n)\| \right. \\
&\qquad + \sum_{j=1}^{q} \beta_j h_n^j \|(D_j\, y)\,(x_{n+1}, y(x_{n+1})) - (\widetilde{D}_j\, y)\,(x_{n+1}, y_{n+1})\| \\
&\qquad \left. + c_{pq}\, h_n^{p+q+1} \, \|y^{(p+q+1)}\| \right].
\end{aligned}
\tag{3.18}
$$

For $f \in \mathcal{F}_1$ and A-stable methods we have $\|R_{pq}(h_n A)\| \leq 1$, and from $(x_n, y_n) \in V$ it follows that

$$
\begin{aligned}
\|y(x_{n+1}) - y_{n+1}\| &\leq r_V \\
&\quad + \|Q_{pq}(h_n A)^{-1}\| \left[\sum_{i=1}^{p} \alpha_i h_n^i \|(D_i\, y)\,(x_n, y(x_n)) - (\widetilde{D}_i\, y)\,(x_n, y_n)\| \right. \\
&\qquad + \sum_{j=1}^{q} \beta_j h_n^j \|(D_j\, y)\,(x_{n+1}, y(x_{n+1})) - (\widetilde{D}_j\, y)\,(x_{n+1}, y_{n+1})\| \\
&\qquad \left. + c_{pq}\, h_n^{p+q+1} \, \|y^{(p+q+1)}\| \right].
\end{aligned}
\tag{3.19}
$$

Because of (**??**), (**??**) and (**??**) we obtain

$$
\begin{aligned}
\|y(x_{n+1}) - y_{n+1}\| &\leq r_V + Q_{pq}(h_n \mu)^{-1} \left(r_V \sum_{i=1}^{p} \alpha_i L_i\, h_n^i \right. \\
&\qquad \left. + r_W \sum_{j=1}^{q} \beta_j L_j\, h_n^j + c_{pq}\, h_n^{p+q+1} \, \|y^{(p+q+1)}\| \right)
\end{aligned}
\tag{3.20}
$$

and

$$
\|y(x_{n+1}) - y_{n+1}\| \leq r_V + r_V \sum_{i=1}^{p} \alpha_i L_i h_n^i + r_W \sum_{j=1}^{q} \beta_j L_j h_n^j + c_{pq} h_n^{p+q+1} \|y^{(p+q+1)}\|.
$$

Let

$$h_{VW_1} := \frac{r_W - r_V}{r_V \sum_{i=1}^{p} \alpha_i L_i + r_W \sum_{j=1}^{q} \beta_j L_j + c_{pq} \|y^{(p+q+1)}\|}$$

and

$$h_{21} := \begin{cases} \min(1, h_{VW_1}), & \text{if} \quad (\textbf{??}) \quad \text{holds} \\ \min(h_{11}, 1, h_{VW_1}), & \text{otherwise.} \end{cases} \tag{3.21}$$

For $0 < h_n \leq \min(h_{21}, x_e - x_n)$ we then have

$$\|y(x_{n+1}) - y_{n+1}\| \leq r_W. \tag{3.22}$$

This means $(x_{n+1}, y_{n+1}) \in W$, so that y_{n+1} is also a solution of the corresponding equation (**??**), respectively (**??**). Under the conditions stated, y_{n+1} is the unique solution of (**??**). This is because if there was a second solution, it would also have to be a solution of (**??**), but those are unique. ■

Theorem 3.2. *Suppose method* (**??**) *is A-stable and* $p, q \leq 16$. *If* (**??**) *holds and* V *and* W *are defined by* (**??**) *and* (**??**), *then there exists a constant* $h_{22} > 0$, *such that for all* $f \in \mathcal{F}_2$, *all* $(x_n, y_n) \in V$ *and* $0 < h_n \leq \min(h_{22}, x_e - x_n)$, (**??**) *has a unique solution* y_{n+1} *with* $(x_{n+1}, y_{n+1}) \in W$. h_{22} *depends only on* L_j $(j = 1, \ldots, q)$, μ, $\|y^{(p+q+1)}\|$, r_V, r_W *and the coefficients of the method.*

Proof. This proof follows the lines of the proof of Theorem **??**. From (**??**) it follows that for $f \in \mathcal{F}_2$ again (**??**) holds. At least for $0 < h_n \leq \min(h_{12}, x_e - x_n)$ (h_{12} be defined by (**??**)), the related equation (**??**) has a unique solution y_{n+1}, and as in the proof of Theorem **??** we have (**??**). Because of (**??**), (**??**) and (**??**), we now deduce

$$\begin{aligned} \|y(x_{n+1}) - y_{n+1}\| \leq r_V & \\ + Q_{pq}(h_n \lambda \mu)^{-1} \Bigg(r_V \sum_{i=1}^{p} \alpha_i \lambda^{i-1} L_i \, h_n^i + r_W \sum_{j=1}^{q} \beta_j \lambda^{j-1} L_j \, h_n^j & \\ + c_{pq} \, h_n^{p+q+1} \|y^{(p+q+1)}\| \Bigg) & \end{aligned} \tag{3.23}$$

and

$$\begin{aligned} \|y(x_{n+1}) - y_{n+1}\| \leq r_V & \\ + Q_{pq}(h_n \lambda \mu)^{-1} \left(r_V \sum_{i=1}^{p} \alpha_i \lambda^{i-1} L_i \, h_n^i + r_W \sum_{j=1}^{q} \beta_j \lambda^{j-1} L_j \, h_n^j \right) & \end{aligned}$$

$$+ c_{pq}\, h_n^{p+q+1} \|y^{(p+q+1)}\| \quad (3.24)$$

from (??). With

$$G_2(x) := \frac{\sum_{i=1}^{p} \alpha_i L_i x^{i-1}}{Q_{pq}(x\mu)} \tag{3.25}$$

and with function $G_1(x)$ defined by (??), equation (??) can be written as

$$\|y(x_{n+1}) - y_{n+1}\| \leq r_V + h_n \left(r_V\, G_2(h_n \lambda) + r_W\, G_1(h_n \lambda) \right)$$

$$+ c_{pq}\, h_n^{p+q+1} \|y^{(p+q+1)}\|. \quad (3.26)$$

For the here considered p, q and $x \geq 0$, we have $0 \leq G_2(x) < \infty$. Therefore, it exists a constant $M_2 > 0$, depending only on L_j $(j = 1, \ldots, q)$, μ and the coefficients of the method, such that

$$0 \leq G_2(x) \leq M_2 < \infty \quad \text{for all} \quad x \geq 0 \tag{3.27}$$

holds. Because of (??) and (??) we get

$$\|y(x_{n+1}) - y_{n+1}\| \leq r_V + h_n \left(r_V M_2 + r_W M_1 \right) + c_{pq}\, h_n^{p+q+1} \|y^{(p+q+1)}\|$$

from (??). Let

$$h_{VW_2} := \frac{r_W - r_V}{r_V M_2 + r_W M_1 + c_{pq}\, \|y^{(p+q+1)}\|}$$

and

$$h_{22} := \begin{cases} \min(1, h_{VW_2}), & \text{if} \quad (??) \quad \text{holds} \\ \min(h_{12}, 1, h_{VW_2}), & \text{otherwise.} \end{cases} \tag{3.28}$$

For $0 < h_n \leq \min(h_{22}, x_e - x_n)$, we again have (??). ■

Remark 3.3. Again, the bounds h_{21} and h_{22}, given by (??) are (??) and independent of μ and λ, respectively, and are sufficient so that (??) has a unique solution. Let h_{21}^* and h_{22}^* denote the upper bounds for the step sizes such that (??) has a unique solution. From Remark **??** and from (??) and (??) it follows that $\lim_{\mu \to -\infty} h_{21}^* = \infty$ and $\lim_{\lambda \to \infty} h_{22}^* = \infty$. In the case $p > 1$ from $\mu \to 0$ it follows $M_2 \to \infty$ and $h_{VW_2} \to 0$.

Remark 3.4. For the Lemmas **??**, **??** and the two following Theorems **??** and **??**, we had the restriction $p, q \leq 16$. This restriction, which will also be a constituent part of all the following Theorems, originates from Theorem **??** and Corollary **??**. There the estimation of $\|Q_p(A)^{-1}\|$ is done only for these p and q. By this restriction all A-stable methods up to order 30 are included. Looking at it from the numerical point of view this should be sufficient. Usually, stiff IVPs are solved with lower order methods. In Remark **??** it is suggested that the estimation is valid for $p, q > 16$ and it may be valid for all A-stable methods (??).

4 C-stability and contractivity

Let

$$\varphi_{R_{pq}}(x) := \sup_{\mathrm{Re} z \le x} |R_{pq}(z)|$$

and with functions G_1 and G_2, defined by (**??**) and (**??**), let

$$G_3(x) := \frac{\varphi_{R_{pq}}(x\mu) + x\, G_2(x)}{1 - x\, G_1(x)} \tag{4.1}$$

Theorem 4.1. *Let conditions* (**??**) *and* (**??**) *be valid and* $q - 2 \le p \le q \le 16$. *Then at least for* $0 < h_n \le \min(h_{11}, x_e - x_n)$ *the difference of two numerical solutions of* (**??**) *can be estimated by*

$$\|y_{n+1} - \hat{y}_{n+1}\| \le G_3(h_n)\, \|y_n - \hat{y}_n\|. \tag{4.2}$$

If we have (**??**), (x_n, y_n), $(x_n, \hat{y}_n) \in V$, $f \in \mathcal{F}_1$, *and a* A*-stable method* (**??**) *then estimate* (**??**) *holds at least for* $0 < h_n \le \min(h_{21}, x_e - x_n)$.
h_{11} *and* h_{21} *are given by* (**??**) *and* (**??**).

Proof. From Lemma **??** it follows that for all (x_n, y_n), $(x_n, \hat{y}_n) \in [x_0, x_e) \times \mathbb{R}^m$ and at least for $0 < h_n \le \min(h_{11}, x_e - x_n)$, equation (**??**) has unique solutions y_{n+1}, $\hat{y}_{n+1} \in \mathbb{R}^m$ with

$$\begin{aligned} \|y_{n+1} - \hat{y}_{n+1}\| \le{}& \|R_{pq}(h_n A)\|\, \|y_n - \hat{y}_n\| \\ &+ \|Q_{pq}(h_n A)^{-1}\| \left[\sum_{i=1}^{p} \alpha_i h_n^i \|(\widetilde{D}_i\, y)\,(x_n, y_n) - (\widetilde{D}_i\, y)\,(x_n, \hat{y}_n)\| \right. \\ &\left. + \sum_{j=1}^{q} \beta_j h_n^j \|(\widetilde{D}_j\, y)\,(x_{n+1}, y_{n+1}) - (\widetilde{D}_j\, y)\,(x_{n+1}, \hat{y}_{n+1})\| \right]. \end{aligned} \tag{4.3}$$

Because of (**??**) it follows that

$$\begin{aligned} \|y_{n+1} - \hat{y}_{n+1}\| \le{}& \|R_{pq}(h_n A)\|\, \|y_n - \hat{y}_n\| \\ &+ \|Q_{pq}(h_n A)^{-1}\| \left[\sum_{i=1}^{p} \alpha_i L_i h_n^i \|y_n - \hat{y}_n\| + \sum_{j=1}^{q} \beta_j L_j h_n^j \|y_{n+1} - \hat{y}_{n+1}\| \right], \end{aligned}$$

and because of (**??**),

$$\|y_{n+1} - \hat{y}_{n+1}\| \le \varphi_{R_{pq}}(h_n \mu)\, \|y_n - \hat{y}_n\|$$

$$+ Q_{pq}(h_n\mu)^{-1}\left[\sum_{i=1}^{p} \alpha_i L_i h_n^i \|y_n - \hat{y}_n\| + \sum_{j=1}^{q} \beta_j L_j h_n^j \|y_{n+1} - \hat{y}_{n+1}\|\right],$$

$$(1 - h_n G_1(h_n)) \|y_{n+1} - \hat{y}_{n+1}\| \le (\varphi_{R_{pq}}(h_n\mu) + h_n G_2(h_n)) \|y_n - \hat{y}_n\|,$$

and

$$\|y_{n+1} - \hat{y}_{n+1}\| \le \frac{\varphi_{R_{pq}}(h_n\mu) + h_n G_2(h_n)}{1 - h_n G_1(h_n)} \|y_n - \hat{y}_n\|.$$

If we restrict the step size by $0 < h_n \le \min(h_{21}, x_e - x_n)$ then the same estimates are valid for all (x_n, y_n), $(x_n, \hat{y}_n) \in V$, $f \in \mathcal{F}_1$ and A-stable methods (**??**). ■

Corollary 4.1. *Let conditions* (**??**) *and* (**??**) *be valid. Then the A-stable methods* (**??**)*, at least for $p, q \le 16$, are C-stable. If* (**??**) *holds, then for (x_n, y_n), $(x_n, \hat{y}_n) \in V$ the A-stable methods* (**??**)*, at least for $p, q \le 16$, are C-stable on $\mathcal{F}_1$.*

Proof. Let

$$G_4(x) := \frac{1 + \sum_{i=1}^{p} \alpha_i L_i x^i}{1 - \sum_{j=1}^{q} \beta_j L_j x^j}. \tag{4.4}$$

Because of $\mu \le 0$ and for x_1 as defined in the proof of Lemma **??**, we have

$$G_3(x) \le G_4(x) \quad \text{for} \quad 0 \le x < x_1. \tag{4.5}$$

From (**??**) we get

$$G_4(0) = 1 \tag{4.6}$$

and

$$G_4'(x) = \left[\sum_{i=1}^{p} i\alpha_i L_i x^{i-1}\left(1 - \sum_{j=1}^{q} \beta_j L_j x^j\right) + \left(1 + \sum_{i=1}^{p} \alpha_i L_i x^i\right) \sum_{j=1}^{q} j\beta_j L_j x^{j-1}\right]\left(1 - \sum_{j=1}^{q} \beta_j L_j x^j\right)^{-2}. \tag{4.7}$$

Let h_{31} be the smallest positive root of $\sum_{j=1}^{q} \beta_j L_j x^j = \frac{1}{2}$ and let

$$C_{01} := 4\left[\sum_{i=1}^{p} i\alpha_i L_i h_{31}^{i-1} + \left(1 + \sum_{i=1}^{p} \alpha_i L_i h_{31}^i\right) \sum_{j=1}^{q} j\beta_j L_j h_{31}^{j-1}\right]. \tag{4.8}$$

Therefore it follows from (**??**) and from (**??**) – (**??**) that for $0 < h_n \le \min(h_{31}, x_e - x_n)$ the difference of two numerical solutions of (**??**) can be estimated by

$$\|y_{n+1} - \hat{y}_{n+1}\| \le (1 + C_{01}\, h_n) \|y_n - \hat{y}_n\|.$$

If we restrict the step size by $0 < h_n \le \min(h_{21}, h_{31}, x_e - x_n)$, then the same estimates are valid for all (x_n, y_n), $(x_n, \hat{y}_n) \in V$, $f \in \mathcal{F}_1$ and method (**??**). ■

The condition $\mu + L_1 \le 0$ is sufficient so that any two solutions of an ODE of the class $\mathcal{F}_1$ approach each other. For the numerical solutions we have

Corollary 4.2. *Let (**??**) hold. For the L-stable methods (**??**) with $p, q \le 16$ there exists a constant $h_{41} > 0$, so that for all $f \in \mathcal{F}_1$ with $\mu + L_1 < 0$ and all (x_n, y_n), $(x_n, \hat{y}_n) \in V$*

$$\|y_{n+1} - \hat{y}_{n+1}\| \le \|y_n - \hat{y}_n\| \quad \textit{for} \quad 0 < h_n \le \min(h_{41}, x_e - x_n). \tag{4.9}$$

h_{41} depends on L_j $(j = 1, \ldots, q)$, $\|y^{(p+q+1)}\|$, r_V, r_W, the coefficients of the method and on μ but not on $\|A\|$ (which represents the stiffness of the problem).

Proof. We have

$$\varphi_{R_{qq}}(x) = 1 \quad \text{for} \quad q > 0, \quad x \le 0$$

and for $q - 2 \le p \le q - 1$

$$\varphi_{R_{pq}}(x) = 1 + x + o(x) \quad \text{for} \quad x \to 0$$

(cf., e.g. [?] or [?]). From (**??**) we then get

$$G_3(0) = 1 \tag{4.10}$$

and

$$G_3'(0) = \begin{cases} L_1, & \text{if} \quad p = q > 0 \\ \mu + L_1, & \text{if} \quad q - 2 \le p \le q - 1. \end{cases} \tag{4.11}$$

For $q - 2 \le p \le q - 1$ let

$$x_{21} := \max\{x : G_3(z) \le 1,\ 0 < z \le x \le h_{21}\}. \tag{4.12}$$

From (**??**) and (**??**), (**??**) then it follows, that for

$$h_{41} := \min(x_{21}, x_e - x_n)$$

(**??**) holds. ∎

Remark 4.1. For A-stable methods and all $x \ge 0$ with $x\, G_1(x) < 1$ function $G_3(x)$ can also be estimated by

$$G_5(x) := \frac{1 + x\, G_2(x)}{1 - x\, G_1(x)} \tag{4.13}$$

with $G_3(x) \le G_5(x)$. If (**??**) holds, then there exists a $C_{01}^* = C_{01}^*(\mu) > 0$ so that for all $0 < h_n \le x_e - x_n$ the difference of two numerical solutions of (**??**) can be estimated by

$$\|y_{n+1} - \hat{y}_{n+1}\| \le (1 + C_{01}^* h_n)\, \|y_n - \hat{y}_n\|. \tag{4.14}$$

From (**??**) we get $\lim_{\mu \to -\infty} C_{01}^*(\mu) = 0$. If we restrict the step size by $0 < h_n \le \min(h_{21}^*, x_e - x_n)$ then, for all (x_n, y_n), $(x_n, \hat{y}_n) \in V$, $f \in \mathcal{F}_1$, and methods (**??**), the estimate (**??**) is also valid.

Remark 4.2. For L-stable methods $\lim_{x\to\infty} G_3(x) = 0$ and $\lim_{\mu\to-\infty} G_3(x) = 0$ holds. Therefore, for large step sizes or/and $\mu \to -\infty$ contractivity can be expected.

Let us define

$$G_6(x) := \frac{\varphi_{R_{pq}}(x\lambda\mu) + x\,G_2(x\lambda)}{1 - x\,G_1(x\lambda)}. \tag{4.15}$$

Analogous to Theorem **??**, we have

Theorem 4.2. *Let conditions* (**??**) *and* (**??**) *be valid and* $q-2 \le p \le q \le 16$. *Then, at least for* $0 < h_n \le \min(h_{12}, x_e - x_n)$, *the difference of two numerical solutions of* (**??**) *can be estimated by*

$$\|y_{n+1} - \hat{y}_{n+1}\| \le G_6(h_n)\,\|y_n - \hat{y}_n\|. \tag{4.16}$$

If we have (**??**) *then, for* (x_n, y_n), $(x_n, \hat{y}_n) \in V$, $f \in \mathcal{F}_2$, *and the A-stable methods* (**??**), *estimate* (**??**) *holds at least for* $0 < h_n \le \min(h_{22}, x_e - x_n)$.
h_{12} *and* h_{22} *are given by* (**??**) *and* (**??**).

Proof. From Lemma **??** it follows that for all (x_n, y_n), $(x_n, \hat{y}_n) \in [x_0, x_e) \times \mathbb{R}^m$ and at least for $0 < h_n \le \min(h_{12}, x_e - x_n)$ equation (**??**) has unique solutions $y_{n+1}, \hat{y}_{n+1} \in \mathbb{R}^m$ so that (**??**) holds. Because of (**??**) and (**??**) it then follows that

$$\|y_{n+1} - \hat{y}_{n+1}\| \le \varphi_{R_{pq}}(h_n\lambda\mu)\,\|y_n - \hat{y}_n\|$$

$$+\, Q_{pq}(h_n\lambda\mu)^{-1}\left[\sum_{i=1}^{p} \alpha_i \lambda^{i-1} L_i\, h_n^i \|y_n - \hat{y}_n\| + \sum_{j=1}^{q} \beta_j \lambda^{j-1} L_j\, h_n^j \|y_{n+1} - \hat{y}_{n+1}\|\right],$$

$$(1 - h_n G_1(h_n\lambda))\,\|y_{n+1} - \hat{y}_{n+1}\| \le (\varphi_{R_{pq}}(h_n\lambda\mu) + h_n G_2(h_n\lambda))\,\|y_n - \hat{y}_n\|,$$

and

$$\|y_{n+1} - \hat{y}_{n+1}\| \le \frac{\varphi_{R_{pq}}(h_n\lambda\mu) + h_n G_2(h_n\lambda)}{1 - h_n G_1(h_n\lambda)}\,\|y_n - \hat{y}_n\|.$$

If we restrict the step size by $0 < h_n \le \min(h_{22}, x_e - x_n)$, then for all (x_n, y_n), $(x_n, \hat{y}_n) \in V$, $f \in \mathcal{F}_2$ and method (**??**), the same estimates are valid. ∎

Corollary 4.3. *Let conditions* (**??**) *and* (**??**) *be valid. Then the A-stable methods* (**??**), *at least for* $p, q \le 16$, *are C-stable. The A-stable methods* (**??**), *at least for* $p, q \le 10$, *are C-stable on* $\mathcal{F}_2$ *for* (x_n, y_n), $(x_n, \hat{y}_n) \in V$ *if* (**??**) *holds.*

Proof. With the constants M_1 and M_2 as defined in the proofs of Lemma **??** and Theorem **??**, let

$$G_7(x) := \frac{1 + xM_2}{1 - xM_1}. \tag{4.17}$$

Because of $\lambda\mu < 0$, we have

$$G_6(h_n) \leq G_7(h_n) \quad \text{for} \quad 0 < h_n < \frac{1}{M_1}. \tag{4.18}$$

From (**??**) we get

$$G_7(0) = 1 \tag{4.19}$$

and

$$G_7'(x) = \frac{M_1(1 + xM_2) + M_2(1 - xM_1)}{(1 - xM_1)^2}. \tag{4.20}$$

Let

$$h_{32} := \frac{1}{2M_1} \tag{4.21}$$

and

$$C_{02} := 4M_1 + 6M_2. \tag{4.22}$$

From (**??**) and (**??**) – (**??**) it follows now that for $0 < h_n \leq \min(h_{32}, x_e - x_n)$ the difference of two numerical solutions of (**??**) can be estimated by

$$\|y_{n+1} - \hat{y}_{n+1}\| \leq (1 + C_{02}\, h_n)\, \|y_n - \hat{y}_n\|.$$

If we restrict the step size by $0 < h_n \leq \min(h_{22}, h_{32}, x_e - x_n)$ then, for all (x_n, y_n), $(x_n, \hat{y}_n) \in V$, $f \in \mathcal{F}_2$ and method (**??**), the same estimates are valid. ■

Condition $\lambda\mu + L_1 \leq 0$ is sufficient so that any two solutions of an ODE from the class $\mathcal{F}_2$ approach each other. For the numerical solutions we have

Corollary 4.4. *Let (**??**) hold. For the L-stable methods (**??**) with $p, q \leq 16$ there exists a constant $h_{42} > 0$, so that for all $f \in \mathcal{F}_2$ with $\lambda\mu + L_1 < 0$ and all (x_n, y_n), $(x_n, \hat{y}_n) \in V$*

$$\|y_{n+1} - \hat{y}_{n+1}\| \leq \|y_n - \hat{y}_n\| \quad \text{for} \quad 0 < h_n \leq \min(h_{42}, x_e - x_n). \tag{4.23}$$

h_{42} depends on L_j ($j = 1, \ldots, q$), μ, $\|y^{(p+q+1)}\|$, r_V, r_W, the coefficients of the method and on λ but not on $\|A\|$.

Proof. From (**??**) we get

$$G_6(0) = 1 \tag{4.24}$$

and

$$G_6'(0) = \begin{cases} L_1, & \text{if} \quad p = q > 0 \\ \lambda\mu + L_1, & \text{if} \quad q-2 \le p \le q-1. \end{cases} \tag{4.25}$$

For $q-2 \le p \le q-1$ let

$$x_{22} := \max\{x : G_6(z) \le 1,\ 0 < z \le x \le h_{22}\}. \tag{4.26}$$

From (**??**) and (**??**), (**??**) it follows that (**??**) holds for

$$h_{42} := \min(x_{22}, x_e - x_n).$$

∎

Analogously to Remarks **??** and **??** we have

Remark 4.3. For A-stable methods and all $x \ge 0$ with $x\,G_1(x\lambda) < 1$ function $G_6(x)$ can also be estimated by

$$G_8(x) := \frac{1 + x\,G_2(x\lambda)}{1 - x\,G_1(x\lambda)} \tag{4.27}$$

with $G_6(x) \le G_8(x)$. If (**??**) holds, then there exists a $C_{02}^* = C_{02}^*(\lambda) > 0$ so that for all $0 < h_n \le x_e - x_n$ the difference of two numerical solutions of (**??**) can be estimated by

$$\|y_{n+1} - \hat{y}_{n+1}\| \le (1 + C_{02}^* h_n)\,\|y_n - \hat{y}_n\|. \tag{4.28}$$

From (**??**) we get $\lim_{\lambda\to\infty} C_{02}^*(\lambda) = 0$. If we restrict the step size by $0 < h_n \le \min(h_{22}^*, x_e - x_n)$ then, for all (x_n, y_n), $(x_n, \hat{y}_n) \in V$, $f \in \mathcal{F}_2$, and methods (**??**), estimate (**??**) is also valid.

Remark 4.4. For L-stable methods $\lim_{x\to\infty} G_6(x) = 0$ and $\lim_{\lambda\to\infty} G_6(x) = 0$ holds. Therefore for large step sizes or/and $\lambda \to \infty$ contractivity can be expected.

5 B-convergence

Lemma 5.1. *Let (**??**) and (**??**) or (**??**) and (**??**) hold. Then the A-stable methods (**??**), at least for $p, q \le 16$, are B-consistent of order $p+q$. On the classes $\mathcal{F}_1$ and $\mathcal{F}_2$ the A-stable methods (**??**) , at least for $p, q \le 16$, are also B-consistent of order $p+q$.*

Proof. a) Let (**??**) and (**??**) hold. From Lemma **??** it follows that for all $(x_n, y_n) \in [x_0, x_e) \times \mathbb{R}^m$ and at least for $0 < h_n \le \min(h_{11}, x_e - x_n)$, equation (**??**) has a unique solution $y_{n+1} \in \mathbb{R}^m$. From the proof of Theorem **??** it follows that (**??**) holds. For $y_n = y(x_n)$ we get from (**??**)

$$\|y(x_{n+1}) - y_{n+1}\| \le$$

$$\|Q_{pq}(h_n A)^{-1}\| \left[\sum_{j=1}^{q} \beta_j h_n^j \|(D_j\, y)\,(x_{n+1}, y(x_{n+1})) - (\widetilde{D}_j\, y)\,(x_{n+1}, y_{n+1})\| \right.$$

$$\left. + \, c_{pq}\, h_n^{p+q+1}\, \|y^{(p+q+1)}\| \right], \quad (5.1)$$

$$(1 - h_n G_1(h_n))\, \|y(x_{n+1}) - y_{n+1}\| \le Q_{pq}(h_n \mu)^{-1} c_{pq}\, h_n^{p+q+1}\, \|y^{(p+q+1)}\|$$

and

$$\|y(x_{n+1}) - y_{n+1}\| \le \frac{Q_{pq}(h_n \mu)^{-1}}{1 - h_n G_1(h_n)}\, c_{pq}\, h_n^{p+q+1}\, \|y^{(p+q+1)}\|\,. \quad (5.2)$$

For $0 < h_n \le \min(h_{31}, x_e - x_n)$ (h_{31} defined in the proof of Corollary **??**) and with

$$C_1 := 2\, c_{pq}\, \|y^{(p+q+1)}\| \quad (5.3)$$

it follows that

$$\|y(x_{n+1}) - y_{n+1}\| \le \frac{C_1}{Q_{pq}(h_n \mu)}\, h_n^{p+q+1} \quad (5.4)$$

and

$$\|y(x_{n+1}) - y_{n+1}\| \le C_1\, h_n^{p+q+1}. \quad (5.5)$$

For $0 < h_n \le \min(h_{31}, \left(\frac{r_W}{C_1}\right)^{\frac{1}{p+q+1}}, x_e - x_n)$ we have (**??**). y_{n+1} is then also the solution of equation (**??**) for the corresponding function $f \in \mathcal{F}_1$.

b) Let (**??**) and (**??**) hold. As above, according to Lemma **??** and the proof of Theorem **??**, for $y_n = y(x_n)$ and at least for $0 < h_n \le \min(h_{12}, x_e - x_n)$, we have (**??**). Now it follows

$$(1 - h_n G_1(h_n \lambda))\, \|y(x_{n+1}) - y_{n+1}\| \le Q_{pq}(h_n \lambda \mu)^{-1} c_{pq}\, h_n^{p+q+1}\, \|y^{(p+q+1)}\|$$

and for $0 < h_n \le \min(h_{32}, x_e - x_n)$ (h_{32} given by (**??**)) we get

$$\|y(x_{n+1}) - y_{n+1}\| \le \frac{C_1}{Q_{pq}(h_n \lambda \mu)}\, h_n^{p+q+1} \quad (5.6)$$

and (**??**). For $0 < h_n \le \min(h_{32}, \left(\frac{r_W}{C_1}\right)^{\frac{1}{p+q+1}}, x_e - x_n)$ we have (**??**) again. ∎

Theorem 5.1. *The A-stable methods (??), at least for $p, q \leq 16$, are B-convergent of order $p+q$ on the classes $\mathcal{F}_1$ and $\mathcal{F}_2$.*

Proof. We start our proof by considering method (??) and on condition that (??) and (??) or (??) and (??) hold. Under these conditions method (??) is C-stable and B-consistent of order $p+q$. Let $\tilde{y}_{n+1}$ denote the numerical solution obtained by (??) from the initial value $\tilde{y}_n = y(x_n)$. Then we have

$$y(x_{n+1}) - y_{n+1} = y(x_{n+1}) - \tilde{y}_{n+1} + \tilde{y}_{n+1} - y_{n+1}$$

and

$$\|y(x_{n+1}) - y_{n+1}\| \leq \|y(x_{n+1}) - \tilde{y}_{n+1}\| + \|\tilde{y}_{n+1} - y_{n+1}\|. \tag{5.7}$$

With constant C_1, defined by (??), let

$$C_{11}(h_n) := \frac{C_1}{Q_{pq}(h_n\mu)}, \qquad C_{12}(h_n) := \frac{C_1}{Q_{pq}(h_n\lambda\mu)}. \tag{5.8}$$

From the B-consistence it follows that

$$\|y(x_{n+1}) - \tilde{y}_{n+1}\| \leq C_{1i}(h_n)\, h_n^{p+q+1} \tag{5.9}$$

for $0 < h_n \leq \min(h_{3i}, x_e - x_n)$ and from the C-stability we have

$$\|\tilde{y}_{n+1} - y_{n+1}\| \leq (1 + C_{0i}h_n)\, \|y(x_n) - y_n\| \tag{5.10}$$

with the same restriction on the step size and with $i = 1$ if (??) and (??) and $i = 2$ if (??) and (??) hold. C_{01} and C_{02} are defined by (??) and (??).

If we start the integration with the exact initial value y_0 then it follows from (??) – (??) (cf., e.g. [?], [?] or [?]) that

$$\|y(x_{n+1}) - y_{n+1}\| \leq C_{1i}(h_{min})\, h_{max}^{p+q}\, e^{C_{0i}(x_e - x_0)}(x_e - x_0) \tag{5.11}$$

and

$$\|y(x_{n+1}) - y_{n+1}\| \leq C_1\, h_{max}^{p+q}\, e^{C_{0i}(x_e - x_0)}(x_e - x_0)$$

with $h_{min} = \min h_i$ and $h_{max} = \max h_i \leq \min(h_{3i}, x_e - x_n)$. This means B-convergence of order $p+q$ for method (??). If we demand that

$$h_{max} \leq \min\left(h_{3i}, \left(\frac{r_W}{C_1\, e^{C_{0i}(x_e - x_0)}(x_e - x_0)}\right)^{\frac{1}{p+q}}, x_e - x_n\right),$$

then we also have (??) so that for all $n = 0, 1, \ldots$ the y_{n+1} are the solutions of method (??) for the corresponding function $f \in \mathcal{F}_i$. ∎

6 Asymptotic error estimates

Andreas Griewank [?] was the first who investigated the accuracy of the implicit Taylor, or HOP method as he it calls, applied to the test equation of Prothero and Robinson [?]. He discovered the, compared to other methods, favorable behavior of the asymptotic error: For the IVP

$$y' = \lambda\,(y - \varphi(x)) + \varphi'(x), \qquad y(x_0) = \varphi(x_0), \qquad \mathrm{Re}\,\lambda \le 0 \tag{6.1}$$

we have

$$(D_i\, y)(x,z) = \sum_{k=0}^{i-1} \lambda^k g^{(i-1-k)}(x) \qquad \text{for} \qquad i > 0.$$

If we apply method (**??**) with step size h to (**??**), and use the notation $z = \lambda h$, from (**??**) and (**??**) then we get the recursion

$$\varphi(x_{n+1}) - y_{n+1} = R_{pq}(z)\,(\varphi(x_n) - y_n) + Q_{pq}(z)^{-1}\,\delta_h(x_n) \tag{6.2a}$$

with

$$\delta_h(x_n) = (-1)^q\, c_{pq}\, h^{p+q+1} \varphi^{(p+q+1)}(\xi_n), \tag{6.2b}$$

which leads to the following formula for the global error:

$$\begin{aligned}\varphi(x_{n+1}) - y_{n+1} = R_{pq}(z)^{n+1}\,(\varphi(x_0) - y_0)& \\ + Q_{pq}(z)^{-1} \sum_{j=0}^{n} R_{pq}(z)^{n-j}\delta_h(x_j).&\end{aligned} \tag{6.3}$$

When solving stiff ODEs one is interested in step sizes h which are much larger than $|\lambda|^{-1}$. We therefore study the error under the assumption that simultaneously $h \to 0$ and $z = \lambda h \to \infty$. In Table **??**, we collect the results for the A- and L-stable methods. There, in the last column (variable h), the symbols h and z have to be interpreted as $\max h_i$ and $z = \lambda \min h_i$.
Verification of Table **??**.
The formulas for the local error follow immediately from (**??**) and from the definition of the function $Q_{pq}(z)$. In the case $0 < p = q$ it then follows from (**??**) (for constant and variable h) that the global error behaves like $\mathcal{O}(z^{-q})\,\mathcal{O}(h^{p+q})$ because of $|R_{pq}(z)| \le 1$. For odd p we have $R_{pp}(\infty) = -1$ and the global error estimate can be improved in the case of constant step sizes. This follows, as for the Gauss methods, from partial summation of the sum in (**??**) (c.f., e.g. [?, p. 242]). Since $R_{pq}(z) = \mathcal{O}(z^{p-q})$ for the L-stable methods, the error propagation in (**??**) is negligible and the local and global errors have the same asymptotic behavior. ■

Table 6.1: Error for (??) when $h \to 0$ and $z = \lambda h \to \infty$

Method	local error	global error	
		constant h	variable h
$0 < p = q \begin{cases} p & \text{odd} \\ p & \text{even} \end{cases}$	$z^{-q}\, h^{p+q+1}$	$\begin{cases} z^{-q}\, h^{p+q+1} \\ z^{-q}\, h^{p+q} \end{cases}$	$z^{-q}\, h^{p+q}$
$1 \leq q - p \leq 2$	$z^{-q}\, h^{p+q+1}$	$z^{-q}\, h^{p+q+1}$	$z^{-q}\, h^{p+q+1}$

Table 6.2: Error for classes $\mathcal{F}_1$ and $\mathcal{F}_2$ when $h \to 0$ and $z \to -\infty$

Class	Method	local error	global error (variable h)
$\mathcal{F}_1$	$0 < p = q$	$z^{-q}\, h^{p+q+1}$	$z^{-q}\, h^{p+q}$
$(z = \mu h)$	$1 \leq q - p \leq 2$	$z^{-q}\, h^{p+q+1}$	$z^{-q}\, h^{p+q+1}$
$\mathcal{F}_2$	$0 < p = q$	$z^{-q}\, h^{p+q+1}$	$z^{-q}\, h^{p+q}$
$(z = \lambda\mu h)$	$1 \leq q - p \leq 2$	$z^{-q}\, h^{p+q+1}$	$z^{-q}\, h^{p+q+1}$

If we put $z = \mu h$ for class $\mathcal{F}_1$ and $z = \lambda\mu h$ for class $\mathcal{F}_2$ then we get analogous estimates for the errors of method (??) applied to these classes of IVPs. These estimates are given in Table ??. In the last columns the symbols h and z again have to be interpreted as $\max h_i$ and $z = \mu \min h_i$ or $z = \lambda\mu \min h_i$ respectively.
Verification of Table ??.
The estimates for the local error follow immediately from (??) and from (??). From (??) and (??) we get the estimates for the global error for the A-stable methods. For the L-stable methods this estimate can be improved. For both classes we get the estimate

$$\|y(x_{n+1}) - y_{n+1}\| \leq \frac{\varphi_{R_{pq}}(z) + h\, G_2(z)}{1 - h\, G_1(z)} \|y(x_n) - y_n\| + \frac{1}{1 - h\, G_1(z)} \frac{1}{Q_{pq}(z)} c_{pq}\, h_n^{p+q+1} \|y^{(p+q+1)}\| \quad (6.4)$$

from (??). For $z \to -\infty$ we have $R_{pq}(z) = \mathcal{O}(z^{p-q})$ and $\varphi_{R_{pq}}(z) = \mathcal{O}(|z|^{p-q})$. Therefore, for L-stable methods the error propagation in (??) is negligible and the local and global errors have the same asymptotic behavior. ■

Appendix A

An estimate for $\|Q_{pq}(hA)^{-1}\|$

Let $Q_{pq}(z)$ be defined by (**??**). Simply by calculating the modulus of $Q_{pq}(iy)$ we get

Theorem 0.1. *At least for all* $0 \le p, q \le 16$ *with* $0 \le q - p \le 2$ *we have*

$$\min_{Rez \le 0} |Q_{pq}(z)| = Q_{pq}(0).$$

Proof. From the minimum principle it follows that

$$\min_{\mathrm{Re} z \le 0} |Q_{pq}(z)| = \min_{y \in \mathbb{R}} |Q_{pq}(iy)|.$$

With $\beta_j = \beta_j(p,q)$, defined by (**??**), for $0 \le j \le q$ let

$$a_j = a_j(p,q) := (-i)^j \beta_j, \qquad b_j = b_j(p,q) := i^j \beta_j,$$

and

$$c_j = c_j(p,q) := \sum_{k=0}^{j} a_{j-k}\, b_k, \quad d_j = d_j(p,q) := \sum_{k=0}^{j} a_{q-j+k}\, b_{q-k}.$$

With these abbreviations we have

$$\begin{aligned} |Q_{pq}(iy)|^2 &= Q_{pq}(iy)\, Q_{pq}(-iy), \\ &= \sum_{j=0}^{q} a_j\, y^j \sum_{j=0}^{q} b_j\, y^j, \\ &= \sum_{j=0}^{q} \sum_{k=0}^{j} a_{j-k}\, b_k\, y^j + \sum_{j=0}^{q-1} \sum_{k=0}^{j} a_{q-j+k}\, b_{q-k}\, y^{2q-j}, \end{aligned}$$

$$= \sum_{j=0}^{q} c_j\, y^j + \sum_{j=0}^{q-1} d_j\, y^{2q-j},$$

$$|Q_{pq}(iy)|^2 = \sum_{k=0}^{2k\le q} c_{2k}\, y^{2k} + \sum_{k=0}^{2k\le q-1} d_{2k}\, y^{2q-2k}.$$

In the Tables **??** and **??** the modified coefficients

$$\tilde{c}_{2k} = \frac{k!\,(p+q)!\binom{p+q}{k}}{p!\binom{q}{k}}\, c_{2k}$$

and

$$\tilde{d}_{2k} = \frac{k!\,((p+q)!)^2}{p!\,(p+k)!\,q!}\, d_{2k}$$

for $k = 0, 1, \ldots, 8$ are given. From these tables we see that for the p and q in which we are interested, the c_{2k} and d_{2k} are non-negative. ■

Corollary 0.1. *Assume that the matrix A satisfies (**??**) and $h\mu \le 0$. Then at least for all $0 \le p, q \le 16$ with $0 \le q - p \le 2$ we have*

$$\|Q_{pq}(hA)^{-1}\| \le \sup_{Re z \le h\mu} |Q_{pq}(z)^{-1}| = Q_{pq}(h\mu)^{-1}.$$

Proof. For Re $z \le 0$ the function $Q_{pq}(z)^{-1}$ is bounded and rational. Therefore for the special case $\mu = 0$ the statement of the Corollary follows immediately from Neumann's Theorem and from the Theorem given above. In the case $\mu < 0$ apply the special case to $\tilde{Q}_{pq}(z) = Q_{pq}(z + \mu)$ and $\tilde{A} = A - \mu I$. ■

Remark 0.1. Essential for the Proof of Theorem **??** is the non-negativity of the coefficients c_{2k} and d_{2k}. In order to save space they are given here only for $0 \le k \le 8$. But for larger p and q these coefficients are also non-negative. Experiments with the symbolic manipulation package Maple suggest that for all $k \ge 2$

$$c_{2k} = \frac{p!\binom{q}{k}}{k!\,(p+q)!\binom{p+q}{k}} \frac{(p+q-2k)!}{(p-k)!}$$

and

$$d_{2k} = \frac{p!\,(p+k)!\,q!}{k!\,((p+q)!)^2} \frac{(p+2k-q)!}{(p+k-q)!\,(q-k)!}$$

Table 0.1: Coefficients $\tilde{c}_{2k}$ for $k = 0, 1, \ldots, 8$.

$$
\begin{array}{lll}
\tilde{c}_0 = \dfrac{(p+q)!}{p!} & \tilde{c}_2 = \dfrac{(p+q-2)!\,p}{p!} & \tilde{c}_4 = \dfrac{(p+q-4)!}{(p-2)!} \\[2ex]
\tilde{c}_6 = \dfrac{(p+q-6)!}{(p-3)!} & \tilde{c}_8 = \dfrac{(p+q-8)!}{(p-4)!} & \tilde{c}_{10} = \dfrac{(p+q-10)!}{(p-5)!} \\[2ex]
\tilde{c}_{12} = \dfrac{(p+q-12)!}{(p-6)!} & \tilde{c}_{14} = \dfrac{(p+q-14)!}{(p-7)!} & \tilde{c}_{16} = \dfrac{(p+q-16)!}{(p-8)!}
\end{array}
$$

Table 0.2: Coefficients $\tilde{d}_{2k}$ for $k = 0, 1, \ldots, 8$.

$$
\begin{array}{lll}
\tilde{d}_0 = \dfrac{1}{q!} & \tilde{d}_2 = \dfrac{p+2-q}{(q-1)!} & \tilde{d}_4 = \dfrac{(p+4-q)!}{(p+2-q)!\,(q-2)!} \\[2ex]
\tilde{d}_6 = \dfrac{(p+6-q)!}{(p+3-q)!\,(q-3)!} & \tilde{d}_8 = \dfrac{(p+8-q)!}{(p+4-q)!\,(q-4)!} & \tilde{d}_{10} = \dfrac{(p+10-q)!}{(p+5-q)!\,(q-5)!} \\[2ex]
\tilde{d}_{12} = \dfrac{(p+12-q)!}{(p+6-q)!\,(q-6)!} & \tilde{d}_{14} = \dfrac{(p+14-q)!}{(p+7-q)!\,(q-7)!} & \tilde{d}_{16} = \dfrac{(p+16-q)!}{(p+8-q)!\,(q-8)!}
\end{array}
$$

holds, so that the estimates probably apply to A-stable Taylor series methods of any order.

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