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Stability of the Richardson Extrapolation combined with some implicit Runge–Kutta methods

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ABSTRACT

The implementation of the Richardson Extrapolation in combination with different numerical methods for solving systems of ordinary differential equations (ODEs) is relatively simple, but the important requirement for stability of the computational process may cause serious difficulties. For example, the commonly used by scientists and engineers Trapezoidal Rule has good stability properties, but its combination with the Richardson Extrapolation is unstable. Therefore, it is necessary to study in advance and very carefully the stability of the new numerical methods arising when the scientists and the engineers use this computational device in combination with different algorithms for solving systems of ODEs.

We are presenting a systematic investigation of the implementation of Richardson Extrapolation for two implicit Runge–Kutta methods. Three numerical examples, including an atmospheric chemical scheme used successfully in several extensive environmental studies and described mathematically by a very stiff and badly scaled nonlinear system of ODEs, are presented to illustrate the advantages of the presented approach. The numerical results show that not only are the computations stable, but also the achieved accuracy is higher when the Richardson Extrapolation is additionally applied. It will be possible to derive similar stability and accuracy results for other implicit Runge–Kutta methods.

1. Statement of the problem

Consider the initial-value problem for first-order nonlinear systems of ordinary differential equations, ODEs, described in the following way:

$$\frac{dy}{dt} = f(t, y), \quad t \in [a, b], \ a < b, \ y \in \mathbb{R}^s, \ s \geq 1, \ f \in D \subset \mathbb{R} \times \mathbb{R}^s, \ y(a) = \eta, \tag{1}$$

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where

(a) t is the independent variable (in most of the problems arising in physics and engineering t is the time-variable),
(b) the positive integer s is the number of equations
(c) f is a given function (it will be assumed that f is a *one-valued* function in the whole domain D)

and

(d) the unknown function $y = y(t)$ is a real vector of dimension s that depends of the time-variable t.

Assume that the system defined by (1) is stiff. Then special methods, which are necessarily implicit, because of the second Dahlquist barrier, [1], should be used in the solution process in order to ensure (or, at least, to try to ensure) the robustness of the computational process.

It is highly desirable to select numerical methods, which have good stability properties. In fact, this is not only desirable, but also must be satisfied when the system of ODEs is very stiff. A-stable, strongly A-stable or L-stable methods are very popular and commonly used. It is not necessary to describe here in detail the properties of these numerical methods, because such information can be found in relevant textbooks on numerical solution of systems of ODEs (see, for example, [2–7]), but two facts are very important and must be emphasized:

(a) all these methods are, as mentioned above, implicit

and

(b) their absolute stability regions contain the whole $\mathbb{C}^-$, i.e. the part of the complex plane located to the left of the imaginary axis.

The second of these two facts, condition (b), ensures the stability of the computational process, for any choice of the time-stepsize, but only in the very special case where the *scalar and linear* test-problem $dy/dt = \lambda y,\ t \in [0, \infty], y \in \mathbb{C}, \lambda = \alpha + \beta i \in \mathbb{C},\ \alpha \leq 0, y(0) = \eta \in \mathbb{C}$ proposed in 1963 by G. Dahlquist in [1], is solved. One should expect that if the numerical method is stable for this simple test-problem, then it is stable also when other problems are treated numerically (see, for example, Remark 13 on p. 37 in [6]).

In the remaining part of this paper, we shall assume that

(A) implicit Runge–Kutta methods with good stability properties are used in the numerical treatment of the system of ODEs described by (1)

and

(B) the Richardson Extrapolation is additionally implemented in an attempt to improve the accuracy of the results.

We shall study the stability properties of *the new numerical methods* obtained when the Richardson Extrapolations is combined with some *stable* implicit Runge–Kutta methods.

2. Implicit Runge–Kutta methods

Implicit Runge–Kutta Methods can be introduced by the following formula:

$$y_n = y_{n-1} + h \sum_{i=1}^{m} c_i k_i^n. \tag{2}$$

The coefficients c_i are given constants (the requirement to achieve at least first-order of accuracy implies that the sum of the coefficients c_i should be equal to one), while at an arbitrary time-step n the stage vectors k_i^n are defined by

$$k_i^n = f\left(t_{n-1} + ha_i, y_{n-1} + h \sum_{j=1}^{m} b_{ij} k_j^n\right), \quad a_i = \sum_{j=1}^{m} b_{ij},\ i = 1, 2, 3, \ldots, m \tag{3}$$

where b_{ij} are also some given constants, which depend on the particular numerical method.

Several alternative, but in some of the cases equivalent, formulations of implicit Runge–Kutta methods can be found for example in [3–6].

The numerical method defined by the equalities (2) and (3) is an m-stage Fully Implicit Runge–Kutta (FIRK) Method. The implicitness arises in (3), because the stage vectors k_i^n appear in both sides of these m relationships. This implies that at every time-step we have to solve a system of ms algebraic equations, which is in general nonlinear.

The FIRK Methods have two major advantages:

(a) high order of accuracy can, in principle, be achieved

and

(b) numerical schemes from this class, which have very good stability properties, can be derived.