A NOTE ON STABILITY INVESTIGATIONS FOR ROSENBROCK-TYPE METHODS FOR QUASILINEAR-IMPLICIT DIFFERENTIAL EQUATIONS

M. BÜTTNER, R. WEINER AND K. STREHMEL

Abstract — Zusammenfassung

The solution of quasilinear-implicit ODEs using Rosenbrock type methods may suffer from stability problems despite of stability properties as A-stability or L-stability, respectively. These problems are caused by inexact computation of artificial introduced components (transformation to DAE system). The paper investigates the source of the numerical difficulties and shows modifications to overcome the problems.

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Key words: Rosenbrock-type methods, quasilinear-implicit differential equations, GMRES, Arnoldi method

Bei der Lösung quasilinear-impliziter ODE's mittels Rosenbrock-Typ-Methoden können trotz guter Stabilitätseigenschaften (A- bzw. L-Stabilität) des Grundverfahrens Stabilitätsprobleme auftreten. Diese Schwierigkeiten sind auf Ungenauigkeiten bei der Berechnung künstlich eingeführter Komponenten (Überführung in DAEs) zurückzuführen. Die Arbeit untersucht die Ursachen für diese Effekte und zeigt Möglichkeiten, die Probleme zu überwinden.

1. Introduction

We consider quasilinear-implicit differential equations with solution-dependent matrix multiplying the derivative.

$$B(y(t))y'(t) = f(y(t)), \quad t \in [t_0, t_e] \tag{1.1}$$
$$y(t_0) = y_0$$

These equations arise e.g. in electrical network simulation [3], and modelling combustion problems and in chemical reaction kinetics [2].

The matrix B may be singular. The conditions

(1.2) $f(y_0) \in \text{range}(B(y_0))$,

(1.3) B is of constant rank in a neighbourhood of the solution,

(1.4) the matrix pencil $\{A + \lambda B\}$, with $A = \frac{\partial}{\partial y}(f(y) - B(y)y')$ has index 1 of nilpotency along the solution

guarantee the existence of a unique, smooth solution y of (1.1) [5].

For such problems, also with regular $B(y)$, Hairer/Wanner [4] propose to formulate the system (1.1) in the equivalent form

$$
\begin{aligned}
y' &= z \\
0 &= f(y) - B(y)z.
\end{aligned} \tag{1.5}
$$

Then codes like RADAU5 can be applied directly, there is no need for explicit computation of $B(y)^{-1}$. Lubich/Roche [5] use the same approach to construct Rosenbrock type methods for (1.1) under conditions (1.2)–(1.4) of the form

$$
y_{m+1} = y_m + h\sum_{i=1}^{s} b_i k_i^{(y)} \qquad\qquad z_{m+1} = z_m + h\sum_{i=1}^{s} b_i k_i^{(z)} \tag{1.6}
$$

$$
\begin{aligned}
Ek_i^{(y)} &= f(y_{m+1}^{(i)}) + [B(y_m) - B(y_{m+1}^{(i)})]z_{m+1}^{(i)} + h\,\frac{\partial}{\partial y}[f(y) - B(y)z_m)]\Big|_{y=y_m} \sum_{j=1}^{i-1} \gamma_{ij} k_j^{(y)} \\
k_i^{(z)} &= \frac{1}{h\gamma}\left\{ k_i^{(y)} - \left[z_{m+1}^{(i)} + \sum_{j=1}^{i-1} \gamma_{ij} k_j^{(z)} \right] \right\}, \quad i = 1, \ldots, s \\
E &= \left\{ B(y_m) - h\gamma\,\frac{\partial}{\partial y}[f(y) - B(y)z_m]\Big|_{y=y_m} \right\}
\end{aligned}
$$

$$
y_{m+1}^{(i)} = y_m + h\sum_{j=1}^{i-1} a_{ij} k_j^{(y)} \qquad\qquad z_{m+1}^{(i)} = z_m + h\sum_{j=1}^{i-1} a_{ij} k_j^{(z)}.
$$

The analytical computation of the product $\frac{\partial}{\partial y}B(y)z_m$ can be avoided, using the Fréchet derivative

$$
\frac{\partial}{\partial y}B(y)z_m\Big|_{y=y_m} \approx (B(y_m + \delta z_m) - B(y_m))/\delta. \tag{1.7}
$$

Our aim is to study the stability of this method.

For stiff explicit ODEs the stability of numerical methods is studied for the test equation of A-stability

$$
y' = \lambda y, \quad \mathrm{Re}\,\lambda < 0. \tag{1.8}
$$

One step methods give for (1.8)

$$
y_{m+1} = R_0(h\lambda)y_m, \tag{1.9}
$$

where $R_0(h\lambda)$ is the stability function. For ROW-methods the stability function is given by (see [4])

$$
\begin{aligned}
R_0(\zeta) &= 1 + \sum_{k=0}^{s-1} b^T \beta^k \mathbb{1}(1-\gamma\zeta)^{-(k+1)}\zeta^{k+1}, \\
b &= (b_1, \ldots, b_s)^T \\
\mathbb{1} &= (1, \ldots, 1)^T \\
\beta &= (\beta_{ij}), \quad \beta_{ij} = a_{ij} + \gamma_{ij}.
\end{aligned} \tag{1.10}
$$

For systems of the form (1.1) it seems natural to study the stability with respect to the semi-implicit form of (1.8)

$$\frac{1}{\lambda y}y' = 1, \qquad y(t_0) = y_0. \tag{1.11}$$

Applying (1.6) to (1.11) in form (1.5) with exact initial values we get

$$y_1 = \tilde{R}_0(\zeta)y_0, \tag{1.12}$$

where $\tilde{R}_0(\zeta) = R_0(\zeta)$, i.e. the method is stable for (1.11), if it is A-stable for problem (1.8). However practical tests give surprising results. In Lubich/Roche [5] an 4-stage ROW-method of order $p = 3$ for problem (1.1) is developed, where because of $\beta_{sj} = b_j$, $(j = 1, \ldots, s)$ the stability function satisfies $R_0(\infty) = 0$. With $\gamma = 0.3$ this method is A-stable for ODE's.

We applied this method to (1.11) and got the results presented in table 1.1

TOL	λ	accepted steps	rejected steps
10^{-2}	-10	23	0
	-10^3	1127	668
	-10^5	103818	66830
10^{-4}	-10	85	0
	-10^3	1128	604
	-10^5	108416	66379
10^{-6}	-10	382	0
	-10^3	2310	641
	-10^5	105314	68738

TABLE 1.1. Numerical results for the method of Lubich/Roche for example (1.11)

This clearly indicates stability problems for the method.

Remark 1.1. The above mentioned stability problems are not due to $y \to 0$. Similar results were obtained on a modified Prothero-Robinson equation

$$\begin{aligned} \frac{1}{\lambda(y(t) - g(t)) + g'(t)}y'(t) = 1, \quad t \in [0, 1] \\ g(t) = 2t + \sin(t) \quad \square \end{aligned} \tag{1.13}$$

In the following we will explain the poor performance of the method. We will see, that in general L-stable methods have some stability problems for (1.11).

2. Stability investigations

For the linearly implicit Euler method, when applied to (1.11), we have to solve $(\frac{1}{\lambda y_m} - h\frac{z_m}{\lambda y_m^2})k_1 = 1$. Then we get

$$
\begin{aligned}
y_{m+1} &= R_0^{(y)} \cdot y_m \\
z_{m+1} &= R_0^{(z)} \cdot y_m
\end{aligned} \tag{2.1}
$$

where with $\alpha_m = \frac{z_m}{y_m}$

$$
\begin{aligned}
R_0^{(y)} &= \frac{1 + (\lambda - \alpha_m)h}{1 - h\alpha_m} \\
R_0^{(z)} &= \frac{\lambda}{1 - h\alpha_m}.
\end{aligned} \tag{2.2}
$$

For $z_m \approx z(t_m)$, $y_m \approx y(t_m)$ we have $\alpha \approx \lambda$, for which both $R_0^{(y)}$ and $R_0^{(z)}$ are reasonably bounded. We observed, that the instability of the method was due to large variations of α. From (2.1) we have

$$
\begin{aligned}
\alpha_{m+1} &= \frac{R_0^{(z)}}{R_0^{(y)}} \\
&= \frac{\lambda}{1 + (\lambda - \alpha_m)h} \\
&= \Phi(\alpha_m).
\end{aligned} \tag{2.3}
$$

It is clear λ is a fixed point of the iteration (2.3). To obtain stability we have to ensure, that Φ is contractive, i.e. $|\Phi'(\lambda) < 1|$. We now investigate a general s-stage method.

Applying (1.6) to (1.11) we get with $K_i = k_i^{(y)}/y_m$, $L_i = k_i^{(z)}/y_m$ and $\alpha_m = z_m/y_m$

$$
\begin{aligned}
K_i &= \frac{1}{1 - h\gamma\alpha_m}\left[\lambda + \left(1 - \frac{1}{1 + h\sum_{j=1}^{i-1} a_{ij}K_j}\right)\left(\alpha_m + h\sum_{j=1}^{i-1} a_{ij}L_j\right) + \alpha_m h\sum_{j=1}^{i-1}\gamma_{ij}K_j\right] \\
L_i &= \frac{1}{h\gamma}\left[K_i - \alpha_m - h\sum_{j=1}^{j-1}\beta_{ij}L_j\right]
\end{aligned} \tag{2.4}
$$

and

$$
\begin{aligned}
\alpha_{m+1} &= \Phi(\alpha_m) \\
&= \frac{z_{m+1}}{y_{m+1}} \\
&= \frac{\alpha_m + h\sum_{i=1}^{s} b_i L_i}{1 + h\sum_{i=1}^{s} b_i K_i}
\end{aligned} \tag{2.5}
$$

Starting from consistent initial values we have to ensure, that the mapping Φ is contractive.

We now investigate $\frac{\partial \Phi}{\partial \alpha}\Big|_{\alpha=\lambda}$.

(2.6)

$$\frac{\partial \Phi}{\partial \alpha} = \left(1 + h\sum_{i=1}^{s} b_i K_i\right)^{-2} \left[\left(1 + h\sum_{i=1}^{s} b_i L_i'\right)\left(1 + h\sum_{i=1}^{s} b_i K_i\right) - \left(\alpha + h\sum_{i=1}^{s} b_i L_i\right)\left(h\sum_{i=1}^{s} b_i K_i'\right)\right]$$

The derivatives $\frac{\partial K_i}{\partial \alpha}$ and $\frac{\partial L_i}{\partial \alpha}$ are recursively determined and needed for $\alpha = \lambda$ only.

Lemma 2.1. *It holds*

$$L_j(\lambda) = \lambda K_j(\lambda). \tag{2.7}$$

Proof. (by induction) Let $j = 1$:

$$\begin{aligned} L_1(\lambda) &= \frac{1}{h\gamma}\left[K_1 - \alpha\right]\Big|_{\alpha=\lambda} \\ &= \frac{\lambda - \alpha(1 - h\gamma\alpha)}{h\gamma(1 - h\gamma\alpha)}\Bigg|_{\alpha=\lambda} \\ &= \frac{\lambda}{1 - h\gamma\lambda}\lambda \\ &= \lambda K_1(\lambda) \end{aligned} \tag{2.8}$$

Let (2.7) hold for $j = 1, \ldots, i-1$.

(2.9)

$$\begin{aligned} L_i(\lambda) =& \frac{1}{h\gamma}\left\{\frac{1}{1 - h\gamma\lambda}\left[\lambda + \left(1 - \frac{1}{1 + h\sum_{j=1}^{i-1} a_{ij}K_j(\lambda)}\right)(\lambda + h\sum_{j=1}^{i-1} a_{ij}L_j(\lambda)) + h\lambda\sum_{j=1}^{i-1}\gamma_{ij}K_j(\lambda)\right]\right. \\ & \left. - \lambda - h\sum_{j=1}^{i-1}\beta_{ij}L_j(\lambda)\right\} \\ =& \frac{1}{h\gamma(1 - h\gamma\lambda)}\left\{\lambda\left(1 + h\sum_{j=1}^{i-1}\beta_{ij}K_j(\lambda)\right) - \lambda(1 - h\gamma\lambda)\left[1 - h\sum_{j=1}^{i-1}\beta_{ij}K_j(\lambda)\right]\right\} \\ =& \lambda K_i(\lambda) \end{aligned}$$

■

With Lemma 2.1 the evaluation of (2.6) at $\alpha = \lambda$ simplifies to

$$\frac{\partial \Phi}{\partial \alpha}\Big|_{\alpha=\lambda} = \left(1 + h\sum_{i=1}^{s} b_i K_i(\lambda)\right)^{-1}\left(1 + h\sum_{i=1}^{s} b_i L_i'(\lambda) - h\lambda\sum_{i=1}^{s} b_i K_i'(\lambda)\right) \tag{2.10}$$

with
(2.11)

$$
\begin{aligned}
K_i(\lambda) &= \frac{\lambda}{1-h\gamma\lambda}\left[1+h\sum_{j=1}^{i-1}\beta_{ij}K_j(\lambda)\right] \\
K_i'(\lambda) &= \frac{1}{1-h\gamma\lambda}\left[1+h\gamma K_i(\lambda)+h\sum_{j=1}^{i-1}\gamma_{ij}K_j(\lambda)+h\lambda\sum_{j=1}^{i-1}\gamma_{ij}K_j'(\lambda)+h\sum_{j=1}^{i-1}a_{ij}L_j'(\lambda)\right. \\
&\qquad\left.-\frac{1+h\sum_{j=1}^{i-1}a_{ij}(L_j'(\lambda)-\lambda K_j'(\lambda))}{1+h\sum_{j=1}^{i-1}a_{ij}K_j(\lambda)}\right] \\
L_i'(\lambda) &= \frac{1}{h\gamma}\left[K_i'(\lambda)-1-h\sum_{j=1}^{i-1}\beta_{ij}L_j'(\lambda)\right]
\end{aligned}
$$

We now have to fulfil $|\Phi'(\lambda)| < 1$ to ensure convergence of the iteration (2.5), i.e. the desired stability property.

For the method of Lubich/Roche we have plotted $\Phi'(\lambda)$ in figure 2.1 with different scalings for λ in order to show the poles of Φ' as well as the bounded stability interval.

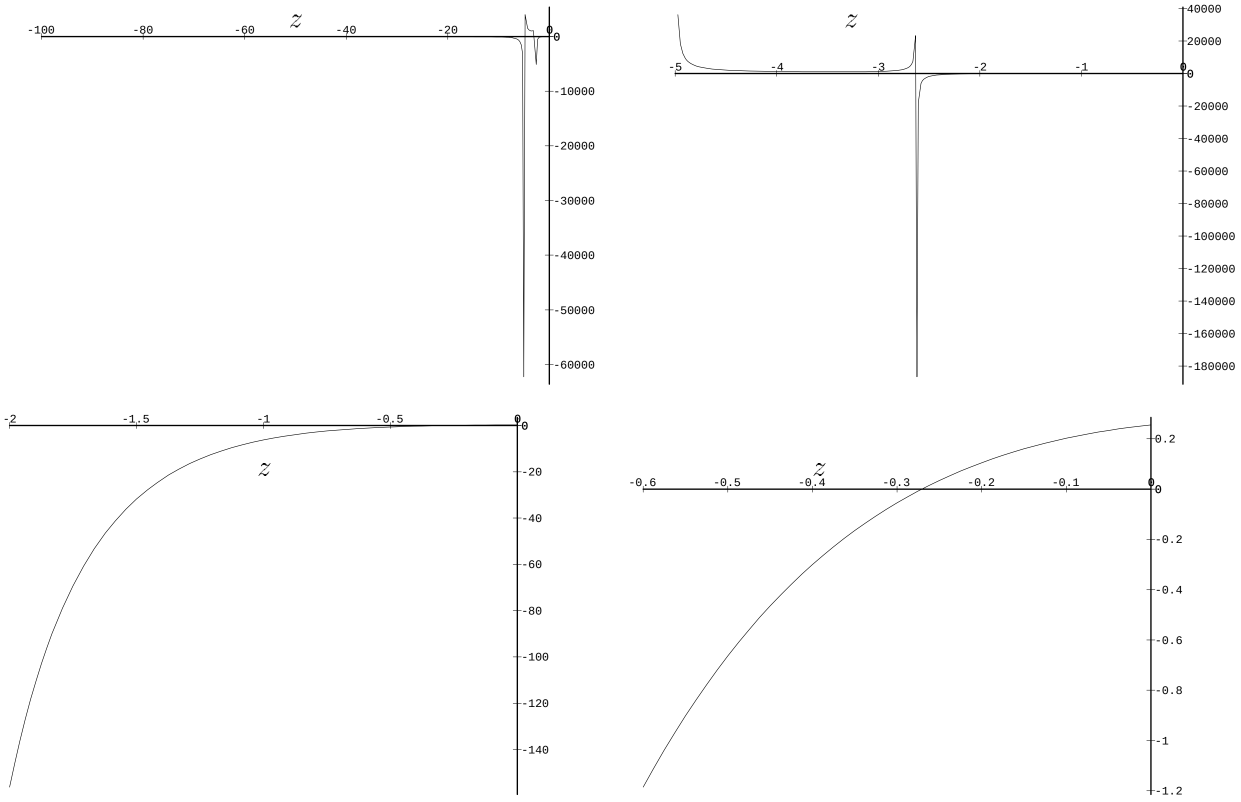

FIGURE 2.1. Stability ($\Phi'(\lambda)$) of the method of Lubich/Roche

The tests with the 4-stage method of Lubich/Roche [5] (c.f. table 1.1) showed a strong restriction in the stepsize. This is due to the lack of stability with respect to α, as the figures 2.1 demonstrate.

The stability domain is on the real axis bounded by about $z := h\lambda = -0.5683687354$. Thus the restrictions are very stringent with respect to h with moderate λ already.

Remark 2.1. In general one could not expect L-stable methods to be unrestricted stable for problem (1.11). This is due to the fact, that the denominator of (2.10) is just the stability function $R_0(z)$ of standard ROW methods. Additionally, as (2.11) indicates, the denominator of (2.10) will also contain the internal stability functions via $K_i'(\lambda)$. If in this situation the zeros of the stability functions are not met by an zero of equal multiplicity of the numerator of Φ', the function $\Phi'(\lambda)$ will not be bounded in this points.

3. Construction of stable methods

The methods have to be constructed with growing stage number s.

Example 3.1. Let $s = 1$. We have

$$\begin{aligned} K_1(\lambda) &= \frac{\lambda}{1 - h\gamma\lambda} \\ K_1'(\lambda) &= \frac{h\gamma\lambda}{(1-h\gamma\lambda)^2} \\ L_1'(\lambda) &= \frac{-1 + 3h\gamma\lambda - h^2\gamma^2\lambda^2}{h\gamma(1-h\gamma\lambda)^2} \end{aligned} \tag{3.1}$$

So we get

$$\left.\frac{\partial\Phi}{\partial\alpha}\right|_{\alpha=\lambda} = \frac{1 - 1/\gamma + (2-\gamma)h\lambda}{1 + (1-\gamma)h\lambda}. \tag{3.2}$$

For $\mathrm{Re}\,\lambda < 0$ the function $\Phi'(\lambda)$ is analytical, if $\gamma > 1$. In fact we have the desired property of $|\Phi'(\lambda)| < 1 \quad (\forall\lambda : \ Re\lambda < 0)$, if $\gamma \in (\frac{3}{2}, \infty)$. According to remark 2.1 we cannot have an L-stable method with unrestricted stability with respect to α. The zero of the denominator is $h\lambda = \frac{1}{1-\gamma}$ and for the numerator it is $h\lambda = \frac{\gamma-1}{\gamma(2-\gamma)}$, which are not identical for all $h\lambda \in \mathbb{C}^-$. The method with $\gamma > \frac{3}{2}$ however is strongly A-stable.

Example 3.2. Let $s = 2$. $K_2(\lambda)$, $K_2'(\lambda)$ and $L_2'(\lambda)$ are computed according to (2.11). The parameters are set to give a method of order 2. The free parameters are set $b_2 = 1/2$, $c_2 = 1$. Thus $\beta_{21} = (1/2 - \gamma)/b_2$ and $\gamma_{21} = \beta_{21} - c_2$. We have to investigate

$$\left.\frac{\partial\Phi}{\partial\alpha}\right|_{\alpha=\lambda} = \frac{P(\lambda)}{\gamma^2(1 + (1-2\gamma)h\lambda + (1/2 - 2\gamma + \gamma^2)h^2\lambda^2)(1 + (1-\gamma)h\lambda)} \tag{3.3}$$

where

$$\begin{aligned} P(\lambda) =& 1/2 - 2\gamma + \gamma^2 + \left(-\frac{7\gamma}{2} + 8\gamma^2 - 3\gamma^3\right) h\lambda + \left(7\gamma^2 - 11\gamma^3 + 3\gamma^4\right) h^2\lambda^2 + \\ & \left(\frac{\gamma^2}{2} - 5\gamma^3 + 5\gamma^4 - \gamma^5\right) h^3\lambda^3 \end{aligned}$$

This 2-stage ROW method is strongly A-stable for values $\gamma \geq \frac{1}{4}$. Figure 3.1 clearly shows the poles of $\Phi'(-\infty)$ for $\gamma \in \{1 - \frac{\sqrt{2}}{2}, 1, 1 + \frac{\sqrt{2}}{2}\}$. It holds $|\Phi'(-\infty)| < 1$ if $\gamma \in (0, 0.1593346776) \cup (1.178963184, 1.25) \cup (2.661702138, \infty)$.

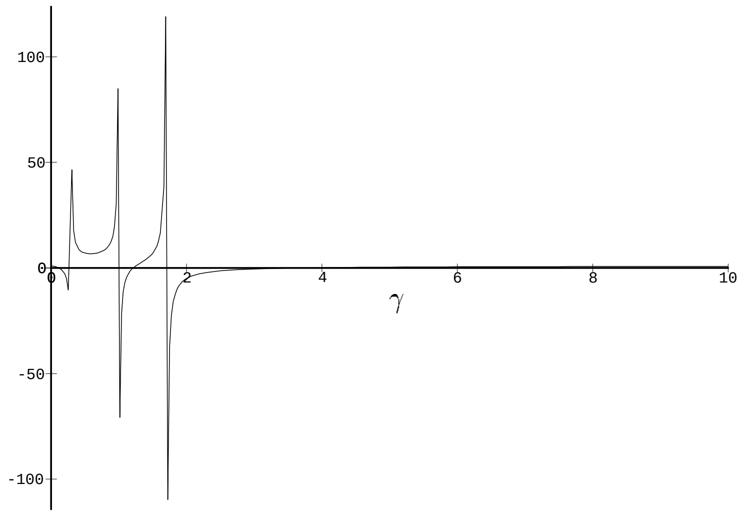

FIGURE 3.1. Maple-plot of $\Phi'(-\infty)$ for method of example 3.2 for $\gamma \in [0,10]$

Especially we have $\Phi'(-\infty) = 0$ for $\gamma \in \{0.1123358146, 1.210391768, 3.677272418\}$. The numerical tests on (1.11) as well as on (1.13) showed good behaviour for $\gamma > 2.7$. The values $\gamma \in (1.178963184, 1.25)$ did not give acceptable numerical results. A plot of $\Phi'(\lambda)$ for those γ would look similar to the plots in figure 2.1, i.e. $\Phi'(\lambda)$ is bounded for $h\lambda \to \infty$, but not bounded for $h\lambda \approx -3.709$ (pole). $|\Phi'(\lambda)| < 1$ we only have for $h\lambda \in (-0.58..., 0)$.

To show the practical behaviour of the methods of example 3.2 we applied it with and without stepsize control to equations (1.11) and (1.13), respectively. The results are presented in table 3.1.

TOL	λ	example (1.11)						example (1.13)					
		$\gamma = 2.7$			$\gamma = 1 - \frac{\sqrt{2}}{2}$			$\gamma = 2.7$			$\gamma = 1 - \frac{\sqrt{2}}{2}$		
		as	rs	le	as	rs	le	as	rs	le	as	rs	le
10^{-2}	-10	24	0	-3.1	20	5	-3.3	15	1	-2.7	15	2	-2.7
	-10^3	25	0	-10.2	3137	1690	-2.3	24	10	-3.1	1976	931	-1.9
	-10^5	30	5	-15.9	311052	175043	-2.4	180	176	-4.2	253565	159820	-1.7
10^{-4}	-10	100	0	-4.5	32	0	-5.5	40	3	-3.5	29	0	-4.6
	-10^3	104	2	-11.6	3125	1899	-4.8	52	2	-4.1	60	2	-5.0
	-10^5	110	4	-18.7	318699	170826	-4.1	79	50	-3.6	222797	115421	-3.6
10^{-6}	-10	480	0	-5.7	109	0	-6.5	221	2	-4.8	100	0	-6.1
	-10^3	498	2	-14.3	3180	1810	-7.0	375	2	-7.2	362	1	-7.3
	-10^5	503	4	-20.8	314465	191365	-7.0	467	2	-6.5	495	3	-7.6

TABLE 3.1. Method 3.2 with stepsize control

The abbreviations in the column headings are:

TOL	prescribed tolerance for the integration method,
as	number of accepted steps,
rs	number of rejected steps,
le	decimal logarithm of the error on t_e.

Here we see, that the choice of γ allows the construction of unrestricted stable methods for $s = 1$ and $s = 2$ for example (1.11). The disadvantages of the construction principle are the rapidly growing number of side conditions, to get stable methods with $s > 2$, and the fact, that these stability properties in general are obtained for large values of γ only, which leads to large error constants of the stability function with respect to the approximation of e^z.

4. GMRES

As the theoretical investigation showed the ROW method is possibly not able to compute the artificial introduced z-components sufficiently exact. Our aim of modification of the ROW method is to improve this value. The matrix E of (1.6) is usually computed by finite difference approximation. Thus the vector $r = f(y_m) - B(y_m)z_m$ is explicit used by the implementation. r should be zero to fulfil the introduced algebraic condition in (1.5). In case of the above mentioned stability problems r becomes large in magnitude. Here an iterative solver as GMRES (Saad [7], Walker [8]), minimizing the residual of a system of linear equations, is used. GMRES computes an approximate solution with monotonically decreasing residual of the systems of equations by use of Krylov subspaces (Arnoldi method). The iterative solution process of GMRES will compute the exact solution with at most $\kappa_{\max} = \operatorname{rank}(B(y))$ steps, if

$$f(u_m) \in \operatorname{range}(B(u_m)), \tag{4.1}$$

what is similar to (1.2). I.e. our modified implementation will also work for problems with singular $B(y)$ satisfying (1.2)–(1.4).

In our numerical tests we used

$$r \leq \mathrm{TOL} \tag{4.2}$$

as stopping criterion for the GMRES process.

The performance of the method of Lubich/Roche with GMRES was improved, as the results in table 4.1 demonstrate.

Further tests were done on a example from Denk [1], modelling the discharge of a capacitor via a resistor. The capacity C is supposed to depend polynomial of the voltage u.

$$C = a_0 + \frac{a_1}{2}u + \frac{a_2}{3}u^2 + \frac{a_3}{4}u^3 + \dots, \tag{4.3}$$

where $a_0, a_1, a_2, a_3, \dots$ are constant coefficients. From the derivation of charge $Q = Cu$ and Kirchhoffs law we have

$$u'(a_0 + a_1 u + a_2 u^2 + a_3 u^3 + \dots) = -\frac{1}{R}u, \tag{4.4}$$

where R is the resistance. The solution u is implicitly defined by

$$a_0 \ln u + a_1 u + \frac{a_2}{2}u^2 + \frac{a_3}{3}u^3 + \dots = -\frac{1}{R}t + const. \tag{4.5}$$

TOL	λ	acc. steps	rej. steps	steps with GMRES
10^{-2}	-10	23	0	0
	-10^3	47	0	5
	-10^5	51	4	13
10^{-4}	-10	85	0	0
	-10^3	250	0	3
	-10^5	256	3	10
10^{-6}	-10	382	0	0
	-10^3	1341	1	5
	-10^5	1347	3	961

TABLE 4.1. Results for method of Lubich/Roche with GMRES on example (1.11)

With cubic controlled capacity $C = 10^{-15} + 10^{-20}u^3$ the above mentioned stability problems were also detected. The numerical test results for different resistances are given in table 4.2 for running the method of Lubich/Roche without and with GMRES.

R	without GMRES		with GMRES		
	as	rs	as	rs	GMRES
10^3	96	30	88	24	5
$5 \cdot 10^3$	94	59	86	22	3
10^4	91	127	85	21	3

TABLE 4.2. Numerical results for example (4.4)

5. Conclusions

At almost all problems (1.1)–(1.4), which we solved by the code of Lubich/Roche it performed excellently. Only at some very extreme problems there arose stability problems, which we not expected. Our investigations at the classical test equation in implicit form (1.11) explained, that the difficulties are due to the insufficient accuracy for the algebraic conditions in (1.5). These problems can be avoided, changing method parameters or by improvement of the artificial introduced derivatives. For ROW methods with $s > 2$ stages only the second way seems applicable, because of the rapidly growing number of conditions ensuring the unrestricted stability. A combination of method (1.6) with GMRES gave good results. The additional effort is low, because GMRES is called only, when there is a great residual in the linear system.

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