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INTEGRATION OF DIFFERENTIAL ALGEBRAIC STIFF SYSTEMS[1]

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Abstract. This paper describes some practical aspects of method of ε enclosure application for differential algebraic systems. An one-stage Rosenbrock scheme is recommended and method of accuracy control is stated.

Key words: stiff systems, differential algebraic systems, Rosenbrock schemes

1. Introduction

In practice we often deal with so-called singular problems with parameter ε. If this parameter is small then the given differential equation is stiff. If ε tends to zero it becomes differential algebraic. Among that sort of problems are the following:

1) Electric circuits described by differential equations together with algebraic Kirchhoff law;

2) Hydrodynamics governed by Euler's equation supplemented by algebraic equations of state;

3) In chemical kinetics it is necessary to take in to account algebraic balance conditions.

In practice such problems are often formulated in implicit form and algebraic equations are not explicitly separated from differential. In most general case such problem can be written in the following form

$$M\frac{du}{dt} = f(u,t)$$

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here u, f are vector-functions and M is square matrix. M is singular if equations are differential-algebraic. These problems have additional difficulty. They are stiff. The meaning of the term *stiff* is intuitively clear, but its strict mathematical definition still causes numerous controversies. It is typical for stiff problems to have both fast varying and slow damping components of the solution. The time characteristics of different physical processes in stiff system vary in a wide range. Therefore these problems require special difference schemes and introduction of new concepts of stability, for example A-stability or Lp-stability (see [1, 2]). Explicit schemes are not applicable.

2. Autonomization

It was turned out that if algebraic equations are not autonomous then effective order of accuracy reduces. But system can be transformed to autonomic form by very simple way. Let's introduce one additional unknown function identically equal to time. Differential equation for new function is very simple. Resulting differential algebraic system is autonomic. Dimension of system becomes greater. It leads to non crucial increasing of calculation volumes but gives significant gain in accuracy. Thus we assume that system is already autonomous.

3. Numerical Solution

For numerical solution of differential-algebraic systems we used the family of Rosenbrock schemes. Those schemes were proposed for pure differential stiff system. The so-called method of ε-enclosure (see [1]) allows us to use any scheme constructed for pure differential system to solve differential-algebraic systems by substituting the unique matrix in initial formula by singular matrix M.

Next we present brief information on one-stage Rosenbrock schemes for solving differential algebraic systems. Its general formula is given by

$$\hat{u} = u + \tau \mathrm{Re} k, \qquad (M - \alpha\tau f_u(u))\, k = f(u).$$

Here f_u is Jacobi matrix of the system. The properties of the scheme depend on parameter α. One case of those schemes has unique properties. It has the complex parameter $\alpha = \frac{1+i}{2}$. It approximates the problems with second order of accuracy and is L_2 stable so absolutely stable. Thus it is suitable for very stiff systems. We denote it CROS (see [5]). Just this scheme gives the best results on tests and can be recommended for wide applications. Two-stages Rosenbrock schemes allow to get a higher accuracy (see [3]).

4. Accuracy Control

For testing numerical methods and for practical application of numerical results the method of accuracy control is necessary. The well known method of accuracy control is the Richardson method, offered in 1927. It allows to estimate the accuracy of the discrete solution aposteriori:

$$\Delta^{(2N)} = \frac{u^{(2N)} - u^{(N)}}{2^p - 1}.$$

Here $u^{(2N)}$ is a numerical solution when grid has $2N$ points, $u^{(N)}$ is a numerical solution when grid has N points, p is the order of accuracy. This formula is asymptotically exact when N tends to infinity and allows carrying out calculations with assured accuracy (see [4]).

5. Transistor Amplifier

Let us consider simulation of the transistor amplifier as an example of differential algebraic stiff system. There is the electrical circuit on Fig. 1.

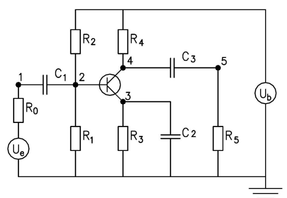
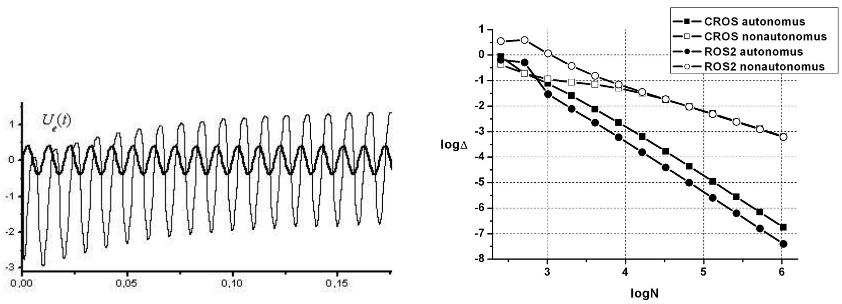


Figure 1. An electrical circuit of transistor amplifier.

Voltage values in points 1,2,3,4,5 are unknown. The same example is used by Hairer and Wanner for testing package RADAU5 in their classic monograph about stiff differential equations (see [1]). The base of this program is 3-stages implicit Runge-Kutta scheme. It is A-stable and has third order of accuracy. The algorithm carries out automatic step selection. Application of Kirchhoff law to the electric circuit of transistor amplifier gives us the following differential algebraic system

$$\begin{cases} \dfrac{U_e\left(U_6\right)}{R_0} - \dfrac{U_1}{R_0} + C_1\left(U_2' - U_1'\right) = 0, \\ \dfrac{U_b}{R_2} - U_2\left(\dfrac{1}{R_1} + \dfrac{1}{R_2}\right) + C_1\left(U_1' - U_2'\right) - 0.01 f\left(U_2 - U_3\right) = 0, \\ f\left(U_2 - U_3\right) - \dfrac{U_3}{R_3} - C_2 U_3' = 0, \\ \dfrac{U_b}{R_4} - \dfrac{U_4}{R_4} + C_3\left(U_5' - U_4'\right) - 0.99 f\left(U_2 - U_3\right) = 0, \\ -\dfrac{U_5}{R_5} + C_3\left(U_4' - U_5'\right) = 0, \\ U_6' = 1. \end{cases}$$

Dimension of singular matrix M is 6 and $\mathbf{rank}M$ is equal to 4. This system is nonlinear but it is necessary to solve only linear system. Results of simulation are presented on Fig. 2*a*. There is dependence on time of input and output voltages.



a) b)

Figure 2. Results of simulations: a) dependence on time of input and output voltages of the transistor amplifier, b) decreasing the error of numerical solution with increasing the number of nodes in double logarithmic scale.

Two processes are present in this stiff system: fast periodical alternation and slow increasing of amplitude. Amplitude of output voltage is increased, it means that our amplifier does work.

We carried out a set of calculation of transistor amplifier on embedded analytical grids by CROS scheme and one of the 2-stages scheme. These results are presented in Fig. 2*b*. Decreasing the error with increasing the number of nodes in double logarithmic scale confirms theoretical order of accuracy for autonomous system. But as shown in Fig. 2*b* if we apply those schemes for differential-algebraic system written in non-autonomic form results are much worse: order of accuracy is below than the theoretical one.

Then we compared CROS and RADAU5 schemes. The dependence of errors on time is shown in Fig. 3. We see that CROS has lower accuracy at the beginning but soon RADAU5 error begins to increase and then gets the order of the solution. Thus, CROS has the following advantages:

- it is applicable for very stiff problems,
- it lets to get assured accuracy,
- it has essentially higher accuracy when calculations are carried out on long time intervals.

6. Complex-Value DE

The 1-stage Rosenbrock scheme with complex parameter may be applied for nonautonomus complex differential equations

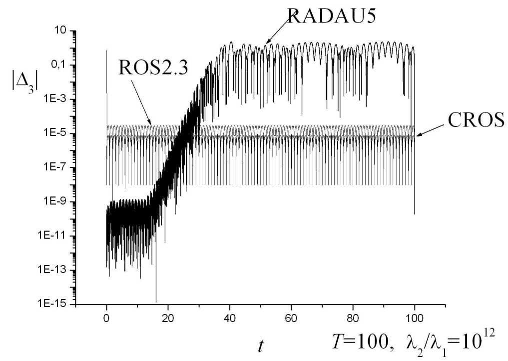


Figure 3. Error of CROS is stable and error of RADAU5 is lower at the beginning, but then it increases.

$$M\frac{du}{dt} = f\left(u,t\right).$$

In this case the scheme is defined as follows:

$$\begin{aligned}
&\hat{u} = u + \tfrac{1}{2}\tau\left(\upsilon + w\right),\\
&\left[M - 0.5\left(1+i\right)\tau f_u\right]\upsilon = f\left(u, t + 0.5\tau\right),\\
&\left[M - 0.5\left(1-i\right)\tau f_u\right]w = f\left(u, t + 0.5\tau\right).
\end{aligned}$$

This scheme is L_2-stable.

Let's give an example. Sivashinsky has shown in 1977 that in suitable asymptotic regime the dynamics of wrinkled flame front is governed by a non linear pseudo differential equation (see [6]). In the one-dimensional case it is written down in the following way:

$$u_t + uu_x = \Lambda u + \nu u_{xx}.$$

Here Λ is linear singular operator defined conveniently in terms of the spatial Fourier transform:

$$u\left(t,x\right) = \int\limits_{-\infty}^{+\infty} e^{ikx}\tilde{u}\left(t,k\right)dk, \quad \Lambda : \tilde{u}\left(t,k\right) \mapsto \left|k\right|\tilde{u}\left(t,k\right),$$

$u = \varphi_x$ and φ is the flame front displacement.

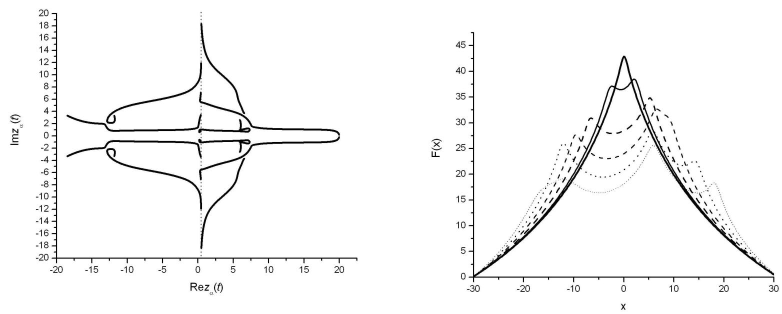
The results of various studies of the Sivashinsky equation the following. Solutions are highly organized in the form of one or several wrinkles. At the root of simple behaviour of the Sivashinsky equation is the fact that it possesses a pole decomposition: this equation admits solutions of the form

$$u\left(t,x\right) = -2\nu\sum_{\alpha=1}^{2M}\frac{1}{x - z_\alpha\left(t\right)}.$$

There $z_\alpha(t)$ are poles in the complex plane (consisting of complexly conjugate pairs) moving according to the laws of motion of poles:

$$\dot{z}_\alpha(t) = -2\nu \sum_{\beta \neq \alpha} \frac{1}{z_\alpha - z_\beta} - i\,\mathrm{sign}\left(\mathrm{Im}\left(z_\alpha\right)\right), \quad 1 \leq \alpha \leq 2M.$$

We have applied the complex Rosenbrock scheme for numerical solution of the given system of complex ODE. Fig. 4*a* reflects the dynamics of 5 pairs of random poles.



a) b)

Figure 4. Results of numerical experiments: a) the poles of pole decomposition of Sivashinsky equation stable along the same line, b) dynamics of the flame front of Sivashinsky equation.

It is obvious that they are stable along the same line. This fact agrees with a theoretical result. In this case flame front changes with time as shown in Fig. 4*b*.

The exact solution of the given system of ODE for complex functions $z_\alpha(t)$ can be written explicitly in simple cases, e.g. in a case of two poles (see [7]). When 2π spatial periodicity is assumed it is enough to restrict to poles with real part between 0 and 2π:

$$u(t,x) = -\nu \sum_{\alpha=1}^{2M} \mathrm{ctg}\frac{x - z_\alpha(t)}{2},$$
$$\dot{z}_\alpha(t) = -\nu \sum_{\beta \neq \alpha} \mathrm{ctg}\frac{z_\alpha - z_\beta}{2} - i\,\mathrm{sign}\left(\mathrm{Im}\left(z_\alpha\right)\right), \quad 1 \leq \alpha \leq 2M.$$

7. Conclusions

The practical aspects of application the method of e-enclosure for differential algebraic stiff systems

$$M\frac{du}{dt} = f\left(u,t\right)$$

was investigated. The comparison of few concrete schemes is carried out and it is shown that the most effective is 1-stage complex Rosenbrock scheme with accuracy $O\left(N^2\right)$.

It is shown that the mentioned schemes realize they theoretical order of accuracy for differential-algebraic systems in autonomic form. Simple way of autonomization was illustrated. Effectiveness of complex Rosenbrock scheme for complex value ODE is shown. The applicability of embedded grids Richardson's method for calculation differential-algebraic systems with accuracy control was shown.

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