STIFF SYSTEMS IN THEORY AND PRACTICE

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Abstract

The words ”stiff system” are used frequently in this work as it is the top topic of it. In particular the paper deals with stiff systems of differential equations. To solve this sort of system numerically is a diffult task. In spite of the fact that we come across stiff systems quite often in the common practice, it was real challenge even to find suitable articles or other bibliography that would discuss the matter properly.
On the other hand a very interesting and promissing numerical method of solving systems of ordinary differential equations based on Taylor series has appeared. The question was how to harness the said ”Modern Taylor Series Method” for solving of stiff systems.
The potential of the Taylor series has been exposed by many practical experiments and a way of detection and solution of large systems of ordinary differential equations has been found.
Generally speaking, a stiff system contains several components, some of them are heavily suppressed while the rest remain almost unchanged. This feature forces the used method to choose an extremely small integration step and the progress of the computation may become very slow. However, we often need to find out the solution in a long range. It is clear that the mentioned facts are troublesome and ways to cope with such problems have to be devised.
There are many (implicit) methods for solving stiff systems of ODE’s, from the most simple such as implicit Euler method to more sophisticated (implicit Runge-Kutta methods) and finally the general linear methods. The mathematical formulation of the methods often looks clear, however the implicit nature of those methods implies several implementation problems. Usually a quite complicated auxiliary system of equations has to be solved in each step. These facts lead to immense amount of work to be done in each step of the computation.
These are the reasons why one has to think twice before using the stiff solver and to decide between the stiff and non-stiff solver.

Keywords: Stiff systems, Modern Taylor Series Method, Differential equations, Continous system modelling

Jiří Kunovský graduated at Brno University of Technology, in 1967. During most of his time at BUT he has taught and directed research in Computer Science, specially in simulations of ”Security-Oriented Research in Information Technology”. He has created the simulation language TKSL (II-2007/TKSL is available now).

1 Introduction

This paper is related with computer simulations of continuous systems. The research group HPC ("High performance computing") has been working on extremely exact and fast solutions of homogenous differential equations, nonlinear ordinary and partial differential equations, stiff systems, large systems of algebraic equations, real time simulations and corresponding software and hardware (parallel) implementations since 1980.

The Modern Taylor series method (MTSM) developed at our university is an original mathematical method which uses the Taylor series method for solving differential equations in a non-traditional way. It has been verified that the computation quite naturally uses the full hardware accuracy of the computer. Taylor series computations are based on an automatic integration method order setting, i.e using as many Taylor series terms for computing as needed to archive the required accuracy.

Unfortunately, it is easier said than done as there are some peculiar systems of differential equations, which cannot be solved by commonly used (explicit) methods - the stiff systems. While the definition of this kind of systems is intuitively clear to the mathematicians the exact definition has not been yet specified.

The selected problems are taken from the common practice - they represent physical or chemical phenomenons, simulation of electrical circuits etc. Each of the selected problems has special features so as the variety of stiff system is shown.

An original numerical method suitable for solving stiff systems is suggested - again, the method is based on Modern Taylor series method.

2 Stiff systems in theory

One of the most frequently mentioned definition of stiff systems is:
Let

$$\mathbf{y}' = \mathbf{f}(y,t) \tag{1}$$

be a system of n ordinary differential equations. Let $\mathcal{J}$ be the Jacobian of the Eq. (1) and λ_i the eigenvalues of $\mathcal{J}$ .The eigenvalues λ_i are generally timedependent. Let the eigenvalues λ_i be arranged in the following way:

$$\text{Re}|\lambda_{max}| \geq \text{Re}\lambda_i \geq \text{Re}|\lambda_{min}| \quad i = 1 \cdots n-2 \tag{2}$$

The *stifness ratio* is

$$r = \frac{\text{Re}|\lambda_{max}|}{\text{Re}|\lambda_{min}|} \tag{3}$$

The stiffness ratio r is a coefficient that helps to decide whether a problem is stiff or not. A higher r indicates a more stiff system. However, there is no exact value of the stiffness ratio r that would distinguish the non-stiff problems from the stiff-problems. For many problems in common practice the stiffness ratio r is "very high" (say $1 \cdot 10^6$ or higher).

2.1 Test example

Let us examine system

$$\begin{array}{rcl} y' &=& z \\ z' &=& -a \cdot y - (a+1) \cdot z \qquad a \in (1,\infty) \end{array} \tag{4}$$

with initial conditions $y(0) = 1$, $z(0) = -1$. Typically we calculate the Jacobian of the system Eq. (4)

$$\mathcal{J} = \begin{pmatrix} 0 & 1 \\ -a & -a-1 \end{pmatrix}$$

then we specify the eigenvalues of the system Eq. (4):

$$\begin{array}{rcl} \lambda_1 &=& -1 \\ \lambda_2 &=& -a \end{array}$$

The stiffness ratio is $r = \frac{\text{Re}|\lambda_{max}|}{\text{Re}|\lambda_{min}|} = a$.

The system Eq. (4) is "stiff" for large constant a and "non-stiff" for small a. Let us create an analytic solution of Eq. (4).

Eq. (4) can be rewritten into:

$$\begin{array}{rcl} y'' &=& z' \\ y'' &=& -a \cdot y - (a+1) \cdot z \\ y'' &=& -a \cdot y - (a+1) \cdot y' \end{array}$$

or

$$\begin{array}{rcl} y'' + a \cdot y - (a+1) \cdot y' &=& 0 \\ \lambda^2 + (a+1) \cdot \lambda + a &=& 0 \\ \hline \lambda_1 &=& \frac{-(a+1)+\sqrt{(a+1)^2-4\cdot a}}{2} \\ \lambda_2 &=& \frac{-(a+1)-\sqrt{(a+1)^2-4\cdot a}}{2} \end{array}$$

$$\lambda_1 = \underline{\underline{-1}}, \quad \lambda_2 = \underline{\underline{-a}}$$

Solution is expected in the form:

$$\begin{array}{rcl} y &=& C_1 \cdot e^{\lambda_1 \cdot t} + C_2 \cdot e^{\lambda_2 \cdot t} \\ \hline y &=& C_1 \cdot e^{-t} + C_2 \cdot e^{-a \cdot t} \\ y' &=& -C_1 \cdot e^{-t} + -a \cdot C_2 \cdot e^{-a \cdot t} \end{array}$$

with initial conditions

$$\begin{array}{rcl} & y(0) = 1, \quad z(0) = -1 & \\ 1 &=& C_1 + C_2 \\ -1 &=& -C_1 - a \cdot C_2 \end{array}$$

we get

$$C_1 = 1, \quad C_2 = 0$$

The particular solution of the system Eq. (4) is:

$$\begin{array}{rcl} y &=& e^{-t} \\ z &=& -e^{-t} \end{array} \tag{5}$$

New equivalent system with respect to system Eq. (4) and its particular solution Eq. (5) is:

$$\begin{array}{rclcrcl} y' &=& -y & & y(0) &=& 1 \\ z' &=& -z & & z(0) &=& -1 \end{array} \tag{6}$$

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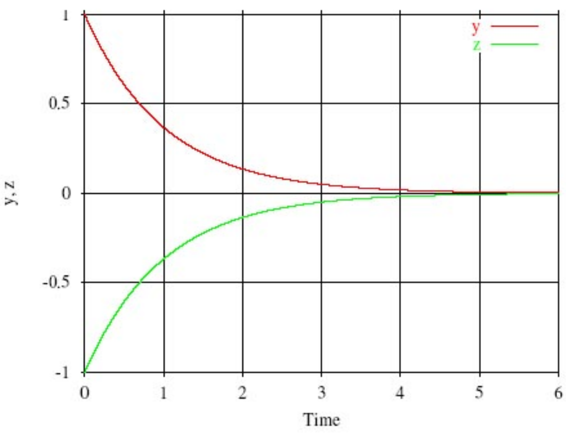

Fig. 1 II-2007/TKSL

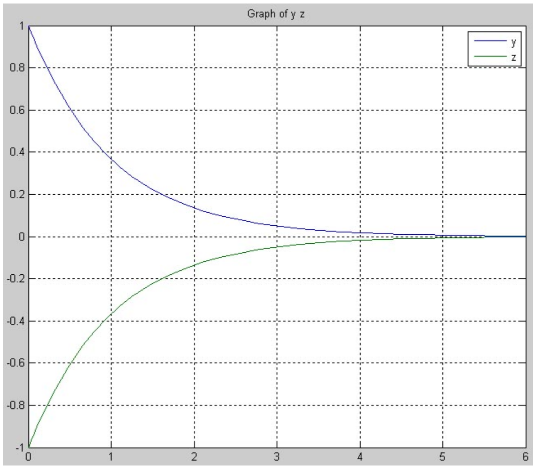

Fig. 2 MatLab

Corresponding time functions in TKSL and MatLab are in Fig. 1, Fig. 2.

Conclusion:
After some mathematical computations we have changed and simplified the given stiff problem Eq. (4) into non-stiff problem Eq. (6) with stiffnes ratio $r = 1$.

3 Stiff systems in practice

The selected problems are taken from the common practice - they represent physical or chemical phenomenons, simulation of electrical circuits etc. The problems are introduced together with their description, solutions and some other characteristics in this section. Several aspects have been watched, especially the stiffness ratio which is a widely used stiffness indicator. The numerical solutions were computed using the simulator II-2007/TKSL.

3.1 Problem 1

Stiff systems appear in simulation of electrical circuits very often. For example, in the case when we consider parasitic parameters of the circuit (such as parasitic resistance, inductance or capacity). Even a simple system of differential equation describing its model may become very stiff easily.

In many cases we need to solve the system on a relatively very large interval as we have to find the steady state. The stiffness makes it difficult or even impossible.

Let us consider the eletrical circuit in Fig. 3 The time

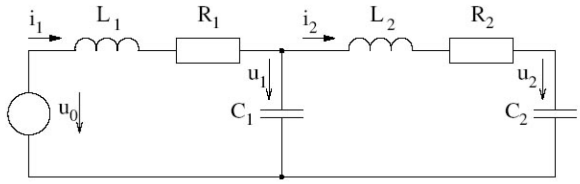

Fig. 3 Eletrical circuit with parasitic parameters

behavior of voltages and currents in the circuit is described by system Eq. (7)

$$\begin{aligned} i_1' &= \tfrac{1}{L_1}\cdot(u_0 - u_1 - R_1\cdot i_1) \\ i_2' &= \tfrac{1}{L_2}\cdot(u_1 - u_2 - R_2\cdot i_2) \\ u_1' &= \tfrac{1}{C_1}\cdot(i_1 - i_2) \\ u_2' &= \tfrac{1}{C_2}\cdot i_2 \end{aligned} \tag{7}$$

All the initial conditions are zeroes, $u0 = 1\text{V}$.

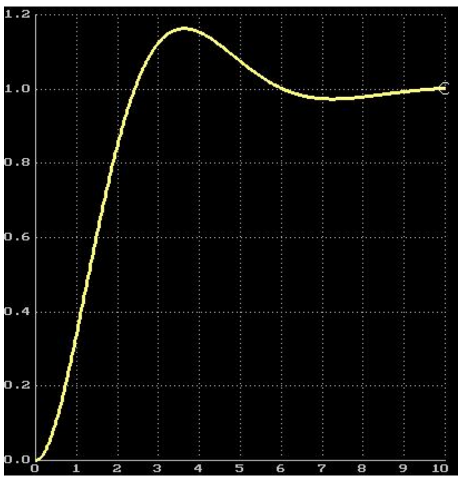

Fig. 4 II-2007/TKSL: Time function u_2

An expected result (without parasitic elements) representing voltage u_2 across C_2 for parameters $C_2 = 1\text{F}$, $L_2 = 1\text{H}$, $R_2 = 1\Omega$ can be seen in Fig. 4.

Parastic elements (such as $C_1 = 0.001\text{F}$, $L_1 = 0.001\text{H}$, $R_1 = 0.006\Omega$) practically doesn't change time function u_2 Fig. 5. Time functions u_1, u_2 are presented together in Fig. 5

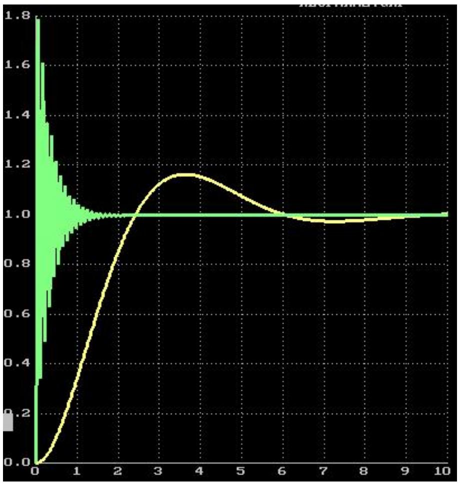

Fig. 5 II-2007/TKSL: Time functions u_1, u_2

The same is true for the eletrical circuit with parasitic elements $C_1 = 10^{-12}$F, $L_1 = 10^{-12}$H, $R_1 = 10^{-3}\Omega$. In this case electrical circuit becomes stiff system.

Jacobian of this system Eq. (7) is:

$$\mathcal{J} = \begin{pmatrix} -10^9 & 0 & -10^{12} & 0 \\ 0 & -1 & 1 & -1 \\ 10^{12} & -10^{12} & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

The eigenvalues of the eletrical circuit are:

$$\begin{aligned} \lambda_{1,2} &= -0.5 \pm 0.8657i \\ \lambda_{3,4} &= -5 \cdot 10^8 \pm 1 \cdot 10^{12} i \end{aligned}$$

The stiffness ratio is $r = \frac{5 \cdot 10^8}{5 \cdot 10^{-1}} = 1 \cdot 10^9$.

Conclusion:
The eletric circuit with parasitic elements represents stiff system. The same time function u_2 can be obtained without parasitic elements.

3.2 Problem 2

The problem *Van der Pol Oscillator* was proposed by Bathasar van der Pol in the 1920s and describes the behavior of nonlinear vacuum tube circuits. It consists of a second order differential Eq. (8).

$$y'' + \mu \cdot (y^2 - 1) \cdot y' + y = 0, \qquad \mu > 0 \tag{8}$$

The solution is a periodical function and it doesnt depend on initial conditions for certain parameters (after the transient part).

The Eq. (8) may be written as a system of ordinary differential equations of the first order

$$\begin{aligned} y_1' &= y_2 \\ y_2' &= \mu \cdot (1 - y_1^2) \cdot y_2 - y_1, \qquad \mu > 0 \end{aligned} \tag{9}$$

The significant feature of Eq. (9) is that the small oscillations are amplified and the large oscillations are damped. The coefficient μ influences the stiffness of the system.

The solution of Eq. (9) for initial conditions $y_1(0) = 2$, $y_2(0) = 0$ and parameter $\mu = 0.01$ for typical application of generating harmonic signals is shown in Fig. 6.

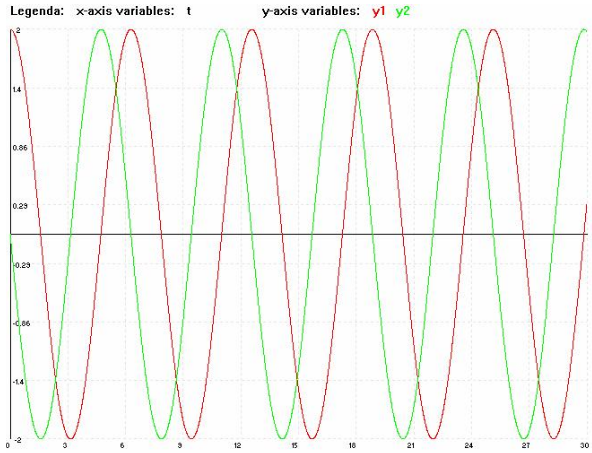

Fig. 6 II-2007/TKSL: $\mu = 0.01$

A result of "mathematical" experiments (without electronic background) of Eq. (9) for initial conditions $y_1(0) = 2$, $y_2(0) = 0$ and parameter $\mu = 10$ is shown in Fig. 7. Actually, stiff system has been created.

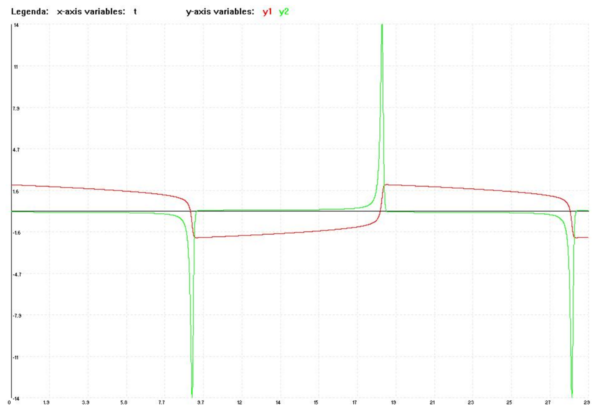

Fig. 7 II-2007/TKSL

The Jacobian of the system Eq. (9) is

$$\mathcal{J} = \begin{pmatrix} 0 & 1 \\ -2 \cdot \mu \cdot y_1 \cdot y_2 - 1 & \mu \cdot (1 - y_1^2) \end{pmatrix}$$

As the system is nonlinear, the eigenvalues change in the time and so does the stiffness ratio.

Conclusion:
It must be noted again, that Van der Pol equation has been developed for generation of harmonic signals. "Mathematical" experiments with large μ have no practical use as non-linear waves for $\mu = 10$ (Fig. 7) can easily be obtained with a well-known astabile multivibrator.

3.3 Problem 3

The eletricial problem - *Telegraph equation* models the behaviour of eletrical signals on a telegraph line. The first step in building the model is to replace a small piece of the wire by quadrupole build from resistors, capacitors and coils Fig. (8). Letting the size of this piece go to zero we obtain a partial differential equation describing the behaviour of signals on the wire Eq. (10)

$$
\begin{aligned}
L \cdot C \tfrac{\partial^2 u(x,t)}{\partial t^2} + (L \cdot G + C \cdot R) \tfrac{\partial u(x,t)}{\partial t} + & \\
+R \cdot G \cdot u(x,t) - \tfrac{\partial^2 u(x,t)}{\partial x^2} &= 0 \\
L \cdot C \tfrac{\partial^2 i(x,t)}{\partial t^2} + (L \cdot G + C \cdot R) \tfrac{\partial i(x,t)}{\partial t} + & \\
+R \cdot G \cdot i(x,t) - \tfrac{\partial^2 i(x,t)}{\partial x^2} &= 0
\end{aligned}
\tag{10}
$$

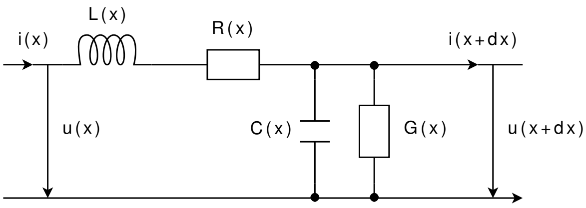

Fig. 8 Modelling a small piece of the wire

Three-point-approximation using 10 segments devides the solution of the partial differential equation into system of the first order differential equations Eq. (11)

$$
\begin{aligned}
u_1' &= v_1 & u_1(0) &= 0 \\
v_1' &= A \cdot (u_2 - 2 \cdot u_1 + u_0) - & v_1(0) &= 0 \\
&\quad -B \cdot v_1 - C \cdot u_1 & & \\
u_2' &= v_2 & u_2(0) &= 0 \\
v_2' &= A \cdot (u_3 - 2 \cdot u_2 + u_1) - & v_2(0) &= 0 \\
&\quad -B \cdot v_2 - C \cdot u_2 & & \\
&\vdots & & \\
u_9' &= v_9 & u_9(0) &= 0 \\
v_9' &= A \cdot (u_{10} - 2 \cdot u_9 + u_8) - & v_9(0) &= 0 \\
&\quad -B \cdot v_9 - C \cdot u_9 & &
\end{aligned}
\tag{11}
$$

where A, B, C are constants of the wire and $u_0 = 1$, $u_{10} = 0$ (short circuit).

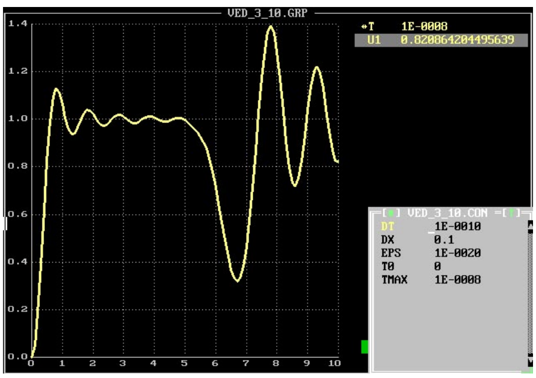

Fig. 9 II-2007/TKSL

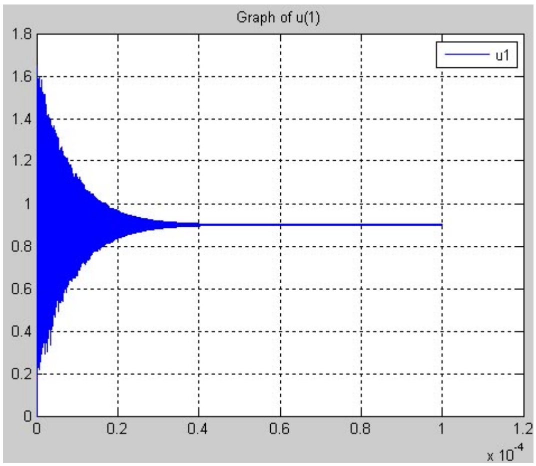

Fig. 10 MatLab

Only "a short" part of time solution of u_1 ($T_{max} = 1 \cdot 10^{-8}$s) is presented in Fig. (9). If we were interested in the steady state (as shown in Fig. (10)) solution in MatLab (function Ode23s) would take as much as $1.390 \cdot 10^4$s.

Conclusion:
Stiffness again complicates solutions when large interval is required.

3.4 Problem 4

The *Robertson's reaction* is very popular in numerical studies. The problem consists of a stiff system of three nonlinear ordinary differential Eq. (12) describing the kinetics of an autocatalytic reaction given by Robertson (1966). The large difference among the reaction rate constants is the reason for stiffness. As is typical for problems arising in chemical kinetics this special system has a small very quick initial transient. This phase is followed by a very smooth variation of the components where a large stepsize would be appropriate for a numerical method.

$$
\begin{array}{rcll}
A & \xrightarrow{0.04} & B & \text{(slow)} \\
B + B & \xrightarrow{3 \cdot 10^7} & C + B & \text{(very fast)} \\
B + C & \xrightarrow{10^4} & A + C & \text{(fast)}
\end{array}
\tag{12}
$$

Let us investigate concentrations of each individual substance. This leads to a system of differential Eq. (13) with initial conditions $y_1(0) = 1, y_2(0) = 0, y_3(0) = 0$. System Eq. (13) was usually treated on the interval $0 \le t \le 40$ until it was discovered that many codes fail if t becomes very large (say $1 \cdot 10^{11}$). The reason is that whenever the numerical solution of y_2 becomes negative, it tends to $-\infty$ and the run ends by overflow.

$$
\begin{aligned}
y_1' &= -0.04 y_1 + 10^4 y_2 y_3 \\
y_2' &= 0.04 y_1 - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2 \\
y_3' &= \qquad\qquad\qquad\qquad\;\; 3 \cdot 10^7 y_2^2
\end{aligned}
\tag{13}
$$

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The solution is shown in Fig. (11).

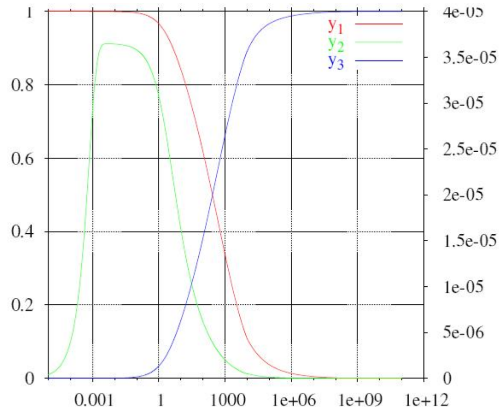

Fig. 11 II-2007/TKSL

The Jacobian of the system Eq. (13) is

$$\mathcal{J} = \begin{pmatrix} -0.04 & 10^4 y_3 & 10^4 y_2 \\ 0.04 & -10^4 y_3 - 6 \cdot 10^7 y_2 & -10^4 y_2 \\ 0 & 6 \cdot 10^7 y_2 & 0 \end{pmatrix}$$

3.5 Problem 5

Belousov–Zhabotinskii reaction is an intriguing experiment that displays unexpected behavior. When certain reactants are combined, an “induction” period of inactivity is followed by a sudden color oscillations from red to blue. The oscillations last about one minute and are repeated over a long period of time. Eventually, the reaction stops oscillating and approaches an equilibrium state. The concentrations of the reactants may be written in a system of differential equations

$$\begin{aligned} y_1' &= 77.27(y_2 + y_1(1 - 8.375 \cdot 10^{-6} y_1 - y_2)) \\ y_2' &= \tfrac{1}{77.27}(y_3 - (1 + y_1) y_2) \\ y_3' &= 0.161(y_1 - y_3) \end{aligned} \tag{14}$$

The initial conditions for this system are $y_1(0) = 1, y_2(0) = 2, y_3(0) = 3$. The solution of system Eq. (14) is shown in the Fig. (12).

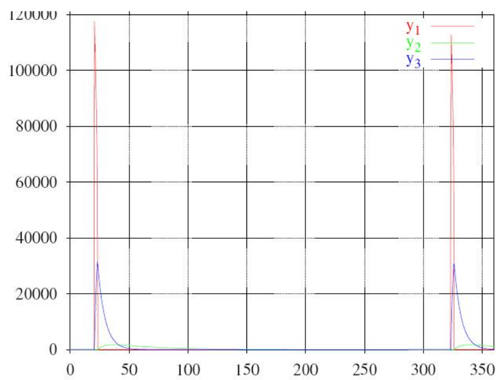

Fig. 12 II-2007/TKSL

The stiffness of Eq. (14) is caused by the fast variations of components y_1 and y_3 compared to y_2.

The Jacobian of the system Eq. (14) is

$$\mathcal{J} = \begin{pmatrix} 77.27(1 - 2 \cdot 8.375 \cdot 10^6 y_1 - y_2) & 77.27(1 - y_1) & 0 \\ -\frac{1}{77.27} y_2 & -\frac{1}{77.27}(1 + y_1) & \frac{1}{77.27} \\ 0.161 & 0 & -0.161 \end{pmatrix}$$

The system is nonlinear and therefore the eigenvalues change in time and so does the stiffness ratio.

4 Conclusions

Linear systems (Eq. (4)), parasitic parameters in electrical circuits (Eq. (7)), Van der Pol oscillator (Eq. (8)), electric line (described by Telegraph Eq. (10)), the reaction of Robertson (Eq. (13)) and Belusov–Zhabotinskii reaction (Eq. (14)) as test examples have been analyzed.

Stiffness ratio r has been specified in presented examples. Stiffness can be eliminated in some examples. All solutions have been created by II-2007/TKSL software, some computations have been created in MatLab, too.

More detailed information will be presented during the conference.

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