Reprinted from

APPLIED NUMERICAL MATHEMATICS

Applied Numerical Mathematics 22 (1996) 35–49

Vienna contributions to the development of RK-methods

Winfried Auzinger*, Reinhard Frank, Hans J. Stetter

Institut für Angewandte und Numerische Mathematik, Technische Universität Wien, Wiedner Hauptstrasse 8-10/1152, A-1040 Vienna, Austria

ELSEVIER

ELSEVIER

Applied Numerical Mathematics 22 (1996) 35–49

APPLIED NUMERICAL MATHEMATICS

Vienna contributions to the development of RK-methods

Winfried Auzinger*, Reinhard Frank, Hans J. Stetter

Institut für Angewandte und Numerische Mathematik, Technische Universität Wien, Wiedner Hauptstrasse 8-10/1152, A-1040 Vienna, Austria

Abstract

In 1965, H.J. Stetter moved from his home in Munich to Vienna, to take a newly created chair for Numerical Mathematics at the Technical University of Vienna. At the Technical University of Munich, since 1953, he had grown up in one of the first major research groups in the new area of Numerical Analysis, with one of the first electronic computers available since 1955. His own interests had been strongly tied to the computational solution of initial value problems in both ordinary and partial differential equations. He took these interests with him to Vienna where they spread to his students and collaborators. Thus, a research group in ODEs originated at the Technical University in Vienna and RK-methods were an important objective. In the following, we sketch the related activities and achievements of this group from 1965 to these days.

The main emphasis has been given to the work related with stiff systems. In particular, Section 5 is devoted to a rather detailed discussion of the nature of stiffness and its implications on the convergence theory of RK-methods for nonlinear stiff problems from a point of view which has originated from the Vienna group since the late seventies.

Keywords: Runge–Kutta methods; Convergence theory; Defect correction

1. Asympotic expansions and composite RK-methods

H.J. Stetter had been involved in the use of Richardson extrapolation in a variety of situations: In Munich, he had used it in supersonic flow computations, during a sabbatical stay at UCLA, he had collaborated with W.B. Gragg who had just finished his thesis [26] on extrapolation for the explicit midpoint rule in ODEs, and he had been associated with the work of Gragg, Bulirsch and Stoer [8] on the generalized Romberg method. Stetter's general formulation [36] of a context in which asymptotic expansions of the global error of a discretization method prevail was a natural step. At first, the unrealistic assumption of constant steps was annoying; but the concept of *coherent grid sequences* [42, 2.1.5] was sufficiently general to extend the use of asymptotic expansions and Richardson extrapolation to many realistic situations.

* Corresponding author. E-mail: winfried@uranus.tuwien.ac.at.

PII S0168-9274(96)00024-4

This background explains why asymptotic expansions and Richardson extrapolation have been an important aspect of the numerical research in Vienna throughout. In the context of RK-methods, a new facet was introduced by J.C. Butcher during his stay in the fall of 1972. He introduced us to his very general approach to the consideration of composite methods. Three main types of composite RK-methods have been studied in Vienna:

(a) *Symmetric methods* which have asymptotic expansions in powers of h^2 for the global discretization error: It was shown [38,42] that each RK-formula has an inverse counterpart such that the combination of the two formulas generates a symmetric RK-method. (This generalizes the combination of the explicit and implicit Euler steps into the implicit trapezoidal and midpoint rules.) Since the inverse of an explicit formula is always implicit, the practical implications remained moderate; also there are well-known self-inverse and hence symmetric RK-formulas of high order, viz. the Gauss formulas.

(b) *Cyclic methods* which use two or more formulas in a cyclic fashion: The mechanism for generating methods whose order is higher than that of their parts has been described in [41]. It is mathematically interesting but not practical because the step size cannot be changed.

(c) *Effective order methods*: They had been introduced in Butcher's contribution to the 1969 Dundee Conference and remained mysterious from an analytic point of view: The possibility to obtain an $O(h^{p+1})$ correct solution value at an arbitrary point in an $O(h^p)$ correct computation implied an asymptotically correct global error estimate from *local data* for an arbitrary differential system! This appeared to contradict the fact that the lowest order part of the global error satisfies an initial value problem for the variational system and must depend on the *history* of the computation. It was finally found [39] that—for these particular combinations of RK-formulas—the error equation becomes an *exact* differential system such that the principal part of the global error is the invariant of the system and may thus be retrieved locally. (It also became clear that the same mechanism may be used more simply in linear multistep methods through particular combinations of predictors and correctors.)

2. Early stability concepts and stability regions

Although G. Dahlquist's pioneering paper [12] had appeared in 1963, the full impact of the stiffness phenomenon was not realized for many years. This may have been partially due to the convincing elegance and simplicity of Henrici's asymptotic error theory: For $h \to 0$, stiffness ceased to be a qualitative phenomenon. Thus the search for high-order methods with $(h \to 0)$-stability (the latter automatically present in RK-methods) was continued for a long time.

Only with growing numerical experience in real-life problems, it became clear that *stability for finite h* was necessary for reliable and economic computations. Various stability concepts were suggested in the literature: Besides the commonly accepted concept of absolute stability (no growth of a perturbation in the discretization), several concepts of *relative stability* were introduced. H.J. Stetter attempted to unify and generalize these concepts through his *strong stability* approach: The growth of a perturbation in the discretization was related to the growth of an analogous perturbation in the differential system, cf. [35,37] and related parts in [42]. More precisely, for a system with (linearized) local eigenvalues λ_j, $j = 1(1)n$, and $\mathrm{Re}(\lambda_1) \geqslant \mathrm{Re}(\lambda_j)$ for all j, an RK-discretization with growth function $\gamma(z)$ was called *locally strongly stable* (at some time t) if

$$|\gamma(h\lambda_j)| \leqslant \max\big(\exp(h\,\mathrm{Re}\,\lambda_1), |\gamma(h\lambda_1)|\big), \quad j = 2(1)n. \tag{1}$$

Related stability regions were plotted and analyzed; but the local character of the concept hindered its application to a wider class of problems.

Another attempt for a generalization was the consideration of *uniformly asymptotically stable* differential systems on "infinite" (= long) intervals. In [42], various concepts from the well-known theory of such dynamical systems were transferred to their discretizations. *Strong exponential stability* required that the properties of the dynamical systems should carry over to their discretizations, either for arbitrary steps or, at least, for steps below some h_0. For RK-methods, a number of positive and negative results were derived (see also [40]); useful results were essentially restricted to the implicit Euler method.

From today's point of view, (1) was a precursor of the order star approach, and investigations of discretization methods which preserve properties of dynamical systems constitute an important part of the research in numerical ODEs. In Vienna, the above considerations led to the important work of R. Frank and a varying group of collaborators on discretizations of stiff differential systems which will be reported in Section 5.

3. Defect correction and applications

At the 1973 Dundee conference, P.E. Zadunaisky, an Argentinian astronomer and numerical analyst, presented a method for the estimation of the global discretization error in numerical ODE integrations which used no explicit estimate of the local error (cf. also Section 4). He could not seriously prove his results; but his experimental data were so convincing that H.J. Stetter could not agree with the widespread low opinion of this idea. Back in Vienna, he was able to interest his collaborators in the analysis of Zadunaisky's approach. For several years, the research at the institute was dominated by the development of a thorough understanding and of new modes of application of what was—following a suggestion by Frank—soon called *defect correction*.

Zadunaisky's original recipe was the following (cf. [48]): Let the numerical integration of the given system $y' = f(t,y)$ generate the approximate values η_ν; then interpolate sets of $m+1$ successive η_ν componentwise by polynomials of degree m each and denote this piecewise polynomial vector function by P. Naturally, P satisfies the "pseudo-problem"

$$z'(t) = f\big(t, z(t)\big) + P'(t) - f\big(t, P(t)\big), \tag{2}$$

which is now integrated by the same numerical procedure on the previous grid yielding the values ζ_ν. Since the exact solution $z(t) = P(t)$ of the pseudo-problem is known, the global error of this auxiliary integration is simply $\zeta_\nu - P(t_\nu)$. This quantity is used as an estimate for $\eta_\nu - y(t_\nu)$, because of the closeness of the two problems and their solutions.

A first analysis of "Zadunaisky's method" was presented by Stetter two months later at a meeting on stiff differential systems because of the presence of a representative group of researchers in numerical ODEs. This analysis [43] was based on asymptotic expansions and proved the appropriateness of the procedure under suitable technical assumptions which were clearly satisfied for RK-methods. At the same time, the potential for an iterative use of this correction method was pointed out. A more detailed analysis, in particular including the important aspect how the approximation properties of the interpolation influence the respective order results, can be found in [16,17,19,20]. The iteration was now called *iterated defect correction method* (IDeC); the asymptotic orders of the iteration steps turned

out to be $O(h^{2p}), O(h^{3p}), \ldots$, where p denotes the order of the method the global error of which is estimated in the single iteration steps. Moreover, it turned out that the maximum attainable order is limited by m (the degree of the interpolating polynomial P used within the algorithm).

In [18,21,22] another type of analysis of IDeC methods was proposed. Instead of analyzing a fixed number of iteration steps asymptotically for $h \to 0$, the question was studied what happened on *fixed* grids if infinitely many iteration steps are performed. This led to an important breakthrough because it became clear that the iteration converges towards a fixed point which in most cases turns out to be a collocating polynomial. Thus, defect correction methods turned out to be potentially attractive stiff solvers, strongly reducing the dimension of the algebraic equations of fully-implicit, high-stage RK methods equivalent to collocation schemes. Further remarks concerning the applicability of the IDeC method in the context of stiff equations will be given in Section 5.3.

The observation that the fixed point of an IDeC iteration can be described independently of asymptotic expansions also showed that the technique was much more general and flexible than originally assumed. A formal description of defect correction techniques from a more general point of view was given in [45].

4. Step size control, global error estimates, ODE codes

In the mid-seventies, it had become clear that the performance of a *general purpose code* for the integration of systems of ODEs depended not only on the approximation quality and stability of its integrator, even with non-stiff systems. Since such a code should not require the specification of any parameters beyond those needed for the problem description (including some specification of the expected accuracy), it had to choose and monitor all procedure-oriented parameters automatically. Some implications of this commonly accepted design principle are still under discussion, notably the automatic switching between stiff and non-stiff integrators.

Regarding the step size selection for a fixed suitable integrator, the following natural requirement was proposed and analyzed, mainly by the Toronto and Vienna groups: For a given ODE problem with solution $y(t) \in \mathbb{R}^n$, the code should select its steps such that the computed values $\eta_\nu \in \mathbb{R}^n$ at the gridpoints t_ν satisfy

$$\|\eta_\nu - y(t_\nu)\| \approx E(t_\nu) \cdot \mathrm{TOL}, \tag{3}$$

where TOL is the value of a scalar accuracy parameter prescribed by the user, and the unknown problem dependent function $E(t)$ is *independent of* TOL. It was established (cf., e.g., [46]) that this *tolerance proportionality* requires the use of an asymptotically correct local error estimate and an error-per-unit-step control of the step size. It was also shown why an error-per-step control for the fictitious local error of a locally extrapolated solution may or may not satisfy (3). Today, a good deal of the available ODE codes strive to achieve tolerance proportionality. Also, this property is one of the criteria evaluated by the testbeds DETEST and STIFF DETEST [15]. Due to their one-step character, RK-codes attain (3) much easier than multistep codes.

Since $E(t)$ in (3) generally remains unknown, the choice of TOL cannot ensure a particular global error level, except through several integrations with different values of TOL. The more important is the (optional) generation of reliable a-posteriori *global error estimates* by the code. Various economic

ways were proposed and analyzed by H.J. Stetter around 1980 (see, e.g., [44]). For RK-codes, the following two procedures have remained useful until today:

(a) Integrators with an asymptotically correct local error estimate: Via a nonstandard application of defect correction, one can form a modified local error estimate such that the integration of the original problem perturbed by this estimate with an Euler integrator generates values permitting an asymptotically correct global error estimate.

(b) Integrators with local extrapolation: The use of a grid with pairs of successive equal steps permits a reintegration and valid Richardson extrapolation on the coarser grid with the equal steps combined into one step.

Step size selection is just one of several control decisions which an ODE code must perform. In connection with the studies of the tolerance proportionality mechanism, a principle for the analysis of decision and control procedures in ODE codes was developed and applied to various situations; see, e.g., [47].

5. Convergence theory of IRK methods for stiff problems

It is well known that certain classes of Implicit Runge–Kutta (IRK) schemes have favorable properties with regard to the numerical integration of stiff initial value problems, and quite a number of theoretical results concerning their convergence properties have been obtained in Vienna. The present section is not merely of a historical nature but includes a rather thorough discussion of the notion of stiffness from our particular point of view. Such a discussion is indispensable for a thorough understanding of our contributions to the convergence theory of RK-methods. An overview on current and forthcoming work on this topic is included at the end of this section.

5.1. Stiffness, notion and effects

Let us begin by recalling the notion of stiffness by means of a phenomenological description: An initial value problem is called stiff if the underlying ODE $y' = f(t, y)$ admits smooth solutions, with moderate derivatives, together with nonsmooth ("transient") solutions rapidly converging towards smooth ones. Stiff problems are assumed to be well-conditioned in a specific global sense (in contrast to the bad local condition which often occurs as a consequence of the transient behavior of nonsmooth solutions).

For linear systems $y' = Ay$ such a solution structure occurs if the matrix A possesses a so-called stiff spectrum, which means that there exist eigenvalues with large moduli all of which have a strongly negative real part. For nonlinear problems there is a long tradition to mathematically formalize stiffness by local linearization: A nonlinear ODE is usually called stiff at a point $\bar{y}$ if the Jacobian $f_y(\bar{y})$ has a stiff spectrum. However, in our opinion such a "definition" of nonlinear stiffness is quite inadequate; our actual investigations are based on a more natural, semi-global way of linearization. We will return to this discussion in Section 5.3.

Before presenting our contributions to the nonlinear stiff convergence theory, let us briefly recapitulate the reasons why classical convergence concepts do not satisfactorily cover stiff problems. This is necessary for an understanding of the ideas behind our theory.

Let η_ν denote an approximation for the exact solution value $y(t_\nu)$ at a grid point t_ν, obtained by a discretization scheme with step size h. A traditional convergence result (of order p) says that $\|\eta_\nu - y(t_\nu)\| = O(h^p)$ holds uniformly for $h \to 0$ for all sufficiently smooth problems, i.e., for problems where f has a sufficiently high degree of differentiability. Stiffness usually does not imply a lack of differentiability, and so the question arises why there should be a need for a particular stiff convergence theory. To motivate this need, let us consider the well-known explicit $O(h)$-error bound for the explicit Euler scheme:

$$\|\eta_\nu - y(t_\nu)\| \leqslant \frac{e^{Lt} - 1}{L} \frac{M_2}{2} h, \tag{4}$$

where L is a Lipschitz bound for f with respect to y and $\|y''(t)\| \leqslant M_2$ for all $t \in [0, T]$. For stiff problems we inevitably have $L \gg 0$, and the bound in (4) becomes very large except for extremely small h. This unsatisfactory error bound is realistic and simply reflects the well-known fact that the explicit Euler scheme is not able to satisfactorily integrate a stiff problem (but produces a strongly oscillating and exponentially increasing error except for extremely small step sizes h). On the other hand certain other, implicit methods (like certain classes of IRK schemes) are able to integrate stiff problems efficiently (on grids adjusted to the smoothness of the solution). Conventional convergence estimates in the spirit of (4) derived for these classes of IRK schemes are useless: Due to their dependence on L they are too pessimistic and do not realistically describe the actual error behavior observed in the stiff case. The crucial point with regard to a satisfactory error analysis is to characterize stiff problems by suitable parameters, *without reference to* L.

In the context of IRK schemes, a further difficulty arises in the *analysis of local errors*. The theory of Butcher trees (cf., e.g., [42]) yields a representation for local errors and is based on the so-called elementary differentials of the right hand side f. In these, the Jacobian f_y is involved, and therefore any local error estimate based on this approach is inevitably influenced by $L \gg 0$:

$$\|\text{local error}\| \leqslant C \cdot h^p, \tag{5}$$

where p is the classical order; but in the stiff case the bound (5) becomes useless because $C = C(L, \ldots) \gg 0$.

In [32], the local error of IRK schemes was systematically studied for a simple scalar model class. It turned out that the order observed for practically relevant step sizes is *reduced* compared to the classical order p; the latter is only observed for extremely small step sizes.

All these observations formed the starting point for a convergence analysis of IRK methods for a specific class of nonlinear stiff problems, including realistic local error estimates.

5.2. *One-sided Lipschitz constant and B-convergence*

For a nonlinear stiff convergence theory, the essential question is how to characterize a sufficiently comprehensive problem class by suitable parameters, avoiding the use the conventional Lipschitz constant L. In his talk given 1975 at the Dundee Conference (cf. [13]), Dahlquist proposed his idea to characterize f by the *one-sided Lipschitz constant* m defined via the one-sided Lipschitz condition

$$\langle y - z, f(t, y) - f(t, z) \rangle \leqslant m \|y - z\|^2. \tag{6}$$

In [13] the notion of one-sided Lipschitz continuity was used as the essential tool in the concept of G-stability, leading to an error analysis of linear multistep methods. In [10], Butcher caught on to this idea: He used the parameter m in the definition of B-stability for IRK schemes and verified this property for relevant classes of IRK schemes (e.g., of Gauss type). Furthermore, in [9] and independently in [11] the notion of algebraic stability was introduced—a natural condition on the coefficients of an IRK scheme which implies B-stability.

As explained above, stability considerations are not sufficient but a careful analysis of local errors is also indispensible, a gap which was closed by a team from Vienna (Frank, Schneid and Ueberhuber, cf. [23–25]). This resulted in the theory of B-convergence, where m is again the essential problem-characterizing parameter. The local error estimates require a refined stability concept called BS-stability, where (in contrast to B-stability) different perturbations are admitted in the individual stages of the IRK scheme. This special stability property can be concluded from a certain algebraic condition on the IRK coefficients, the so-called diagonal stability. Furthermore, in [23–25] positive values of m are admitted (while many other authors restrict their considerations to the dissipative case). Error bounds were derived for Gauss, Radau IA and Radau IIA schemes. The corresponding order of B-convergence is in accordance with the observations by Prothero and Robinson for their model problem (cf. [32]). B-convergence results for Lobatto IIIC schemes were presented in [33,34]. Furthermore, an algebraic characterization of B-convergent Runge–Kutta schemes was given in [29] for the class of problems satisfying the (rather stringent) condition that (6) holds for arbitrary pairs $y, z \in \mathbb{R}^n$.

In [14], Dekker and Verwer presented an overview on the "B-theory" of Runge–Kutta methods for stiff problems characterized by moderate values of m. Significant parts of [14] are devoted to the concept of B-convergence.

Solvability of the algebraic IRK equations

A further important question is concerned with the solvability of the algebraic IRK equations. For this purpose, a further stability concept (BSI-stability) was introduced in [24] to permit the application of the Newton–Kantorovich theorem. BSI-stability is an internal stability property permitting the estimation of the effects of individual perturbations on the internal IRK stages. However, these results are restricted to semi-linear stiff problems $y' = Ay + \phi(t, y)$ with a smooth nonlinearity ϕ.

The solvability of the IRK equations was also studied by a number of other authors; the respective results, however, suffer from the strongly restrictive assumption of global dissipativity (one-sided Lipschitz continuity with $m < 0$ or $m \leqslant 0$ for arbitrary pairs $y, z \in \mathbb{R}^n$). One contribution is due to Kraaijevanger and Schneid (cf. [30]); further results were obtained by Crouzeix, Dekker, Hundsdorfer, Raviart, Spijker, and others (cf., e.g., [14]). More general results for nonlinear problems under realistic local assumptions appear not to be available so far.

Asymptotic error expansions

In the theory of discretization methods, not only bounds for the global errors are derived but also assertions concerning the structure of the global error (asymptotic expansions) are of interest and form the basis for the analysis of acceleration techniques and the design of algorithmic control mechanisms. For stiff problems, asymptotic error expansions are a difficult topic and so far only results for specific problem classes and for simple schemes like implicit Euler, implicit midpoint rule, implicit trapezoidal rule are available. Relevant results have been obtained in Vienna (cf. [1–4]) and also by Hairer and Lubich (cf. [27]).

The point is that the stiffness causes certain imperfections of the error structure: In contrast to non-stiff problems, where one-step methods admit pure asymptotic error expansions, the inherent non-

smoothness of stiff problems gives rise to perturbations. For strongly stable methods like implicit Euler, these perturbations are exponentially descreasing; for the midpoint and trapezoidal rules oscillations occur.[1] The conseqence of these imperfections on the performance of acceleration techniques (extrapolation, defect correction) was studied and demonstrated in [3,4].

The relevance of the one-sided Lipschitz condition in the analysis of stiff problems

All results obtained within the "B-theory" described above rely on the one-sided Lipschitz constant m (cf. (6)) as the essential problem-characterizing parameter. The idea to characterize stiff problems in this way can be motivated by the following considerations: In contrast to the conventional Lipschitz constant $L \in \mathbb{R}^+$, which always becomes large if $f(t,y)$ is strongly varying with respect to varying y, the one-sided Lipschitz constant $m \in \mathbb{R}$ becomes only large and positive if there exist pairs of points y_0, z_0 such that the difference of the solutions $y(t), z(t)$ of the ODE $y' = f(t,y)$ satisfying the initial conditions $y(t_0) = y_0$, $z(t_0) = z_0$ is strongly increasing. In the trivial scalar case $y' = \lambda y$, for instance, we clearly have $L = |\lambda|$ while $m = \lambda$. For systems of ODEs, solutions may be approaching each other in a "spiraling" way, and it is natural to use an inner product to characterize f-differences: In

$$\langle y - z, f(t,y) - f(t,z) \rangle = \|y - z\| \cdot \|f(t,y) - f(t,z)\| \cdot \cos\alpha, \tag{7}$$

where α denotes the angle between $y - z$ and $f(t,y) - f(t,z)$, $\cos\alpha$ becomes negative in the case of converging solutions (i.e., if the difference $f(t,y) - f(t,z)$ has a component opposite to $y - z$). In particular, *rapidly* converging solutions are compatible with moderate (not strongly positive) values of m. A simple calculation shows

$$\frac{\mathrm{d}}{\mathrm{d}t}\|y(t) - z(t)\| = \frac{\langle y(t) - z(t), f(t,y(t)) - f(t,z(t)) \rangle}{\langle y(t) - z(t), y(t) - z(t) \rangle}\|y(t) - z(t)\| \leqslant m\|y(t) - z(t)\|, \tag{8}$$

such that $\|y(t) - z(t)\|$ can be estimated by $\mathrm{e}^{m(t-t_0)}\|y_0 - z_0\|$. Moreover it can be shown that the optimal (smallest possible) value of m with respect to an infinitesimal neighborhood of a point y_0 locally *characterizes* the condition of the initial value problem, i.e., there exists z_0 near y_0 such that the estimate is locally sharp, i.e., $\|y(t) - z(t)\| \doteq \mathrm{e}^{m(t-t_0)}\|y_0 - z_0\|$ for $t \downarrow t_0$. Therefore stability and error bounds based on the parameter m as obtained in the B-theory appear natural and optimal.

Concerning the relevance of the B-theory for stiff problems, however, there remains a gap which was overlooked for a long time: The point is that for most stiff problems there is a strong discrepancy between the local and the global condition: For certain perturbations, a strong local *increase* of the difference of neighboring solutions can occur, such that the problem is locally ill-conditioned. These increases live only on very short t-intervals, leaving the global condition unaffected. But the local effect inevitably implies that the one-sided Lipschitz constant m is *strongly positive*. A typical, linear example is shown in Fig. 1.

Example (see Fig. 1). In this example, A is nonsymmetric with a non-stiff eigenvalue and a stiff eigenvalue $\lambda \ll 0$. Transient solutions are rapidly varying in vertical direction (= stiff eigendirection). Due to the fact the eigendirections are not orthogonal, many of the transient solutions are rapidly

[1] The situation is similar as already observed for multistep methods applied to non-stiff problems (cf., e.g., [26]).

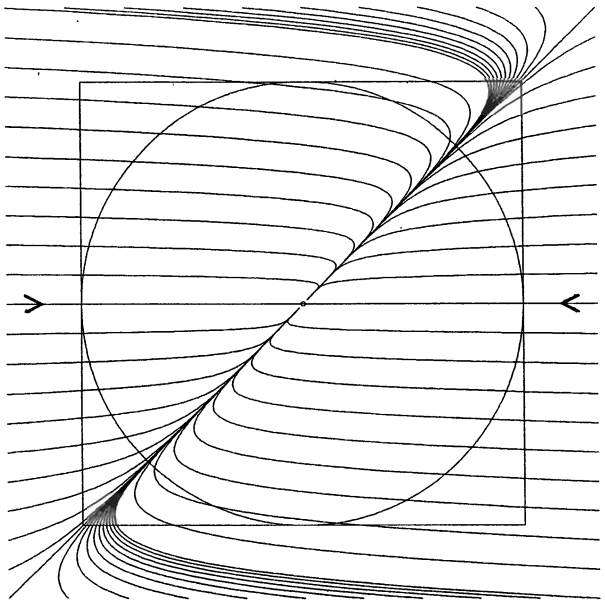

Fig. 1. Phase portrait of a stiff 2×2-system $y' = Ay$.

increasing with respect to the L_2-norm before becoming smooth. Consequently, the difference of the solutions starting at

$$y_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ (equilibrium)} \quad \text{and} \quad z_0 = \begin{pmatrix} -k \\ 0 \end{pmatrix}$$

increases very fast:

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(z(t) - y(t)\big)\big|_{t=0} = \frac{\mathrm{d}}{\mathrm{d}t}z(t)|_{t=0} = A \cdot \begin{pmatrix} -k \\ 0 \end{pmatrix} = \mathrm{O}(|\lambda|).$$

This indicates the very bad local condition of the problem, such that $m = \mathrm{O}(|\lambda|) \gg 0$. Nevertheless, the difference $\|y(t) - z(t)\|$ remains moderate for all t, indicating that the very fast local increase does not contradict the good global condition.

For a more detailed discussion we refer to [5], where it has been shown that m remains moderate only for a very restricted class of stiff problems, namely those where the Jacobians are very close to

normal throughout. In general, however, m is very large and positive, i.e., affected by the stiffness, and therefore the B-convergence bounds based on the parameter m become unrealistically large.

For linear problems $y' = Ay$ where the matrix of (generalized) eigenvectors is well-conditioned, this difficulty can be overcome by means of an elliptic vector norm carefully adapted to the eigendirections of A. In the nonlinear case, however, it appears impossible to find a fixed elliptic norm such that the corresponding one-sided Lipschitz constant is moderate uniformly in the region considered.

5.3. Recent developments

As just mentioned, the one-sided Lipschitz constant m is very often strongly positive, such that the B-theory appears much more restrictive than usually believed. In the analysis of stiff systems, an alternative approach is to consider stiff problems in singular perturbation form; a number of theoretical results for this class are available (for an overview of results, cf., e.g., [28]; see also [31]). However, stiff ODEs in singular perturbation form have a special geometry; in particular, the variation of the "stiff eigendirections" is only $O(\varepsilon)$ ($\varepsilon \ll 1$), such that the phase portrait resembles that of a linear constant coefficient problem.

As a consequence of these observations, it can be seen that even linear stiff problems of the form $y' = A(t)y$ are neither covered by the B-theory nor by the singular perturbation approach. This motivated the paper [6], where the B-theory was extended to a class of semilinear problems with strongly positive m: Satisfactory global error bounds were derived for semi-linear stiff problems $y' = A(t)y + \phi(t, y)$ where $A(t)$ has a smoothly varying eigensystem and where $\phi(t, y)$ is smooth (with a moderate Lipschitz constant). However, this extension of the B-theory is too weak to cover a sufficiently large class of practically relevant nonlinear problems.

With this background in mind, we have been striving for a more comprehensive theory. Here the point is to describe stiffness axiomatically in a way which can be considered as a natural formalization of the qualitative, phenomenological notion of stiffness.[2] The basic idea is to respresent discretization errors as a sum of "smooth" and "stiff" components. The natural underlying assumption is the existence of an *invariant smooth solution manifold* $\mathcal{M} \in \mathbb{R}^n$; furthermore, the idea of linearization is not applied locally but in a more natural, semi-global way: Instead of considering the Jacobians in single points y, each point y is associated with another point $u \in \mathcal{M}$ such that $y - u$ can be considered as a linear combination of stiff eigendirections in a generalized sense: Consider the identity

$$f(y) - f(u) = J(y,u) \cdot (y - u), \quad \text{where } J(y,u) := \int_0^1 f_y\big(u + \tau(y-u)\big)\, \mathrm{d}\tau. \tag{9}$$

For each y, a point u on $\mathcal{M}$ is determined by the requirement that $y - u$ is a linear combination of stiff eigendirections of $J(y,u)$ only. (Here we refer to the usual notion of a stiff eigendirection corresponding to a stiff eigenvalue λ with $\mathrm{Re}\,(\lambda) \ll 0$; but we apply this definition to the "generalized Jacobian" $J(y,u)$ instead of the local Jacobians f_y.)

[2] In the following we restrict our considerations to autonomous systems $y' = f(y)$.

For an illustration of this approach, consider the case where $\mathcal{M}$ is of dimension $n-1$ (n denoting the dimension of the given ODE system). Here the above requirement specializes as follows: For y in a neighborhood of $\mathcal{M}$, determine $u \in \mathcal{M}$ via

$$f(y) - f(u) = \lambda(y) \cdot (y - u), \quad \text{with } \lambda(y) \ll 0. \tag{10}$$

The quantities $\lambda(y)$ respectively $y - u$ are the stiff eigenvalue respectively eigenvector of the corresponding matrix $J(y,u)$.

This semi-global way of linearization forms the basis for our new nonlinear convergence theory using a new formalization of stiffness: Instead of calling a problem stiff at a point y if the local Jacobian f_y has a stiff spectrum, we define stiffness at y via (9), or via (10) in the case $\dim(\mathcal{M}) = n-1$. In the latter case we call a problem stiff if $u = u(y) \in \mathcal{M}$ and $\lambda(y)$ are well-defined by (10) for all y in a certain $O(1)$-neighborhood of $\mathcal{M}$ and if indeed $\lambda(y) \ll 0$. Together with some further natural requirements (e.g., the angle between $y - u$ and $\mathcal{M}$ must not be too small and the stiff eigendirections must be smoothly varying), it is indeed possible to derive convergence results for the relevant classes of IRK schemes.

For a visualization, let us consider the following example:

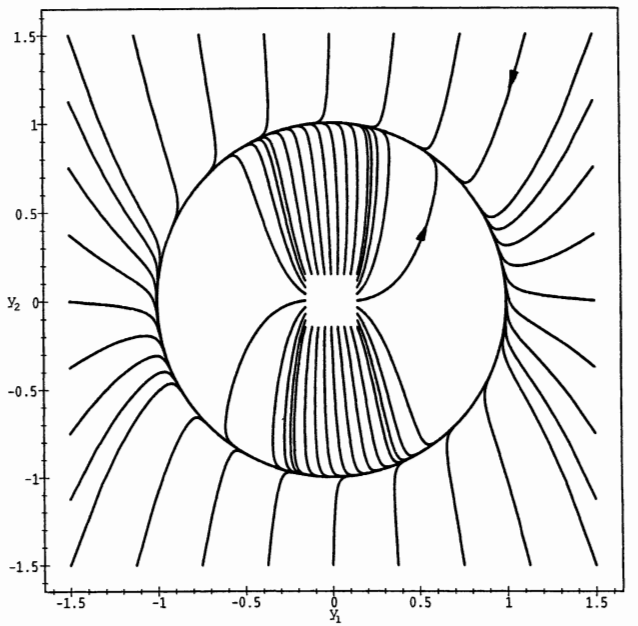

Fig. 2. Phase portrait for example (11).

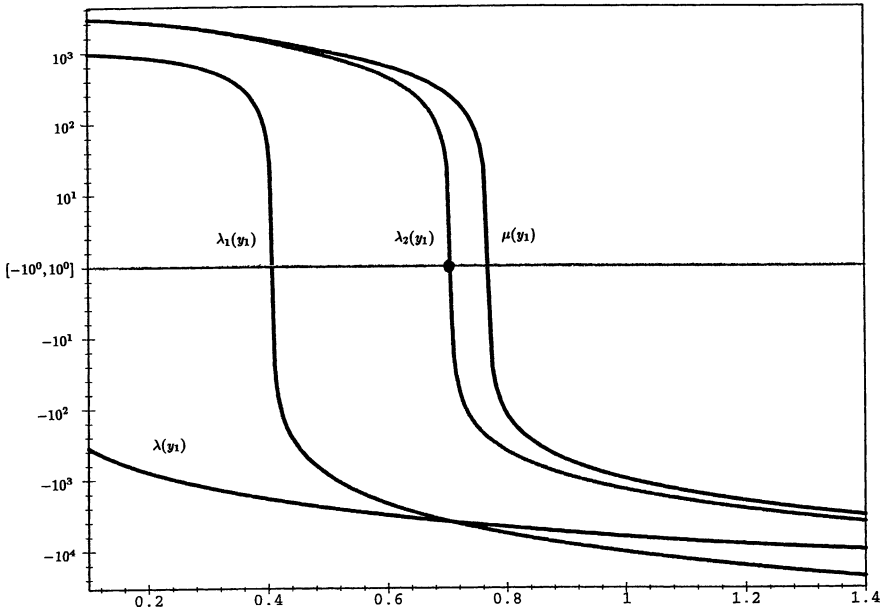

Fig. 3. Eigenvalues and logarithmic norm of the Jacobian and $\lambda(y)$ for example (11).

$$\begin{aligned} y_1' &= -y_2 - \lambda y_1\left(1 - y_1^2 - y_2^2\right), \\ y_2' &= y_1 - \rho\lambda y_2\left(1 - y_1^2 - y_2^2\right), \end{aligned} \tag{11}$$

where $\lambda \ll 0$ characterizes the stiffness and ρ is a moderate positive parameter. For $\lambda = -10$ and $\rho = 3$ the phase portrait is shown in Fig. 2 (the rather moderate value $\lambda = -10$ has been chosen to make the behavior of transient solutions more visible). Obviously, Eq. (11) shows the typical qualitative stiffness properties: The circle $y_1^2 + y_2^2 = 1$ represents an invariant manifold $\mathcal{M}$ on which smooth solutions persist; any other solution starting from an arbitrary point $(y_1, y_2) \in \mathbb{R}^2\backslash(0,0)$ rapidly converges towards such a smooth solution. In this sense (11) is stiff, with $\mathbb{R}^2\backslash(0,0)$ as basin of attraction for $\mathcal{M}$.

Fig. 3 illustrates the spectral behavior of the local Jacobians and displays the quantity $\lambda(y)$ (cf. (10)) for this example. Here, for $\lambda = -10^3$ and $\rho = 3$ the eigenvalues λ_1, λ_2, the logarithmic norm[3] μ of the Jacobian and the quantity $\lambda(y)$ are considered as functions of y_1, along the straight line $y_2 = y_1$ $(0 < y_1 \leqslant 1.4)$. In Fig. 3 the point $y_1 = \sqrt{2}/2$, where $y_2 = y_1$ intersects $\mathcal{M}$, is marked by a bullet. Up to $y_1 \approx 0.4$, λ_1, λ_2 and μ are strongly positive, and the Jacobian does not possess a stiff

[3] Here, μ denotes the logarithmic norm of the Jacobian without restriction to the L_2-norm. Note that μ is the locally optimal one-sided Lipschitz constant without restriction to this norm.

spectrum, although this neighborhood of $(0,0)$ belongs to the basin of attraction of $\mathcal{M}$. Moreover, λ_2 remains strongly positive even very close to $\mathcal{M}$. Thus, not even in a very close neighborhood of $\mathcal{M}$ the Jacobian possesses a stiff spectrum. Furthermore, μ remains strongly positive in a O(1)-neighborhood of $\mathcal{M}$, up to $y_1 \approx 0.8$. In contrast this behavior of the local Jacobians, it can be seen that $\lambda(y)$ remains strongly negative throughout, reflecting the fact that the "transversality condition" (10) is satisfied for all y in the basin of attraction of $\mathcal{M}$.

Numerical evidence shows that the common stiff solvers integrate equation (11) without any difficulties; but none of the conventional theoretical concepts (B-theory, singular perturbation approach) can be used to explain this behavior. Our present approach based on the semi-global linearization concept explained above, however, is sufficiently comprehensive to cover problems with a general nonlinear stiff geometry as in example (11). In [7] (Part I of a series of papers) our basic ideas have been introduced and illustrated under simplified assumptions: Only the implicit Euler scheme is studied, and the considerations are restricted to the case where $\mathcal{M}$ is of dimension $n-1$. In forthcoming papers we shall study the convergence properties of higher-order IRK schemes, together with the locally unique solvability of the respective algebraic equations. The more general problem class with an $(n-k)$-dimensional smooth solution manifold, will be considered.

Concerning order reduction effects in the context of higher order IRK schemes, our new theory reveals some interesting phenomena: It turns out that only the stiff error components are affected by order reductions, whereas the smooth components show the full classical order of superconvergence (similarly as in the case of singularly perturbed models; cf., e.g., [28]).

The performance of codes based on IRK schemes crucially depends on the way the algebraic equations are solved. An efficient approach is iterated defect correction (IDeC, cf. Section 3), an iterative procedure the fixed point of which is the collocating polynomial corresponding to the Runge–Kutta solution (cf. [22]). The implicit equations involved in the IDeC iteration are only of the dimension n (number of given ODEs) in contrast to $n \times s$ for direct solution of the IRK equations (s being the number of IRK stages). However, up to now the applicability of the IDeC approach was restricted to schemes with equidistant internal abscissas, because otherwise the IDeC iteration as proposed in [22] does not converge. This excludes relevant methods like Gauss or Radau schemes. However, in the meantime we have found a way to modify the IDeC algorithm which gives rapid convergence also for non-equidistant collocation abscissas. For stiff problems, the theoretical foundation of this observation is still incomplete; however, together with the superconvergence properties of the smooth error components this gives rise to the hope that such an algorithm may solve a stiff problem in an extremely efficient way.

References

[1] W. Auzinger and R. Frank, Asymptotic error expansions for stiff equations: an analysis for the implicit midpoint and trapezoidal rules in the strongly stiff case, *Numer. Math.* 56 (1989) 469–499.

[2] W. Auzinger, R. Frank and F. Macsek, Asymptotic error expansions for stiff equations: the implicit Euler scheme, *SIAM J. Numer. Anal.* 27 (1990) 67–104.

[3] W. Auzinger, R. Frank and G. Kirlinger, Asymptotic error expansions for stiff equations: applications, *Computing* 43 (1990) 223–253.

[4] W. Auzinger, On error structures and extrapolation for stiff systems, with application in the method of lines, *Computing* 44 (1990) 331–356.

[5] W. Auzinger, R. Frank and G. Kirlinger, A note on convergence concepts for stiff problems, *Computing* 44 (1990) 197–208.
[6] W. Auzinger, R. Frank and G. Kirlinger, An extension of B-convergence for Runge–Kutta methods, *Appl. Numer. Math.* 9 (1992) 91–109.
[7] W. Auzinger, R. Frank and G. Kirlinger, Extending convergence theory for nonlinear stiff problems I, *BIT*, to appear.
[8] R. Bulirsch and J. Stoer, Fehlerabschätzungen und Extrapolation mit rationalen Funktionen bei Verfahren vom Richardson-Typus, *Numer. Math.* 6 (1964) 413–427.
[9] K. Burrage and J.C. Butcher, Stability criteria for implicit Runge–Kutta methods, *SIAM J. Numer. Anal.* 16 (1979) 46–57.
[10] J.C. Butcher, A stability property of implicit Runge–Kutta methods, *BIT* 15 (1975) 358–361.
[11] M. Crouzeix, Sur la B-stabilité des méthodes de Runge–Kutta, *Numer. Math.* 32 (1979) 75–82.
[12] G. Dahlquist, A special stability problem for linear multistep methods, *BIT* 3 (1963) 27–43.
[13] G. Dahlquist, Error analysis for a class of methods for stiff nonlinear initial value problems, in: *Numerical Analysis*, Lecture Notes in Mathematics 506 (Springer, Berlin, 1976) 60–72.
[14] K. Dekker and J.G. Verwer, *Stability of Runge–Kutta Methods for Stiff Nonlinear Differential Equations* (North-Holland, Amsterdam, 1984).
[15] W.H. Enright and J.D. Pryce, Two Fortran packages for assessing initial value methods, *ACM Trans. Math. Software* 13 (1987) 1–27.
[16] R. Frank, Schätzungen des globalen Diskretisierungsfehlers bei Runge–Kutta-Methoden, in: International Series Numerical Mathematics 27 (Birkhäuser, Basel, 1975) 45–70.
[17] R. Frank and C.W. Ueberhuber, Iterated defect correction for Runge–Kutta methods, Report No. 14/75, Institute for Applied and Numerical Mathematics, Technical University of Vienna (1975).
[18] R. Frank and C.W. Ueberhuber, Iterated defect correction for the efficient solution of stiff systems of ordinary differential equations, Report No. 17/76, Institute for Applied and Numerical Mathematics, Technical University of Vienna (1976) (extended version of [22]).
[19] R. Frank, The method of iterated defect-correction and its application to two-point boundary value problems I, *Numer. Math.* 25 (1976) 409–419.
[20] R. Frank, The method of iterated defect-correction and its application to two-point boundary value problems II, *Numer. Math.* 27 (1977) 407–420.
[21] R. Frank and C.W. Ueberhuber, Collocation and iterated defect correction, in: Lecture Notes in Mathematics 631 (Springer, Berlin, 1976) 19–34.
[22] R. Frank and C.W. Ueberhuber, Iterated defect-correction for the efficient solution of stiff systems of ordinary differential equations, *BIT* 17 (1977) 146–159.
[23] R. Frank, J. Schneid and C.W. Ueberhuber, The concept of B-convergence, *SIAM J. Numer. Anal.* 18 (1981) 753–780.
[24] R. Frank, J. Schneid and C.W. Ueberhuber, Stability properties of implicit Runge–Kutta methods, *SIAM J. Numer. Anal.* 22 (1985) 497–515.
[25] R. Frank, J. Schneid and C.W. Ueberhuber, Order results for implicit Runge–Kutta methods applied to stiff systems, *SIAM J. Numer. Anal.* 22 (1985) 515–534.
[26] W.B. Gragg, On extrapolation algorithms for ordinary initial value problems, *SIAM J. Numer. Anal.* 2 (1965) 384–403.
[27] E. Hairer and C. Lubich, Extrapolation at stiff differential equations, *Numer. Math.* 52 (1988) 377–400.
[28] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II. Stiff and Differential–Algebraic Problems* (Springer, Berlin, 1991).
[29] W.H. Hundsdorfer and J. Schneid, An algebraic characterization of B-convergent Runge–Kutta methods, *Numer. Math.* 56 (1990) 695–705.

[30] J.F.B.M. Kraaijevanger and J. Schneid, On the unique solvability of the Runge–Kutta equations, *Numer. Math.* 59 (1991) 129–157.
[31] K. Nipp and D. Stoffer, Invariant manifolds and global error estimates of numerical integration schemes applied to stiff systems of singular perturbation type, *Numer. Math.*, to appear.
[32] A. Prothero and A. Robinson, On the stability and accuracy of one-step methods for solving stiff systems of ordinary differential equations, *Math. Comp.* 28 (1974) 145–162.
[33] J. Schneid, B-convergence of Lobatto IIIC formulas, *Numer. Math.* 51 (1987) 229–235.
[34] J. Schneid, On the maximum order of optimal B-convergence of Lobatto IIIC schemes, *Computing* 39 (1987) 175–181.
[35] H.J. Stetter, A study of strong and weak stability in discretization algorithms, *SIAM J. Numer. Anal.* 2 (1965) 265–280.
[36] H.J. Stetter, Asymptotic expansions for the error of discretization algorithms for nonlinear functional equations, *Numer. Math.* 7 (1965) 18–31.
[37] H.J. Stetter, Stabilitätsbereiche bei Diskretisierungsverfahren für Systeme gewöhnlicher Differentialgleichungen, in: International Series Numerical Mathematics 9 (Birkhäuser, Basel, 1968) 157–167.
[38] H.J. Stetter, Symmetric two-step algorithms for ordinary differential equations, *Computing* 5 (1970) 267–280.
[39] H.J. Stetter, Local estimation of the global discretization error, *SIAM J. Numer. Anal.* 8 (1971) 512–523.
[40] H.J. Stetter, Stability of discretizations on infinite intervals, in: *Proceedings of Conference on Applications of Numerical Analysis*, Lecture Notes in Mathematics 228 (Springer, Berlin, 1971) 207–222.
[41] H.J. Stetter, Cyclic finite-difference methods for ordinary differential equations, in: *Proceedings of Conference on the Numerical Solution of Differential Equations*, Lecture Notes in Mathematics 363 (Springer, Berlin, 1973) 134–143.
[42] H.J. Stetter, *Analysis of Discretization Methods for Ordinary Differential Equations*, Springer Tracts in Natural Philosophy 23 (Springer, New York, 1973).
[43] H.J. Stetter, Economical global error estimation, in: *Stiff Differential Systems* (Plenum, New York, 1974) 245–258.
[44] H.J. Stetter, Global error estimation in ODE-solvers, in: *Numerical Analysis*, Lecture Notes in Mathematics 630 (Springer, Berlin, 1978) 179–189.
[45] H.J. Stetter, The defect correction principle and discretization methods, *Numer. Math.* 29 (1978) 425–443.
[46] H.J. Stetter, Tolerance proportionality in ODE-codes, in: *Proceedings Symposium on ODEs*, University of Illinois, Urbana (1979).
[47] H.J. Stetter, Modular analysis of numerical software, in: *Numerical Analysis*, Lecture Notes in Mathematics 773 (Springer, Berlin, 1980) 133–145.
[48] P.E. Zadunaisky, On the estimation of errors propagated in the numerical integration of ODEs, *Numer. Math.* 27 (1976) 21–39.