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Global error estimation based on the tolerance proportionality for some adaptive Runge–Kutta codes ☆

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Abstract

Modern codes for the numerical solution of Initial Value Problems (IVPs) in ODEs are based in adaptive methods that, for a user supplied tolerance δ, attempt to advance the integration selecting the size of each step so that some measure of the local error is $\simeq \delta$. Although this policy does not ensure that the global errors are under the prescribed tolerance, after the early studies of Stetter [Considerations concerning a theory for ODE-solvers, in: R. Burlisch, R.D. Grigorieff, J. Schröder (Eds.), Numerical Treatment of Differential Equations, Proceedings of Oberwolfach, 1976, Lecture Notes in Mathematics, vol. 631, Springer, Berlin, 1978, pp. 188–200; Tolerance proportionality in ODE codes, in: R. März (Ed.), Proceedings of the Second Conference on Numerical Treatment of Ordinary Differential Equations, Humbold University, Berlin, 1980, pp. 109–123] and the extensions of Higham [Global error versus tolerance for explicit Runge–Kutta methods, IMA J. Numer. Anal. 11 (1991) 457–480; The tolerance proportionality of adaptive ODE solvers, J. Comput. Appl. Math. 45 (1993) 227–236; The reliability of standard local error control algorithms for initial value ordinary differential equations, in: Proceedings: The Quality of Numerical Software: Assessment and Enhancement, IFIP Series, Springer, Berlin, 1997], it has been proved that in many existing explicit Runge–Kutta codes the global errors behave asymptotically as some rational power of δ. This step-size policy, for a given IVP, determines at each grid point t_n a new step-size $h_{n+1} = h(t_n; \delta)$ so that $h(t; \delta)$ is a continuous function of t.

In this paper a study of the tolerance proportionality property under a discontinuous step-size policy that does not allow to change the size of the step if the step-size ratio between two consecutive steps is close to unity is carried out. This theory is applied to obtain global error estimations in a few problems that have been solved with the code Gauss2 [S. Gonzalez-Pinto, R. Rojas-Bello, Gauss2, a Fortran 90 code for second order initial value problems, ⟨http://www.netlib.org/ode/⟩], based on an adaptive two stage Runge–Kutta–Gauss method with this discontinuous step-size policy.

Keywords: Runge–Kutta methods; Global error estimates; Adaptive methods; Tolerance proportionality

1. Introduction

We consider the initial value problem (IVP) for a general differential system

$$y'(t) = f(y(t)), \quad y(0) = y_0 \in \mathbf{R}^m, \quad t \in [0, t_{\text{end}}] \equiv J, \tag{1.1}$$

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which is assumed to possess a unique solution $y(t)$ on J. For simplicity, we will restrict our study to autonomous systems with f sufficiently differentiable in a neighborhood of the trajectory $V_y = \{y = y(t), t \in J\}$. Further, for the derivation of the tolerance proportionality (TP) property, it will be supposed that the product of the length of J by the Lipschitz constant of f in V_y is not too large.

For the numerical solution of (1.1) we consider adaptive Runge–Kutta (RK) methods. That means that for every small tolerance $\delta > 0$, a non-uniform grid $\{t_n\}_{n=0}^{N} \in J$, $t_0 = 0$, $t_N = t_{\text{end}}$, together with approximations $y_n \simeq y(t_n)$, $n = 1, 2, \ldots, N$, both depending on δ, are dynamically generated. In this process the grid is determined so that an estimate of the local errors is maintained under the prescribed tolerance δ. A crucial and natural question is to know how the global errors $\text{ge}_n = y_n - y(t_n)$ depend on the given tolerance. It was established by Stetter [19,20] that for some adaptive RK methods and sufficiently smooth problems the global error has an asymptotically linear dependence on the tolerance in the sense that $\text{ge}_n = v(t_n)\delta + \text{o}(\delta)$, $\delta \to 0^+$, $n = 1, 2, \ldots$, holds for some $\mathscr{C}^1$ function $v(t)$ independent of δ. This property is known in the literature as TP. Later investigations by Higham [10,11] extended Stetter's results to more general adaptive methods that possess a TP dependence of type $\text{ge}_n = v(t_n)\delta^r + \text{o}(\delta^r)$, $\delta \to 0^+$, $n = 1, 2, \ldots$, with a real exponent $r > 0$. A requirement of the Stetter–Higham analysis is the non-vanishing leading term in the local error estimate along the integration interval. When the leading term in the local error estimate vanishes at some isolated points, a modified step-size change technique (regarding the standard one) has been considered in [3] to preserve TP.

In the above-mentioned TP theory developed by Higham [10–12,2] a continuous variation of the step-size along the integration interval was assumed in the sense that the step-size h_{n+1} in advancing from t_n to $t_{n+1} = t_n + h_{n+1}$ satisfies an asymptotic relation $h_{n+1} = \rho(t_n)\delta^{1/q} + \text{o}(\delta^{1/q})$ with a fixed integer $q \geqslant 1$ and a continuous problem-depending function $\rho(t) \geqslant \rho^* > 0$. Such a relation implies that, in general, the step-size will vary from step to step but this does not affect negatively the performance of explicit RK codes in which the computational cost is independent of the size of the step. However, for adaptive codes based on implicit RK formulas, such as Gauss formulas (that may be convenient for special problems which require the preservation of quadratic invariants, simplecticness or some special stability requirements) if the implicit equations of stages are solved by using a simplified Newton iteration, each step-size variation requires a new LU decomposition of the iteration matrix and it increases significantly the computational cost. A way to reduce the number of step-size changes would be to retain the step-size unchanged if h_{n+1}/h_n is close to the unity and this amounts to use a step-size $h_{n+1} = \hat{\rho}(t_n)\delta^{1/q} + \text{o}(\delta^{1/q})$ with a piecewise continuous $\hat{\rho}(t) \geqslant \rho^* > 0$. This technique was already used by Shampine and Gordon in the code DSTEP [17] based on variable coefficient multistep Adams methods to reduce the computational cost. A similar discontinuous strategy have been used in LSODE [13] to improve the stability. Thus, the TP theory of Higham developed under the assumption of a continuous step-size variation cannot be directly applied to those adaptive methods allowing a piecewise constant step-size variation.

On the other hand, in convergent adaptive ODE solvers an integration with tolerance δ does not imply that the global errors are smaller than δ. A desirable practical feature of a numerical integration code is the possibility to provide to the interested user, information on the magnitude of the global errors. As remarked in [1] one may wish to improve the numerical solution when the global error estimation is not good enough. In such a case the technique must be reliable, in the sense that the estimation has some significant digits or it is in the size of the true global errors. An overview about most of global error estimations considered in the literature can be seen in [1,18] and the references therein. In general, these estimations are costly, fail in problems with stability difficulties or when the numerical method is near the limit of accuracy and they are not included in standard integrators. An alternative less demanding is to make use of the TP property exhibited for many adaptive codes, in which case the existence of an asymptotic expansion on the tolerance (δ), allows to derive an estimate of the global error [10,11,16,19,20]. This estimation is based on global extrapolation when considering two independent integrations for different tolerances. Observe that since this technique is based on asymptotic expansions on δ, it may fail at crude tolerances because the asymptotic expansion may not be present and also for very stringent tolerances because of the effects of finite precision. In any case it is important to remark that this technique can be easily applied to any standard integrator.

The aim of this paper is two-fold: firstly, to study the TP property for adaptive codes with the abovementioned discontinuous step-size changing policy and secondly, to apply it to estimate the global error in the code [6,7], which is based on the fully implicit two stage RK Gauss method, intended to integrate second order problems. The paper is organized as follows: in Section 2 we collect a number of definitions and results following the ideas of Higham [10,11] that will be used in the rest of the paper. In Section 3 we study the effect of a discontinuous step-size policy on the numerical integration and a suitable modification of the TP theory of Higham is given. In Section 4 we present a global error estimation based on TP. Finally, in Section 5, the results of some numerical experiments with the code [6] for