Stiff Systems Analysis

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Abstract

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, a very interesting and promising numerical method of solving systems of ordinary differential equations (ODE) based on Taylor series has appeared. The question was how to harness the said "Modern Taylor Series Method" (MTSM) for solving of stiff systems.

The potential of the Taylor series has been exposed by many practical experiments and a way of detection and explicit solution of large systems of ODE has been found. Detailed analysis of stability and convergence of explicit and implicit Taylor series is presented and a new algorithm using implicit Taylor series based on recurrent calculation of Taylor series terms and Newton iteration method (ITMRN) is described. The new method reducing stiffness in system based on finding new equivalent system of ODE "without stiffness" is introduced.

Categories and Subject Descriptors

G.1.7 [**Numerical Analysis**]: Ordinary Differential Equations—*convergence and stability, error analysis, initial value problems, one-step (single step) methods, stiff equations*

Keywords

Stiff Systems of Differential Equations, Taylor Series Method, Ordinary Differential Equations, Initial Value Problems, Numerical Solutions of Differential Equations, TKSL software

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1. Introduction

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.

Unfortunately, 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.

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.

2. Modern Taylor Series Method

The "Modern Taylor Series Method" (MTSM) [22] is used for numerical solution of differential equations. The MTSM is based on a recurrent calculation of the Taylor series terms for each time interval. Thus the complicated calculation of higher order derivatives (much criticised in the literature) need not be performed but rather the value of each Taylor series term is numerically calculated. Solving the convolution operations is another typical algorithm used.

An important part of the MTSM is an automatic integration order setting, i.e. using as many Taylor series terms as the defined accuracy requires. Thus it is usual that the computation uses different numbers of Taylor series terms for different steps of constant length. On the other hand, for a pre-set integration order, the integration step length may be selected. This fact positively affects the stability and speed of the computation.

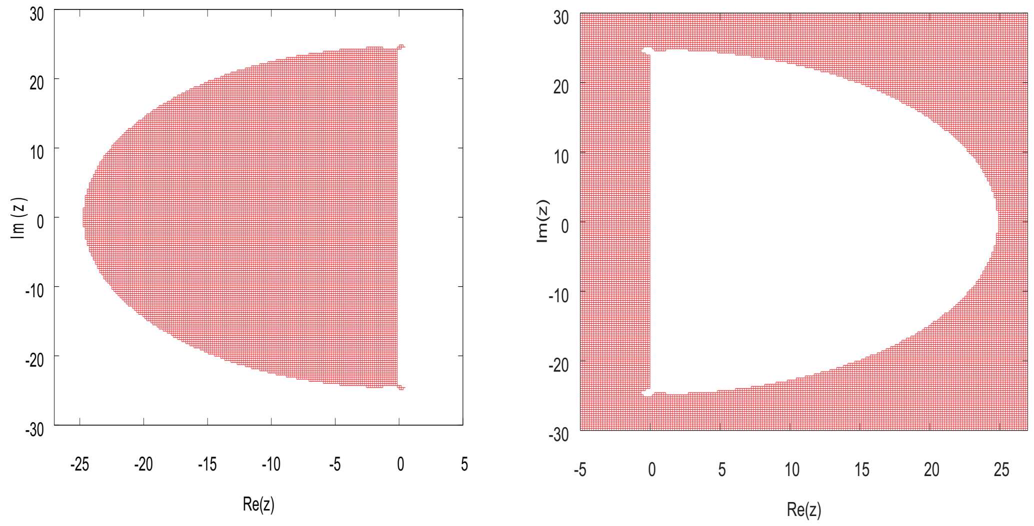

Figure 1: Stability domain for explicit (left) and implicit (right) Taylor $ORD = 63$.

An automatic transformation of the original problem is a necessary part of the MTSM [24]. The original system of differential equations is automatically transformed to a polynomial form, i.e. to a form suitable for easily calculating of the Taylor series forms using recurrent formulae.

The MTSM also has some properties very favourable for parallel processing.

Since the calculations of the transformed system (after the automatic transformation of the initial problem) use only the basic mathematical operations (+,-,*,/), simple specialised elementary processors can be designed for their implementation thus creating an efficient parallel computing system.

An original numerical method (Implicit Taylor Series Method with Reccurent Calculation of Taylor Series Terms and Newton Method - ITMRN) suitable for solving stiff systems is suggested - again, the method is based on MTSM. The MTSM has been implemented in TKSL software [29].

There are several papers that focus on computer implementations of the Taylor series method in different context "a variable order and variable step" (see, for instance, [2, 3]). Another more detailed description of a variable step size version and software implementation of the Taylor series method can be seen in [20]. The stability domain for several Taylor methods is presented in [1]. Promising A-stable combination of implicit Taylor series method with Trapezoidal rule is described in [9, 10].

2.1 Taylor Series

The best-known and most accurate method of calculating a new value of a numerical solution of ordinary differential equation (ODE) - initial value problem

$$y' = f(t, y), \quad y(0) = y_0\,, \tag{1}$$

is to construct the Taylor series [17].

Methods of different orders can be used in a computation. For instance the order method ($ORD = n$) means that when computing the new value y_{i+1} uses n Taylor series terms in the form

$$\begin{aligned} y_{i+1} &= y_i + h \cdot f(t_i, y_i) + \frac{h^2}{2!} \cdot f'(t_i, y_i) + \\ &+ \cdots + \frac{h^n}{n!} \cdot f^{(n-1)}(t_i, y_i)\,, \end{aligned} \tag{2}$$

or

$$y_{i+1} = y_i + DY1_i + DY2_i + \cdots + DYn_i\,, \tag{3}$$

where h is integration step and DYn_i are Taylor series terms.

Similarly we can construct implicit Taylor series method of order n in the form

$$\begin{aligned} y_{i+1} &= y_i + h \cdot f(t_{i+1}, y_{i+1}) - \frac{h^2}{2!} \cdot f'(t_{i+1}, y_{i+1}) - \\ &- \cdots - \frac{(-h)^n}{n!} \cdot f^{(n-1)}(t_{i+1}, y_{i+1})\,, \end{aligned} \tag{4}$$

or

$$y_{i+1} = y_i + DY1_{i+1} + DY2_{i+1} + \cdots + DYn_{i+1}\,. \tag{5}$$

3. Explicit and Implicit Taylor Series Analysis

Let's analyse well known Dahlquist's equation [11], [18]

$$y' = \lambda y\,, \quad y(t_0) = y_0\,, \quad \lambda < 0\,, \tag{6}$$

with analytic solution

$$y = y_0 e^{\lambda t}\,. \tag{7}$$

Approximate solution with explicit Taylor series is in the form

$$\begin{aligned} y_{i+1} &= y_i + hy_i' + \frac{h^2}{2} y_i'' + \frac{h^3}{3!} y_i''' + \cdots + \frac{h^n}{n!} y_i^{(n)} \\ y_{i+1} &= y_i + h\lambda y_i + \frac{h^2}{2}\lambda^2 y_i + \frac{h^3}{3!}\lambda^3 y_i + \cdots + \frac{h^n}{n!}\lambda^n y_i \\ y_{i+1} &= \sum_{k=0}^{n} \frac{(\lambda h)^k}{k!} y_i\,, \end{aligned} \tag{8}$$

where h is integration step.

Similarly implicit Taylor series is in the form

$$y_{i+1} = (\sum_{k=0}^{n} \frac{(-\lambda h)^k}{k!} y_i)^{-1}\,. \tag{9}$$

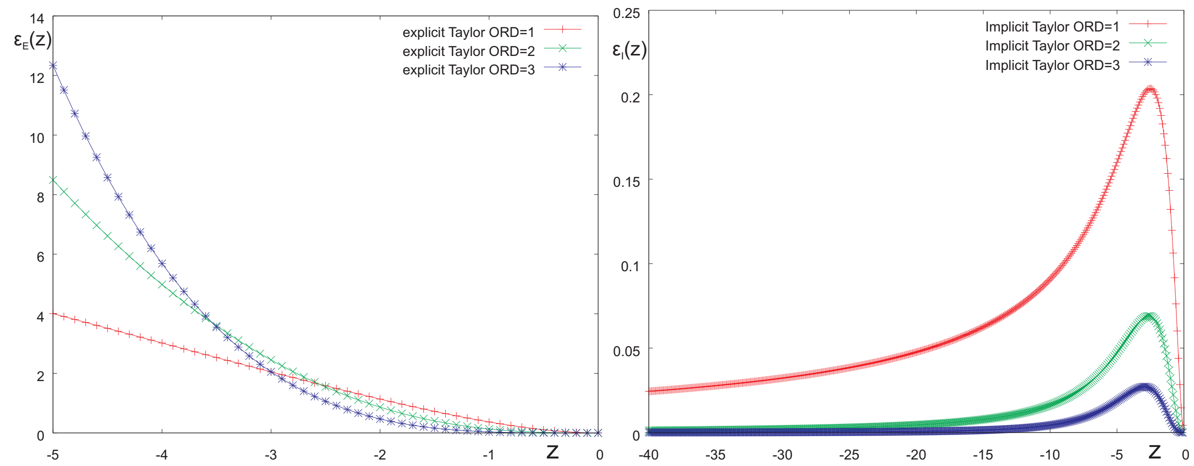

Figure 2: Local error of explicit (left) and implicit (right) Taylor series $ORD = 1, 2, 3$.

3.1 Stability and Convergence

Let $z = \lambda h$ then *stability function* $R(z) = \frac{y_{i+1}}{y_i}$ for explicit Taylor series is in the form

$$R_{ET}(z) = \sum_{k=0}^{k=n} \frac{z^k}{k!}\,, \tag{10}$$

similarly for implicit Taylor series stability function is in the form

$$R_{IT}(z) = (\sum_{k=0}^{k=n} \frac{-z^k}{k!})^{-1}\,. \tag{11}$$

Some *stability domains* $R(z) < 1$ for explicit (10) and implicit (11) Taylor series method $ORD = 63$ can be seen in Fig. 1.

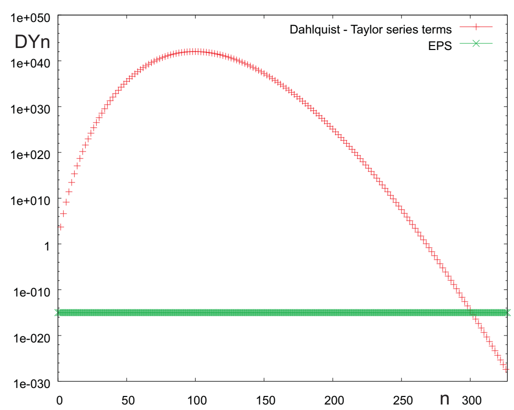

Figure 3: Explicit Taylor series terms, $\lambda = -100$, $h = 1$.

Let us concern in the relative error of the first step, defined as difference between numeric (8), (9) and analytic solution of (7). The relative error for explicit Taylor series is

$$\varepsilon_E(z) = |R_{ET}(z) - e^z|\,, \tag{12}$$

similarly for implicit Taylor series we have

$$\varepsilon_I(z) = |R_{IT}(z) - e^z|\,. \tag{13}$$

Local error of explicit (12) and implicit (13) Taylor series in the first step for $ORD = 1, 2, 3$ can be seen in Fig. 2.

Let's have the example

$$y' = -100y\,, \quad y(t_0) = 1\,, \tag{14}$$

with integration step $h = 1$.

In Fig. 3 can be seen how many Taylor series terms (about 300) are needed in explicit Taylor series to achieve a required accuracy $EPS = 1 \cdot 10^{-15}$ in solution of (14).

The values of explicit Taylor series terms are large (about 10^{40}). Multiple arithmetic for solution (14) with explicit Taylor series must be used Tab. 1.

Table 1: Multiple arithmetic in explicit Taylor series - absolute error in first step ($z = -100$)

bits	$\lvert\varepsilon_E(z)\rvert$
64	$1.3875808066 \times 10^{19}$
128	1.5807982421
256	$3.27147256574024 \times 10^{-39}$
512	"ZERO"

Local error (13) of implicit Taylor series method in the first step can be seen in Tab. 2.

Table 2: Implicit Taylor series - absolute error in first step $\varepsilon_I(z)$

	$\lvert\varepsilon_I(z)\rvert$		
z	$ORD = 1$	$ORD = 3$	$ORD = 5$
-1	0.132121	0.00712056	0.000218718
-10	0.0908637	0.00434699	0.000631343
-50	0.0196078	4.5178×10^{-5}	3.4641×10^{-7}
-100	0.00990099	5.8218×10^{-6}	1.1406×10^{-8}
-500	0.00199601	$4.7712e \times 10^{-8}$	3.8016×10^{-12}
-1000	0.0009990	5.9820×10^{-9}	1.1940×10^{-13}

Conclusion:
Explicit Taylor series method (8) for $n \to \infty$ becomes *A-stable*. With growing number of Taylor series terms multiple arithmetic must be used.

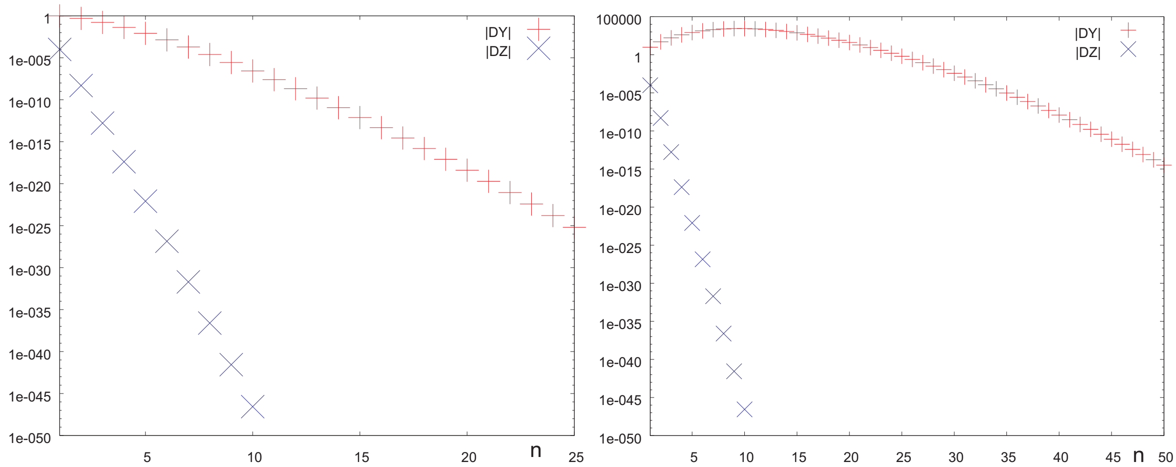

Figure 4: Absolute value of the Taylor series terms, $a = 1$ - left, $a = 10$ - right.

Implicit Taylor series method (9) is *A-stable* numerical method for $ORD = 1, 2$. With growing number of Taylor series terms small instability domains near imaginary axe $\mathrm{Im}(z)$ are occurred. For $n \to \infty$ in (9) instability domains are smaller and instability domains shift to infty along $\mathrm{Im}(z)$. Implicit Taylor series (9) for $\lambda \in \mathcal{R}$ and $n = 1, 2, \dots$ is *L-stable* numerical method

$$\lim_{z\to-\infty} \frac{1}{1 - z + \frac{z^2}{2} - \frac{z^3}{3!} + \dots + \frac{(-z)^n}{n!}} = 0\,.$$

Implicit Taylor series method appear as suitable for stiff systems where eigenvalues $\mathrm{Re}(\lambda) \ll 0$ are occured.

4. Stiff Systems

Let

$$y'_j = f_j(t, y_1, y_2, \dots, y_n), \quad j = 1, 2, \dots, n\,, \qquad (15)$$

be a system of n ordinary differential equations. Let $\mathcal{J}$ be the Jacobian of the (15) and λ_j the eigenvalues of $\mathcal{J}$. The eigenvalues λ_j are generally timedependent. Let the eigenvalues λ_j be arranged in the following way:

$$|\mathrm{Re}\lambda_1| \le |\mathrm{Re}\lambda_2| \le \dots \le |\mathrm{Re}\lambda_n|\,, \qquad (16)$$

and let

$$\lambda_{min} = \lambda_1, \quad \lambda_{max} = \lambda_n\,.$$

One of the most frequently mentioned definition of stiff systems [30] is using a stiffness ratio.

The *stifness ratio* is

$$r = \frac{|\mathrm{Re}\lambda_{max}|}{|\mathrm{Re}\lambda_{min}|}\,. \qquad (17)$$

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).

4.1 Stiff Systems Detection Using Taylor Series Terms

A novel stiff systems detection directly using Taylor series terms in MTSM is presented. Neither Jacobian matrix nor eigenvalues need to be computed.

Let us examine a system

$$\begin{aligned} y' &= -ay\,, \quad a > 0\,, \\ z' &= -0.0001z\,, \end{aligned} \qquad (18)$$

with initial conditions $y(0) = 1$, $z(0) = 1$.

Note: well known analytic solution of (18) is in the form

$$\begin{aligned} y &= e^{-at}, \\ z &= e^{-0.0001t}\,, \end{aligned} \qquad (19)$$

Typically we calculate the Jacobian of the system (18)

$$\mathcal{J} = \begin{pmatrix} -a & 0 \\ 0 & -0.0001 \end{pmatrix},$$

then we specify the eigenvalues of the system (18)

$$\begin{aligned} \lambda_1 &= -a\,, \\ \lambda_2 &= -0.0001\,. \end{aligned}$$

We suppose that $a > 0.0001$ then the stiffness ratio of the system (18) is in the form

$$r = \frac{|\mathrm{Re}\lambda_{max}|}{|\mathrm{Re}\lambda_{min}|} = \frac{a}{0.0001}\,. \qquad (20)$$

Many stiff systems solver needs to compute the Jacobian of the ODEs systems to detect the stiffness. Modern Taylor Series Method as implemented in TKSL software needn't compute Jacobian matrix or eigenvalues of the ODEs systems.

Explicit Taylor series solution of (18) is in the form

$$\begin{aligned} y_{i+1} &= y_i - ah \cdot y_i + \frac{(-ah)^2}{2!} \cdot y_i + \\ &+ \dots + \frac{(-ah)^n}{n!} \cdot y_i\,, \qquad (21) \\ y_{i+1} &= y_i + DY1_i + DY2_i + \dots + DYn_i\,, \qquad (22) \end{aligned}$$

similarly

$$\begin{aligned} z_{i+1} &= z_i - 0.0001h \cdot y_i + \frac{(-0.0001h)^2}{2!} \cdot z_i + \\ &+ \dots + \frac{(-0.0001h)^n}{n!} \cdot z_i\,, \qquad (23) \\ z_{i+1} &= z_i + DZ1_i + DZ2_i + \dots + DZn_i\,. \qquad (24) \end{aligned}$$

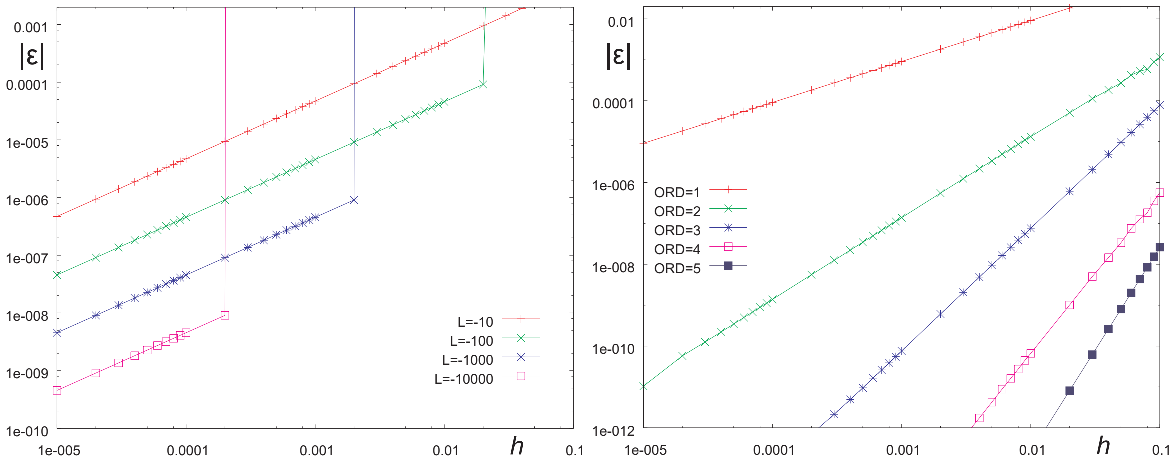

Figure 5: Absolute error at $t = 2$: explicit Euler method - left, explicit Taylor method $L = -10000$ - right.

Let us analyze Taylor series terms in the first step. The absolute value of explicit Taylor series terms $|DZn_i|$ have rapidly decreasing trend. As we can see in Fig. 4 (left) for constant $a = 1$ (respectively $r = 10000$) and integration step size $h = 1$, 15 Taylor series terms are needed to obtain result with local error $EPS = 10^{-10}$.

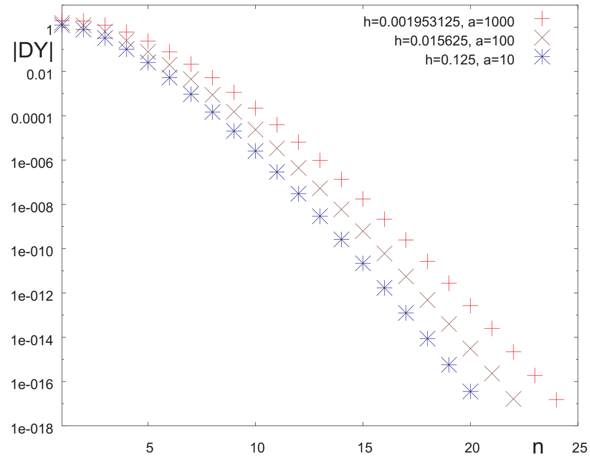

Figure 6: Taylor series terms after automatic step size reduction.

When the constant a is increased (the stiffness ratio r is also increased) we need to use more Taylor series terms to keep the stability of numerical method. In Fig. 4 (right) we can see Taylor series terms for $a = 10$ ($r = 100000$). To obtain local error $EPS = 10^{-10}$ for $a = 10$ we need to use 48 Taylor series terms.

As we can see in Fig. 4 (right) absolute value of explicit Taylor series terms $|DYn_i|$ have increasing character. Modern Taylor series method as implemented in TKSL automatically detects (from different and rapidly growing Taylor series terms) the stiffness in system (18) with growing constant a and automatically reduces integration step size h. Tendency of decreasing Taylor series terms after automatic decreasing step size is shown in Fig. 6.

Conclusion: The TKSL automatically detects stiff system (18) using Taylor series terms and automatically reduces integration step size until the strategy in Fig. 6 is obtained. After detection of stiffness (using explicit MTSM), implicit Taylor series method (ITMRN) must be used as presented in Chapter 4.4.

4.2 Semi-analytic Computation using MTSM

Let us consider the initial value problem [7]

$$y' = L(y - \sin(t)) + \cos(t)\,, \qquad y(0) = 0\,, \qquad L \ll 0\,. \quad (25)$$

the exact solution of which is

$$y = \sin(t)\,. \quad (26)$$

If constant $|L|$ increases as presented in [7] the system (25) becomes "stiff" - explicit numerical methods require smaller integration step size for preserving the stability of computation as we can see in Fig. 5 (left). In Fig. 5 absolute error of numerical solution $|\epsilon(y)|$ which is defined as difference between numerical y_i and exact $y(t_i)$ solution where $t_i = h \cdot i = 2$ can be seen. It is better to use implicit numerical methods for bigger constant $|L|$.

Note: It is an advantage of the explicit Taylor series method using recurrent calculation of the Taylor series terms (implemented in TKSL software) to transform automatically initial value problem (25) into a new system

$$y'_{EKV} = \cos(t)\,, \qquad y(0) = 0\,. \quad (27)$$

which is independent on constant L. The new system (27) has of course the exact solution (26). The new system is non-stiff and absolute error in $t = 2$ is shown in Fig. 5 (right).

Conclusion:
Explicit Taylor series method with recurrent calculation of the Taylor series terms and using auxiliary variables and auxiliary differential equations as is implemented in TKSL automatically transform stiff problem (25) into new equivalent non-stiff problem (27) which is independent on constant L.

4.3 Stiffness Reduction - Using New Equivalent System

Let us examine system

$$\begin{aligned} y' &= z\,, \\ z' &= -a \cdot y - (a+1) \cdot z\,, \qquad a \in (1, \infty)\,, \end{aligned} \quad (28)$$

with initial conditions $y(0) = 1$, $z(0) = -1$.

The eigenvalues of the system (28) are

$$\begin{aligned}\lambda_1 &= -1\,,\\ \lambda_2 &= -a\,,\end{aligned}$$

then the stiffness ratio is $r = \frac{\mathrm{Re}|\lambda_{max}|}{\mathrm{Re}|\lambda_{min}|} = a.$

The system (28) is "stiff" for large constant a and "non-stiff" for small a. Let us create an analytic solution of (28). The system of ODEs (28) can be rewritten into

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

or

$$\begin{aligned}y''+a\cdot y-(a+1)\cdot y' &= 0\\ \lambda^2+(a+1)\cdot\lambda+a &= 0\end{aligned}$$

$$\begin{aligned}\lambda_1 &= \frac{-(a+1)+\sqrt{(a+1)^2-4\cdot a}}{2}\\ \lambda_2 &= \frac{-(a+1)-\sqrt{(a+1)^2-4\cdot a}}{2}\end{aligned}$$

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

Solution is expected in the form

$$y = C_1\cdot e^{\lambda_1\cdot t}+C_2\cdot e^{\lambda_2\cdot t}$$

$$\begin{aligned}y &= C_1\cdot e^{-t}+C_2\cdot e^{-a\cdot t}\\ y' &= -C_1\cdot e^{-t}+-a\cdot C_2\cdot e^{-a\cdot t}\,.\end{aligned}$$

with initial conditions

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

we get

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

The particular solution of the system (28) is

$$\begin{aligned}y &= e^{-t}\,,\\ z &= -e^{-t}\,.\end{aligned}\tag{29}$$

New equivalent system with respect to the system (28) and its particular solution (29) is

$$\begin{aligned}y' &= -y\,, & y(0) &= 1\,,\\ z' &= -z\,, & z(0) &= -1\,.\end{aligned}\tag{30}$$

Conclusion:
After some mathematical computations we have changed and simplified the given stiff problem (28) into non-stiff problem (30) with stiffnes ratio $r = 1$. New non-stiff system of ODEs (30) should be solved with generally used explicit numerical methods.

4.4 ITMRN

Stiff systems in some literature [18] are defined as systems of ODEs where explicit numerical methods don't work and implicit numerical methods must be used.

That is why the new Implicit Taylor Series Method with Reccurrent Calculation of Taylor Series Terms and Newton Iteration Method (ITMRN) is introduced in some special examples.

4.4.1 Stiffness in Electric Circuits

Let's have electric RC circuit Fig. 7 which can be described by differential equation

$$u_C' = \frac{1}{RC}u - \frac{1}{RC}u_C, \tag{31}$$

or

$$u_C' + au_C = au, \quad u_C(0) = 0, \tag{32}$$

where $a = \frac{1}{RC}$.

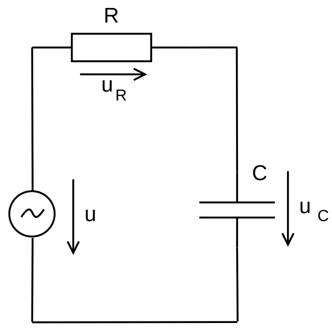

Figure 7: RC circuit.

Analytic solution
To find analytic solution of homogeneous differential equation

$$u_C' + au_C = 0, \tag{33}$$

we start with a characteristic equation

$$\lambda + a = 0, \tag{34}$$

$$\lambda = -a, \tag{35}$$

then eigenvalue (35) is substituted to the expected solution (36) of the homogeneous differential equation (33)

$$u_{Ch} = K(t)e^{\lambda t}. \tag{36}$$

To find non-homogeneous part of solution (32) we use particular integrals

$$u_{Cp} = A\sin(\omega t) + B\cos(\omega t), \tag{37}$$

$$u_{Cp}' = A\omega\cos(\omega t) - B\omega\sin(\omega t). \tag{38}$$

After substitution u_{Cp} (37) and u_{Cp}' (38) into (32) we have

$$\begin{aligned}&A\omega\cos(\omega t) - B\omega\sin(\omega t) + Aa\sin(\omega t) +\\ &+Ba\cos(\omega t) = a\sin(\omega t).\end{aligned}\tag{39}$$

A system of algebraic equations can be obtained as follows

$$A\omega + Ba = 0, \tag{40}$$

$$Aa - B\omega = a. \tag{41}$$

Corresponding solution of (40), (41) is

$$A = \frac{a^2}{a^2+\omega^2}, \tag{42}$$

$$B = -\frac{a\omega}{a^2+\omega^2}. \tag{43}$$

General solution of non-homogeneous differential equation (32) is

$$u_C = u_{Ch} + u_{Cp}, \tag{44}$$

thus

$$u_C = K(t)e^{-at} - \frac{a\omega}{a^2+\omega^2}\cos(\omega t) + \frac{a\omega}{a^2+\omega^2}\sin(\omega t). \tag{45}$$

Particular solution of (32) can be obtained using initial condition $u_C(0) = 0$

$$u_C = \frac{a\omega}{a^2+\omega^2}e^{-at} - \frac{a\omega}{a^2+\omega^2}\cos(\omega t) + \frac{a^2}{a^2+\omega^2}\sin(\omega t)\,. \tag{46}$$

Comparison of analytical (46) and numerical solution using MTSM of RC circuit (32) for $a = 100$, $\omega = 10$ rad/s can be seen in Fig. 8. Note that the printed values of u_C and u_{CA} are the same.

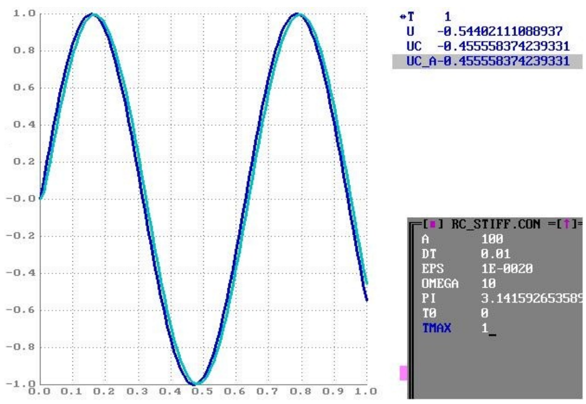

Figure 8: TKSL: numerical and analytical solution of RC circuit.

From analytical solution (46) we can see that

$$\begin{aligned} \lim_{a\to\infty}\left(\tfrac{a\omega}{a^2+\omega^2}\right) &= 0, \\ \lim_{a\to\infty}\left(e^{-at}\right) &= 0, \\ \lim_{a\to\infty}\left(\tfrac{a^2}{a^2+\omega^2}\right) &= 1, \end{aligned}$$

and so

$$\lim_{a\to\infty}(u_C) = \sin(\omega t). \tag{47}$$

Solution (47) is not a surprise. From physical aspect (when we use very small capacitance and resistance than the constant $a = \frac{1}{RC}$ is very large) the differential equation (32) becomes "stiff". Numerical methods have problems with computation (32) for large constant "a" as can be seen in Tab. 3. With increasing constant "a" smaller integration step h must be used. The stiff problem (32) for large "a" can be solved effectively using implicit numerical methods. Basic problem is a "stability problem".

4.4.2 Stability Problem

Let's solve differential equation (well known "Stability problem" [18])

$$y' = -2000(y - \cos(t)), \quad y(0) = 0, \quad t \in \langle 0; 1,5\rangle\,. \tag{48}$$

Table 3: Maximum integration step h_{max} ($a = 2000, \omega = 1$)

numerical method	h_{max}
Euler	4.076×10^{-22}
Runge-Kutta 2. order	1.36×10^{-12}
Runge-Kutta 4. order	5.96×10^{-8}
Taylor (64 terms)	3.125×10^{-3}

Analytic solution is equivalent to RC circuit (32) and for $a = 2000, \omega = 1, u = \cos(t)$ is in the form

$$y = \frac{4000000}{4000001}\cos(t) + \frac{2000}{4000001}\sin(t) - \frac{4000000}{4000001}e^{-2000t} \tag{49}$$

Maximum integration step size of solution (48) using explicit numerical methods can be seen in Tab. 3.

Let's try to find numerical solution of (48) using implicit numerical methods.

Trapezoidal rule

When we use well known formula

$$y_{i+1} = y_i + \frac{1}{2}(hy'_i + hy'_{i+1}), \tag{50}$$

for solution (48) we obtain

$$y_{i+1} = \frac{y_i(1-1000h) + 1000h(\cos(t+h)+\cos(t))}{1+1000h}. \tag{51}$$

Implicit Euler method

When we use well known formula

$$y_{i+1} = y_i + hy'_{i+1}, \tag{52}$$

for solution (48) we obtain

$$y_{i+1} = \frac{y_i + 2000h\cos(t+h)}{1+2000h}. \tag{53}$$

Implicit Taylor series method

When we use well known formula

$$y_{i+1} = y_i + hy'_{i+1} - \cdots - \frac{(-h)^n}{n!}y^{(n)}_{i+1}, \tag{54}$$

for solution (48) we obtain

$$\begin{aligned} y_{i+1} = {} & \frac{y_i + h(-2000(-\cos(t+h))}{1-h(-2000)+\frac{h^2}{2}(-2000)^2-\frac{h^3}{3!}(-2000)^3+\cdots} - \\ & -\frac{\frac{h^2}{2}(-2000(-2000(-\cos(t+h))+\sin(t+h)))}{1-h(-2000)+\frac{h^2}{2}(-2000)^2-\frac{h^3}{3!}(-2000)^3+\cdots} + \\ & +\frac{\frac{h^3}{3!}(-2000(-2000(-2000(-\cos(t+h))+\sin(t+h))+\cos(t+h)))}{1-h(-2000)+\frac{h^2}{2}(-2000)^2-\frac{h^3}{3!}(-2000)^3+\cdots} - \cdots \end{aligned}$$

Numerical solution of (48) using implicit numerical methods (50), (52) and (54) can be seen in Fig. 9. The implicit Taylor series has the best approximation from the previous numerical methods and the largest integration step h can be used.

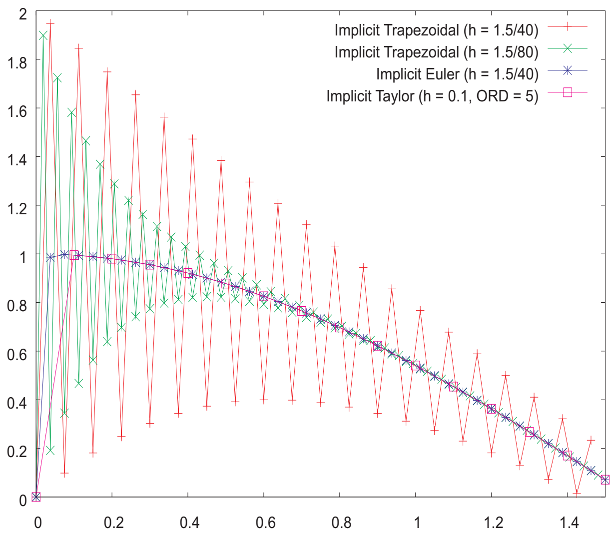

Figure 9: Implicit numerical methods.

Implicit Taylor Series Method with Reccurrent Calculation of Taylor Series Terms and Newton Iteration Method (ITMRN)

For automatic recurrent calculation of higher implicit Taylor series terms we need to use auxiliary variables and differential equations. For solution term y_{i+1} we need to use Newton iteration method.

Absolute error of ITMRN numerical solution is defined as difference between numerical y_i and analytical $y(t_i)$ solution

$$|\text{Error}(y)| = |y_i - y(t_i)|\,, \tag{55}$$

where $t_i = h \cdot i$.

Table 4: ITMRN absolute errors, $ORD = 5, TOL = 10^{-15}$

	$\|\text{Error}(y)\|$		New. iterat.	
t	$h_1 = 0.25$	$h_2 = 0.5$	j_1	j_2
0.25	3.03123×10^{-7}	-	2	-
0.5	5.12372×10^{-7}	1.29815×10^{-5}	2	2
0.75	5.79973×10^{-7}	-	2	-
1	4.73771×10^{-7}	6.16008×10^{-6}	2	2
1.25	1.80985×10^{-7}	-	2	-
1.5	2.89796×10^{-7}	2.2726×10^{-5}	2	2

Table 5: ITMRN absolute errors, $h = 0.5, ORD = 10, TOL = 10^{-15}$

t	$\|\text{Error}(y)\|$	New. iterations
0.5	9.99822×10^{-12}	2
1	2.42912×10^{-11}	2
1.5	3.39579×10^{-11}	2

Absolute errors for different integration step size h and Taylor series terms ORD can be seen in Tab. 4, 5. Take a notice of the same number of Newton iterations j for the different integration step and different number of Taylor series terms.

Absolute errors for different order ORD of ITMRN in first step is shown in Tab. 6.

Table 6: ITMRN absolute errors in first step, $h = 1.5$, $TOL = 10^{-10}$

ORD	$\|\text{Error}(y)\|$	New. iterations
1	0.236354	2
2	0.126078	2
3	0.21045	2
4	0.026256	2
5	0.0144353	2
6	0.00107299	2
7	0.00059927	2
8	3.01715×10^{-5}	2
9	1.51633×10^{-5}	2
10	5.67345×10^{-7}	2
11	2.60475×10^{-7}	2
12	7.66305×10^{-9}	2
13	3.23702×10^{-9}	2
14	7.78821×10^{-11}	2
15	3.04601×10^{-11}	2
16	6.17006×10^{-13}	2
17	2.24515×10^{-13}	2
18	4.02456×10^{-15}	2
19	1.34615×10^{-15}	2

4.4.3 Test Example

Let us analyze system [30]

$$\begin{aligned} y' &= z\,, \\ z' &= -b \cdot y - (b+1) \cdot z\,, \qquad b \in (1, \infty)\,, \end{aligned} \tag{56}$$

with initial conditions $y(0) = 1$, $z(0) = -1$.

Well known analytic solution of (56) is in the form

$$\begin{aligned} y &= e^{-t}\,, \\ z &= -e^{-t}\,. \end{aligned} \tag{57}$$

The system (56) becomes stiff for $b \gg 0$ and stiffness ratio is $r = b$.

Let's try to find the solution of (56) with explicit Taylor series method. Absolute error is shown in Tab. 7. Abbreviation $ORD = 1$ means that 2 Taylor series terms are used during the computation (explicit Euler method) in Tab. 7. Explicit Euler method becomes unstable with growing constant a according to the Tab. 7. We should reduce integration step size, or we must use more Taylor series terms Tab. 8.

Multiple arithmetic: with growing constant a multiple arithmetic is needed. Only 9 Taylor series terms are used for integration step $h = 0.1$ and local error $EPS = 10^{-20}$.

Table 7: Explicit Taylor series method absolute errors, $h = 0.1$, $ORD = 1$

	$\lvert \text{Error}(z) \rvert$			
t	$b = 10^4$	$b = 10^5$	$b = 10^6$	$b = 10^7$
0.1	0.004837	0.004837	0.004837	0.004837
0.2	0.008730	0.008730	0.008730	0.008730
0.3	0.011818	0.011818	0.011818	0.011781
0.4	0.01422	0.014307	0.037502	37.2672
0.5	0.016076	0.856836	2328.16	3.72529×10^7
0.6	0.018722	8727.91	2.328×10^8	3.72529×10^{13}

Table 8: Explicit Taylor series method absolute errors, $h = 0.1$, $b = 100$

	$\lvert \text{Error}(y) \rvert$		
t	$ORD = 2$	$ORD = 3$	$ORD = 4$
0.1	0.000162582	4.0847×10^{-6}	8.1964×10^{-7}
0.2	0.000294247	7.39197×10^{-6}	1.48328×10^{-7}
0.3	0.000399404	1.00328×10^{-5}	2.0132×10^{-7}
0.4	0.000481905	1.2104×10^{-5}	2.4302×10^{-7}
0.5	0.000545106	1.36903×10^{-5}	3.14994×10^{-7}
0.6	0.000591932	1.48514×10^{-5}	1.20207×10^{-5}

Corresponding word length of Taylor series terms for large constant b are shown in Tab. 9.

Table 9: Multiple arithmetic

b	Word length [bits]
10^{10}	3681
10^{20}	8900
10^{50}	24000

TKSL automatically detects stiffness in system (56) (when b is growing) from Taylor series terms and TKSL uses automatically smaller step size.

Implicit Taylor series method has prosperous properties to solve stiff systems especially implicit Taylor series method has bigger absolute stability domain than those of explicit Taylor series method.

Let's solve the system (56) with implicit Taylor series method. Implicit Taylor series is in the form

$$\begin{aligned} y_{i+1} &= y_i + h y'_{i+1} - \cdots - \tfrac{(-h)^n}{n!} y_{i+1}^{(n)} , \\ z_{i+1} &= z_i + h z'_{i+1} - \cdots - \tfrac{(-h)^n}{n!} z_{i+1}^{(n)} , \end{aligned} \qquad (58)$$

where higher derivations are in the form

$$\begin{aligned} y'_{i+1} &= z_{i+1} , \\ z'_{i+1} &= -b y_{i+1} - (b+1) z_{i+1} , \\ \\ y''_{i+1} &= -b y_{i+1} - (b+1) z_{i+1} , \\ z''_{i+1} &= -b y'_{i+1} - (b+1) z'_{i+1} = -b z_{i+1} - \\ &\quad -(b+1)(-b y_{i+1} - (b+1) z_{i+1}) , \\ \\ y'''_{i+1} &= -b z_{i+1} - (b+1)(-b y_{i+1} - (b+1) z_{i+1}) , \\ z'''_{i+1} &= -b(-b y_{i+1} - (b+1) z_{i+1}) - (b+1) \cdot \\ &\quad \cdot (-b z_{i+1} - (b+1)(-b y_{i+1} - (b+1) z_{i+1})) , \\ \\ y^{(4)}_{i+1} &= -b(-b y_{i+1} - (b+1) z_{i+1}) - (b+1) \cdot \\ &\quad \cdot (-b z_{i+1} - (b+1)(-b y_{i+1} - (b+1) z_{i+1})) , \\ z^{(4)}_{i+1} &= -b(-b z_{i+1} - (b+1) z'_{i+1}) - (b+1) \cdot \\ &\quad \cdot (-b z'_{i+1} - (b+1)(-b z_{i+1} - (b+1) z'_{i+1})) , \\ &\vdots \end{aligned}$$

After substitution higher derivations into implicit Taylor series form (58) we obtain numerical solution in the form

$$\begin{aligned} y_{i+1} &= \tfrac{y_i(hb+h+1) + z_i(h)}{1 + h^2 b + hb + h} , \\ z_{i+1} &= -\tfrac{y_i(hb) - z_i}{1 + h^2 b + hb + h} , \end{aligned}$$

for implicit Taylor series order 1 ($ORD = 1$) that is implicit Euler method.

Similarly for $ORD = 2$ we obtain formula in the form

$$\begin{aligned} y_{i+1} &= 2 \tfrac{y_i(h^2b^2 + h^2b + 2hb + h^2 + 2h + 2) + z_i(h^2b + h^2 + 2h)}{2h^2 + 2h^3b^2 + h^4b^2 + 2h^3b + 4 + 4hb + 4h + 4h^2b + 2h^2b^2} , \\ z_{i+1} &= -2 \tfrac{y_i(h^2b^2 + 2hb + h^2b) + z_i(h^2b - 2)}{2h^2 + 2h^3b^2 + h^4b^2 + 2h^3b + 4 + 4hb + 4h + 4h^2b + 2h^2b^2} , \end{aligned}$$

implicit Taylor series $ORD = 3$ is in the form

$$\begin{aligned} y_{i+1} &= 6(y_i(h^3b^3 + h^3b^2 + h^3b + h^3 + 3h^2b^2 + 3h^2b + \\ &\quad +3h^2 + 6hb + 6h + 6) + z_i(6h + h^3b + h^3 + 3h^2 + \\ &\quad +3h^2b + h^3b^2))/(36 + 36h^2b + 6h^3b^3 + 36hb + \\ &\quad +3h^5a^3 + 3h^5b^2 + h^6b^3 + 18h^2 + 18h^3b^2 + 36h + \\ &\quad +18h^3b + 9h^4a^2 + 6h^4b^3 + 6h^4b + 6h^3 + 18h^2b^2) , \\ z_{i+1} &= -6(y_i(3h^2b^2 + 6ha + 3h^2b + h^3b + h^3b^2 + h^3b^3) + \\ &\quad +z_i(-6 + 3h^2b + h^3a^2 + h^3b))/(36 + 36h^2b + \\ &\quad +6h^3b^3 + 36hb + 3h^5b^3 + 3h^5a^2 + h^6b^3 + \\ &\quad +18h^2 + 18h^3b^2 + 36h + 18h^3b + 9h^4b^2 + \\ &\quad +6h^4b^3 + 6h^4b + 6h^3 + 18h^2b^2) , \end{aligned}$$

etc.

Absolute errors of numerical solution using implicit Taylor series method of different order is shown in Tab. 10. Note that constant b has no influence on error of computation.

There is a problem with general formulation of y_{i+1}, z_{i+1} from implicit Taylor series formula (58) - other implicit numerical methods have the same problem. We have to use some iteration method to compute y_{i+1}, z_{i+1} in implicit form.

Implicit Taylor series method with recurrent calculation of Taylor series terms and Newton iteration (ITMRN) was implemented. Absolute errors of ITMRN of $ORD = 2, 3, 4$ are the same as explicit calculations presented in Tab. 10 and only two Newton iterations are needed. Absolute errors of ITMRN $ORD = 5, 6, 7$ and number of

Table 10: Implicit Taylor series method absolute errors $h = 0.1$

	$\vert\text{Error}(y)\vert$: $b = 10^4, 10^5, 10^6, 10^7, 10^8$		
t	$ORD = 2$	$ORD = 3$	$ORD = 4$
0.1	0.000139958	3.48077×10^{-6}	6.93811×10^{-8}
0.2	0.000253297	6.29908×10^{-6}	1.25557×10^{-7}
0.3	0.000343816	8.54948×10^{-6}	1.70413×10^{-7}
0.4	0.000414829	1.03145×10^{-5}	2.05595×10^{-7}
0.5	0.000469227	1.16662×10^{-5}	2.32538×10^{-7}
0.6	0.000509528	1.26673×10^{-5}	2.52491×10^{-7}

Newton iterations j which are needed to obtain numerical results with tolerance $TOL = 10^{-10}$ are shown in Tab. 11.

Table 11: ITMRN absolute errors $h = 0.1$, $ORD = 5, 6, 7$, $TOL = 10^{-10}$, $b = 10^4$

	$ORD = 5$		$ORD = 6$		$ORD = 7$	
t	$\vert\text{Error}(y)\vert$	j	$\vert\text{Error}(y)\vert$	j	$\vert\text{Error}(y)\vert$	j
0.1	1.15×10^{-9}	3	1.64×10^{-11}	3	2.03×10^{-13}	5
0.2	2.08×10^{-9}	3	2.97×10^{-11}	3	3.45×10^{-13}	5
0.3	2.83×10^{-9}	3	4.04×10^{-11}	3	4.84×10^{-13}	5
0.4	3.41×10^{-9}	3	4.87×10^{-11}	3	5.89×10^{-13}	5
0.5	3.86×10^{-9}	3	5.51×10^{-11}	3	6.35×10^{-13}	4
0.6	4.19×10^{-9}	3	5.98×10^{-11}	3	6.99×10^{-13}	5

Problem with increasing the number of Newton iterations j with increasing order of implicit Taylor series method is shown in Tab. 11. We should use multiple arithmetic with growing constant b and order of ITMRN or we should reduce integration step size to obtain better stability of ITMRN (Tab. 12). Absolute errors of ITMRN $ORD = 8$ and number of Newton iterations using in each step are shown in Tab. 12. There are two integration step size used $h_1 = 0.1$ with absolute error $|\text{Error}_1(y)|$ and number of Newton iterations j_1 resp. $h_2 = 0.05$ with absolute error $|\text{Error}_2(y)|$ and number of Newton iterations j_2. The same arithmetic (double precision) is used in both cases.

Table 12: ITMRN absolute errors $h_1 = 0.1$, $h_2 = 0.05$, $ORD = 8$, $TOL = 10^{-10}$, $b = 10^4$

t	$\vert\text{Error}_1(y)\vert$	j_1	$\vert\text{Error}_2(y)\vert$	j_2
0.05	—	—	7.10543×10^{-15}	4
0.1	2.148×10^{-12}	9	1.77636×10^{-15}	4
0.15	—	—	5.00711×10^{-14}	4
0.2	2.753×10^{-14}	8	9.17044×10^{-14}	4
0.25	—	—	8.71525×10^{-14}	5
0.3	6.328×10^{-14}	19	8.23785×10^{-14}	5
⋮	⋮	⋮	⋮	⋮
0.6	4.938×10^{-12}	7	1.77636×10^{-14}	4

5. Conclusions

A very interesting and promising 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 using Taylor series terms and solution of large systems of ordinary differential equations has been found.

The new Implicit Taylor Series Method with Reccurrent Calculation of Taylor Series Terms and Newton Iteration Method (ITMRN) was proposed. ITMRN has prosperous properties to solution "stiff systems" with large eigenvalues $\lambda \ll 0$. ITMRN algorithm is also suitable to parallelization. In many cases multiple arithmetics need to be used.

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