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THE SINGULARITY DIAGNOSTICS BY CALCULATION ON EMBEDDED GRIDS [1]

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Abstract. This paper is devoted to investigation of one algorithm for control of the accuracy of discrete approximations and singularity diagnostics. The algorithm is based on calculation on embedded grids and Richardson's formula giving asymptotically exact estimation for numerical solution error. Application to the Rosenbrock scheme with complex coefficients allows us to determine both the moment of exact solution's singularity and its type.

Key words: numerical methods, ODE, quasi-equidistant grids, Rosenbrock schemes, Richardson's correction

1. Introduction

Requirements to adequacy of mathematical models grow with every year. Accuracy aspects play the significant role in practice of mathematical modelling. For testing numerical methods and for practical application of calculation's results the method of accuracy control is quite necessary.

The well known method of a posteriori accuracy control was offered by the Richardson [8]. The detail review of practical aspects for application of Richardson's method can be found in monograph [10]. In practice, this method is applied not so often and its potential possibilities obviously were not appreciated by investigators. The reason is that Richardson offered his method only for uniform grids.

During last few years so-called quasi-uniform grids were introduced and used in calculation practice by our research group [5]. The Richardson method for estimation the accuracy by calculations on embedded grids is absolutely correct if family of quasi-uniform grids is exploited.

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2. Quasi-Uniform Grids

For the first time quasi-uniform grids were proposed and used by Samarskii in 1952. Later this approach was transform to the following definition.

Let us choose a smooth strict monotone grid generating function $x(\xi)$, which satisfies the following three conditions:

$$1)\ \left|x^{(q)}(\xi)\right| \leq M_q,\ q \gg 1;\ \ 2)\, x'(\xi) \geq m > 0;\ \ 3)\, x(0) = a,\ x(1) = b. \quad (2.1)$$

A family of uniform grids $\xi_n = n/N$ defined on interval $(0,1)$ generates one-parameter family of quasi-uniform grids $x_n = x(\xi_n)$ on a chosen interval (a,b). Quasi-uniform grids are easily adapted to singularity of the solution. In particular, it is possible to construct quasi-uniform grid covering unbounded domain. The last node of such grid is placed on infinity so right boundary condition is taken into account correctly. This approach was successfully applied by authors to solve a wide class of boundary and initially boundary-value problems in unbounded domain [1, 2, 5].

3. Accuracy Control Algorithm

But the main advantage of using the family of quasi-uniform grids in calculations is the possibility to control the accuracy. Algorithm is the same for many finite-difference methods: for numerical integration, solving systems of ODE or PDE. Let us carry out two calculations on embedded uniform or quasi-uniform grids with total number of nodes N and $2N$. All nodes of smaller grid are identical to even nodes of denser grid due to uniformity. Suppose that we use numerical method with order of accuracy p. For smooth enough solution the error can be decomposed into a sum of inverse powers of N. The Richardson formula

$$\Delta_{2N} = \frac{U_{2N} - U_N}{2^p - 1} \quad (3.1)$$

defines the the main term of such sum. This formula is asymptotically exact when $N \to \infty$ if we use uniform or quasi-uniform grids. So it gives the real value of numerical solution error without knowledge of exact solution.

We can apply (3.1) as a single-step approximation correction formula

$$U = U_{2N} + \Delta_{2N} + O\left(N^{-p-s}\right),\quad s \in \{1,2\} \quad (3.2)$$

and increase the order of accuracy of approximation. In (3.2) $s = 1$ for non-symmetrical difference schemes and $s = 2$ for symmetrical ones. Such enlargement of accuracy requires only few arithmetical operations and so it is very cheap.

The algorithm of calculations with accuracy control is illustrated by Fig. 1. We have carried out series of calculations on embedded grids every time doubling the number of grid nodes and evaluating the error by Richardson's

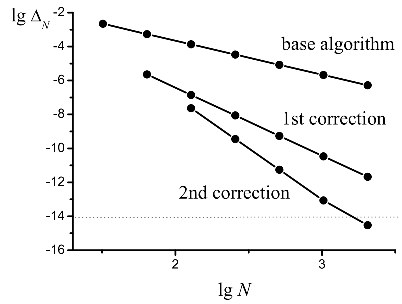

Figure 1. Accuracy control algorithm.

method. The curve of numerical error dependence on a number of nodes in double logarithmic scale is asymptotically close to the straight line with the tangent of inclination angle equal to p. Any other values of inclination angle indicate errors in program or not enough smooth solution. In this case numerical results are possible non adequate.

If inclination angle is near to theoretical value then program is correct, solution is smooth enough and we can carry out Richardson's correction. Result of correction can be interpreted as calculation results obtained by using a method with higher order of accuracy $O\left(N^{-p-s}\right)$.

The error of corrected solution again can be evaluated by the Richardson formula, taking into account the new order of accuracy. Decreasement of the error of corrected solution is substantially faster. Using the same number of grid nodes we obtain much better accuracy. In order to increase the accuracy we have done only few arithmetical operations.

The given Richardson's correction method gives the accuracy on the level of machine round-off error by using $N = 1000$ grid points. Applying the base numerical algorithm without the Richardson correction we achieve the round-off error only using unacceptably large number of grid points $N \sim 10^7$. Including into the program the described algorithm allows us to carry out calculations efficiently with accuracy control. We consecutively double the number of quasi-uniform grid nodes and carry out Richardson's corrections. The process is stopped when the required accuracy level is achieved.

4. Singularity Diagnostics

The natural continuation of accuracy control idea is the method of singularity diagnostics. Let's consider the Cauchy problem for ODE, exact solution of which has the singularity:

$$\frac{du}{dt} = \beta u^{1+\frac{1}{\beta}}, \quad u\left(0\right) = u_0 > 0. \tag{4.1}$$

The exact solution of (4.1) is $u = (t_* - t)^{-\beta}$. If $\beta > 0$, then exact solution of (4.1) $u \underset{t \to t_*}{\to} \infty$. If $\beta \in (-1, 0)$ then the exact solution has singularity of a root type and $u' \underset{t \to t_*}{\to} \infty$. Such differential problems are hard for numerical solution and we call them ill-conditioned to distinguish from stiff systems [4]. Exact solution of (4.1) doesn't exist at $t > t_*$.

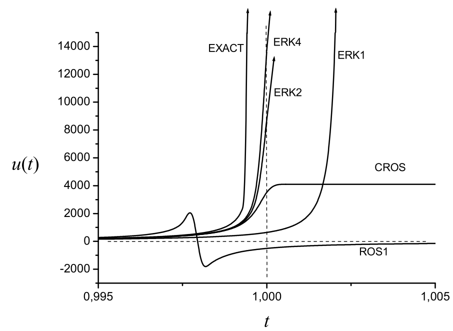

Figure 2. Calculation results for Cauchy problem with singularity of exact solution.

Fig. 2 illustrates the behaviour of numerical solution of (4.1) when different well-known difference schemes are applied. We chose $\beta = 1$, $u_0 = 1$. The exact solution has the vertical asymptotical line at $t = 1$. Abbreviation "ERK" indicates Explicit Runge-Kutta schemes of the first, second and fourth order of accuracy. It is well-known that for ERK schemes a numerical solution of (4.1) exists at any time moment [3]. It is monotone and always positive. It follows from Fig. 2 that all numerical solutions given by ERK schemes cross the asymptote and define numerical solutions in area where the exact solution doesn't exist and so they are non-adequate. More over application of ERK for numerical solution of ill-conditioned ODE leads to overflow in calculations. Unfortunately the moment of overflow is not correlated with the moment of singularity t_*. The similar behavior was demonstrated in tests by other explicit schemes. So they are unsuitable for numerical solution of ill-conditioned problems and singularity diagnostics.

Let us consider implicit one-stage Rosenbrock [9] scheme for numerical solution of the following ODE

$$\frac{du}{dt} = f(u). \tag{4.2}$$

A general formula for obtaining discrete solution at the next temporal level is the following

$$\hat{u} = u + \tau \mathrm{Re}\, k, \quad (E - \alpha \tau f_u)\, k = f(u), \tag{4.3}$$

here $f_u \equiv \partial f / \partial u$ is the Jacobian of the system, E is the identity matrix. Even if the ODE (4.2) is non-linear, the implementation of the scheme requires to solve only linear algebraic system with definitely well-conditioned matrix. It can be solved by some direct method (for example LU decomposition). So transformation onto the next temporal level is carried out by limited number of arithmetic operations, similar to explicit schemes. For this obvious advantage Rosenbrock schemes are often called semi-implicit.

With respect to dependence of the solution on the parameter, the properties of one-stage Rosenbrock schemes (4.3) are different. There is one scheme with complex-valued parameter $\alpha = (1+i)/2$ (CROS) having the unique properties of accuracy and stability. The accuracy in this case is $O\left(N^{-2}\right)$. This scheme is absolutely stable and L_2 stable, so it is suitable for solution of very stiff systems. Just this scheme gives the best results on tests and can be recommended for wide class of applications.

Numerical solutions, given by the Rosenbrock schemes for ill-conditioned Cauchy problem (4.1), have quit different structure. The Rosenbrock schemes with real coefficient give monotone increasing numerical solution, but after definite moment numerical solution suddenly it changes the sign. In some cases using of Rosenbrock schemes with a real coefficient also lead to numerical overflow. This behavior is also inadequate to the behaviuor of the exact solution. A structure of the numerical solution of CROS scheme is cardinally different. Immediately after of singularity moment $t = t_*$ the numerical solution of CROS scheme is stabilized at the constant level u_*.

There is no numerical overflow when CROS scheme is applied for numerical solution of ill-conditioned Cauchy problems. This is its first advantage. The second advantage is the following. First it was noticed in numerical experiments, and then theoretically shown that constant level u_* depends on time grid step τ or (which is the same for quasi-uniform grid) on the number of grids nodes N. Theoretical investigation of the CROS scheme for numerical solution of ill-conditioned Cauchy problem for ODE resulted in following theorems [6, 7].

Theorem 1. *If exact solution of ODE has singularity of power type* $u \sim (t_* - t)^{-\beta}$*, then numerical solution of CROS scheme is stabilized at the constant level* $u_* = [2N/(\beta+1)]^{\beta}$.

While we carry out calculation with the accuracy control on embedded uniform or quasi-uniform grids we have to compute the effective order of accuracy

$$p^{eff}(t) = \frac{\ln \Delta_N(t) - \ln \Delta_{2N}(t)}{\ln 2}. \tag{4.4}$$

Theorem 2. *Effective order of accuracy (4.4) of CROS scheme in the points where exact solution is smooth* ($t < t_*$) *tends to theoretical value* $p^{eff} \underset{N\to\infty}{\to} 2$. *At all points after singularity moment* ($t \geq t_*$) *the effective order of accuracy for CROS scheme is* $p^{eff} \underset{N\to\infty}{\to} -\beta$.

So using CROS scheme in computations on embedded grids allows to determine not only the singularity moment, but also its type.

The similar theoretical results were received for some other singularity types, for example logarithmic. In this case $p^{eff} \underset{N\to\infty}{\to} 0$ at any grid node after the singularity moment $t \geq t_*$.

5. Conclusions

Using quasi-uniform grids in calculation on embedded grids allows us to obtain the a posteriori and asymptotically exact estimation of accuracy. Most well-known standard programs now implements calculations with automatically chosen step size, so grids are not quasi-uniform and accuracy estimation is not asymptotically exact.

For calculation of ill-conditioned ODE's the explicit schemes are unsuitable. In a class of implicit schemes the Rosenbrock scheme with complex coefficient is outstanding. For example, it does not lead to numerical overflow even if the exact solution tends to infinity.

Based on ideas of calculations with accuracy control the algorithm for singularity diagnostics was constructed. Only one-stage Rosenbrock scheme with complex coefficient has appeared to be suitable for such algorithm.

A program realizing the proposed algorithm allows to determine both the moment of singularity and its type.

The proposed approach can be naturally extended to numerical solution of systems of ODE's and PDE's or differential-algebraic systems.

References

[1] A.B. Al'shin, E.A. Al'shina, A.A. Boltnev, O.A. Kacher and P.V. Koryakin. Numerical solution of initial-boundary value problems for Sobolev-type equations on quasi-uniform grids. *Computational Mathematics and Mathematical Physics*, **44**(3), 490 – 510, 2004.

[2] E.A. Alshina and N.N. Kalitkin. Evaluation of spectra of linear differential operators. *Doklady Mathematics*, **64**(2), 208 – 212, 2001.

[3] J.C. Butcher. Coefficients for study of Runge-Kutta integration processes. *J. Austral. Math. Soc.*, **3**, 185 – 201, 1963.

[4] E. Hairer and G. Wanner. *Solving ordinary differential equation II, stiff and differential-algebraic problems.* Springer-Verlag, Berlin, 1991.

[5] N.N. Kalitkin, A.B. Alshin, E.A. Alshina and B.V. Rogov. *Computation on quasi-equidistant grids.* PhysMathLit, Moscow, 2004. (In Russian)

[6] N.N. Kalitkin, E.A. Alshina and P.V. Koryakin. Diagnostics of exact solution singularity by calculations on embedded grids. *Computational Mathematics and Mathematical Physics*, **45**(10), 2005. (in printing)

[7] N.N. Kalitkin, E.A. Alshina and P.V. Koryakin. The singularity diagnostic by the embedded grids method. *Doklady Mathematics*, **68**, 2005. (in printing)

[8] L.F. Richardson. The deferred approach to the limit. *Phil.Trans., A*, **226**, 299 – 349, 1927.

[9] H.H. Rosenbrock. Some general implicit processes for the numerical solution of differential equations. *Comput. J.*, **5**(4), 329 – 330, 1963.

[10] Marchuk G.I.and Shaydurov V.V. *Increasing the accuracy of difference scheme's solutions.* Nauka, Moscow, 1979. (In Russian)