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ROSENBROCK METHODS AND TIME-LAGGED JACOBIAN MATRICES

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Rosenbrock methods and time-lagged Jacobian matrices^{*)}

by

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ABSTRACT

In applications, Rosenbrock-type Runge-Kutta methods for stiff differential equations usually require one Jacobian matrix evaluation and one matrix factorization per integration step. The costs of these computations usually form a large proportion of the total computation cost of one step. This paper investigates the use of time-lagged Jacobian matrices with the aim of reducing the overhead costs. The idea is to integrate with a fixed Jacobian, computed at some previous step, and to maintain the order of consistency by updating the scalar integration parameters.

KEY WORDS & PHRASES: *Numerical Analysis, Stiff Ordinary Differential Equations, Rosenbrock Methods*

^{*)} This report will be submitted for publication elsewhere.

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1. INTRODUCTION

Let

$$(1.1) \quad y' = f(y), \quad y(x_0) = y_0,$$

represent the initial value problem for a stiff system of ordinary differential equations, written in autonomous form, of which the real vector function $f(y)$ is sufficiently differentiable. In this paper we are concerned with the numerical integration of (1.1) by means of a Rosenbrock-type Runge-Kutta method. These particular Runge-Kutta methods are well-known for the possibility to be A-stable and to be of high order. Since the original paper of Rosenbrock [15], several schemes have been proposed in the literature. All these schemes require at least one evaluation of the Jacobian matrix $J(y) = \partial f(y)/\partial y$ and one matrix factorization at each integration step. Since the costs of these computations usually form a large proportion of the total computation costs of one step, an interesting question is whether the costs, or the number of $J(y)$ -evaluations and LU-decompositions can be reduced without a serious loss of accuracy and stability. Bearing this question in mind Steihaug & Wolfbrandt [16] investigated schemes based on non-exact Jacobians. The purpose of this paper is to investigate the application of exact, but time-lagged Jacobian matrices. The idea is to integrate, for some finite number of steps, with a fixed Jacobian computed at some previous time step and to maintain the order of consistency by updating the scalar integration parameters. Herewith we thus avoid a decrease in the order of consistency of the Rosenbrock method, which usually occurs as soon as the $J(y)$ -evaluation is omitted. From a theoretical point of view the use of time-lagged Jacobian matrices is justified by the fact that in the non-transient region many stiff systems almost behave linearly.

Some first theoretical results concerning Rosenbrock-type methods and time-lagged Jacobian matrices, have already been given in [17]. Encouraging numerical results obtained with a particular multistep Rosenbrock method, have already been reported in [21].

2. A CLASS OF ROSENBROCK METHODS

A numerical solution of the following type is studied:

$$\begin{aligned}
 y_{n+1} &= y_n + \sum_{i=1}^m w_i k_i(y_n) + k_{m+1}(y_n), \\
 k_i(y_n) &= h S(\bar{y}_n) f(y_n + \sum_{j=1}^{i-1} \gamma_{ij} k_j(y_n)), \quad i=1(1)m, m \geq 1, \\
 k_{m+1}(y_n) &= S(\bar{y}_n) \sum_{i=1}^m v_i k_i(y_n), \\
 S(\bar{y}_n) &= (I - h\beta J(\bar{y}_n))^{-1}.
 \end{aligned}
 \tag{2.1}$$

The coefficients w_i , γ_{ij} , v_i and β are real parameters, h denotes the stepsize, and I the identity matrix. The vectors k_i , $i=1(1)m+1$, are computed by solving a linear system with $m+1$ different right-hand sides. The vector \bar{y}_n is assumed to be an approximation to an exact solution $y = y(x)$ at some fixed point $x = \bar{x}_n$, such that

$$\bar{y}_n = y(x_n) + \eta h y'(x_n) + \xi h^2 y''(x_n) + O(h^3).
 \tag{2.2}$$

The reals η and ξ are thus prescribed parameters which vary with n . For the moment it is not necessary to make an actual choice for \bar{y}_n . In applications, η and ξ are always of the form

$$\eta = (\bar{x}_n - x_n) h^{-1} + \bar{\eta}, \quad \xi = \frac{1}{2} (\bar{x}_n - x_n)^2 h^{-2} + \bar{\eta} (\bar{x}_n - x_n) h^{-1} + \bar{\xi},
 \tag{2.2'}$$

where $\bar{\eta}$ and $\bar{\xi}$ are fixed and satisfy

$$\bar{y}_n = y(\bar{x}_n) + \bar{\eta} h y'(\bar{x}_n) + \bar{\xi} h^2 y''(\bar{x}_n) + O(h^3).
 \tag{2.2''}$$

Note that almost all Rosenbrock methods, as discussed in the literature, are applied with $\bar{y}_n = y_n$. These methods thus require a $J(y)$ -evaluation per step at the step point $x = x_n$. For methods where $\eta = \bar{\eta} \neq 0$ and $\xi = \bar{\xi} = 0$, see [18,20].

Because (2.1) requires m $f(y)$ -evaluations per step, we call it an m -stage method. If $v_i = 0$ for all i and $\bar{y}_n = y_n$, (2.1) is in fact an

original Rosenbrock formula [15] where the number of $J(y)$ -evaluations per step is limited to 1 (see also [1,2,4]). We added the vector k_{m+1} in order to obtain some more degrees of freedom in choosing the integration parameters. Two-stage and three-stage formulas of a type very similar to (2.1) have already been discussed in [17]. Papers which are concerned with another modification of the original Rosenbrock method are, among others [8,9,10,14,22]. Finally we observe that in the literature Rosenbrock-type methods are also referred to as generalized Runge-Kutta methods (cf. [6,7,9,20]).

Introduce the abbreviations

$$(2.3) \quad \gamma_i = \sum_{j=1}^{i-1} \gamma_{ij}, \quad \beta_{ij} = \gamma_{ij} + \beta \delta_{ij}, \quad \delta_{ij} \text{ the Kronecker symbol,}$$

$$\beta_i = \gamma_i + \beta, \quad \tilde{v}_i = v_i + w_i, \quad \gamma_{ij} = 0 \text{ for } j \geq i.$$

The consistency conditions for order $p=1$ up to order $p=4$ can then be written as in table 2.1 (see e.g. [8,14,22] for a derivation of closely related conditions where $\eta = \xi = 0$).

Table 2.1 Consistency conditions. Summation indices run from 1 to m .

$p=1$	$\sum \tilde{v}_i = 1$	1. f
$p=2$	$\sum \tilde{v}_i \gamma_i + \beta \sum v_i = \frac{1}{2} - \beta$	2. $f_j f^j$
$p=3$	$\sum \tilde{v}_i \gamma_i^2 + 2\beta \eta \sum v_i = \frac{1}{3} - 2\beta \eta$ $\sum \tilde{v}_i \beta_{ij} \beta_j + 2\beta^2 \sum v_i + \beta \sum v_i \gamma_i = \frac{1}{6}$	3. $f_{jk} f^j f^k$ 4. $f_j f_k^j f^k$
$p=4$	$\sum \tilde{v}_i \gamma_i^3 + 3\beta \eta^2 \sum v_i = \frac{1}{4} - 3\beta \eta^2$ $\sum \tilde{v}_i \gamma_i \gamma_{ij} \beta_j + \beta \eta \sum \tilde{v}_i \gamma_i + \beta \eta \sum v_i \gamma_i +$ $(3\beta^2 \eta + \beta \xi) \sum v_i = \frac{1}{8} - \beta^2 \eta - \beta \xi$ $\sum \tilde{v}_i \beta_{ij} \gamma_j^2 + 2\beta \eta \sum \tilde{v}_i \gamma_i +$ $4\beta^2 \eta \sum v_i + \beta \sum v_i \gamma_i^2 = \frac{1}{12} - 2\beta^2 \eta$ $\sum \tilde{v}_i \beta_{ij} \beta_{jk} \beta_k + 2\beta^3 \sum v_i + \beta^2 \sum v_i \gamma_i +$ $\beta \sum v_i \beta_{ij} \beta_j = \frac{1}{24}$	5. $f_{jkl} f^j f^k f^l$ 6. $f_{jk} f_l^j f^k f^l$ 7. $f_j f_k^j f_l^k f^l$ 8. $f_j f_k^j f_l^k f^l$

To study the stability of (2.1) we use the scalar test-equation

$$(2.4) \quad y' = \delta y, \quad y(x_0) = y_0, \quad \delta \in \mathbb{C}.$$

When applied to (2.4) scheme (2.1) yields $y_{n+1} = R(z)y_n$, $z = h\delta$, where the stability function R is a rational function of the form

$$(2.5) \quad R(z) = \frac{\sum_{j=0}^s N_j z^j}{(1-\beta z)^s}, \quad s = \begin{cases} m+1, & \text{if } v_m \neq 0, \\ m, & \text{if } v_m = 0. \end{cases}$$

It has been proved (see [13]) that the order, say q , of this approximation to e^z is always smaller than or equal to $s+1$. Further, if $q \geq s$, the coefficients N_j are determined by β (cf. [12], Proposition 6). We then have

$$(2.6) \quad R(z) = \left(\sum_{j=0}^s z^j \sum_{i=0}^j \binom{s}{i} \frac{(-\beta)^i}{(j-i)!} \right) / (1-\beta z)^s.$$

Thus, if $p=q$ and $s \leq q \leq s+1$, the linear stability of (2.1) is completely determined by β . Ranges of β which produce A-stable methods have, for $1 \leq s \leq 6$ and under the condition that $s \leq q \leq s+1$, been given in [3] (see also [10,22]).

REMARK 2.1. For a discussion on S-stability [11] of generalized Runge-Kutta methods, see [20]. Using the results of [20] it is immediate that (2.1) is S-stable if R is strongly A-acceptable. In the present paper we therefore prefer to use the simple test equation (2.4) \square

REMARK 2.2. In the non-transient region many stiff systems almost behave linearly. In such a situation it is expected that, with respect to accuracy as well as stability, we can fix the Jacobian matrix during a fairly large number of integration steps. Consequently, when solving the order conditions, we have to take into account large negative values for η and large positive values for ξ (see (2.2')). Hence, it is of importance to find integration parameters which are bounded functions of η and ξ (η and ξ restricted to the domain of definition (2.2')). Else we have to reckon with inaccuracies, and probably instabilities, which

can easily annul the expected advantage of using a time-lagged Jacobian matrix. To support this view, consider the internal stability functions (cf. [20])

$$(2.6') \quad R^{(1)}(z) = 1, \quad R^{(i)}(z) = \sum_{j=0}^{i-1} N_j^{(i)} z^j / (1-\beta z)^{i-1}, \quad i=2(1)m.$$

In [20] it was observed that, for highly non-linear problems, it pays to require properties like A-acceptability for these internal stability functions. Now suppose that the integration parameters are not bounded with respect to η and ξ . The coefficients $N_j^{(i)}$ in (2.6') then may become very large. This means that we have to reckon with large internal amplification factors which grow with η and ξ . Even in case of weak non-linearities, such a behaviour cannot be recommended. Therefore, in the following, much attention is paid to finding bounded parameter solutions \square

3. METHODS OF ORDER $p = 3$

In the present section we shall concentrate on 2-stage methods of order $p=3$ ($p=3$ cannot be obtained if $m=1$). For $m=2$ the third order consistency conditions can be simplified to

$$(3.1) \quad \tilde{v}_1 + \tilde{v}_2 = 1,$$

$$(3.2) \quad \tilde{v}_2 \gamma_2 + \beta(v_1 + v_2) = \frac{1}{2} - \beta,$$

$$(3.3) \quad \tilde{v}_2 \gamma_2^2 + 2\beta\eta(v_1 + v_2) = \frac{1}{3} - 2\beta\eta,$$

$$(3.4) \quad \beta v_2 \gamma_2 = \frac{1}{6} - \beta + \beta^2.$$

A necessary condition for the existence of bounded parameters is that $v_1 + v_2 \rightarrow -1$ if $\eta \rightarrow -\infty$. This means that the original Rosenbrock formulas [15] cannot be adapted to time-lagged Jacobians if we also want to fulfil the requirement of boundedness.

The solution of equations (3.1) - (3.4), where β and γ_2 are still

free parameters, is given by

$$(3.5) \quad \begin{aligned} v_2 &= (\frac{1}{6} - \beta + \beta^2) / \beta \gamma_2, \quad v_1 = -v_2 + (\frac{1}{3} - 2\beta\eta - (\frac{1}{2} - \beta)\gamma_2) / (2\beta\eta - \beta\gamma_2), \\ \tilde{v}_2 &= (\frac{1}{2} - \beta(1+v_1+v_2)) / \gamma_2, \quad \tilde{v}_1 = 1 - \tilde{v}_2, \quad \beta, \gamma_2 \neq 0, \gamma_2 \neq 2\eta. \end{aligned}$$

Substitution of some bounded function $\gamma_2 = \gamma_2(\eta)$, leads to a set of bounded integration parameters. If we substitute $\gamma_2 = \frac{2}{3}$, we obtain, somewhat surprisingly, parameters which are independent of η .

If $v_2 \neq 0$, the stability function of a 2-stage method of order 3 is given by (see (2.6))

$$(3.6) \quad R(z) = \frac{1 + (1-3\beta)z + (\frac{1}{2} - 3\beta + 3\beta^2)z^2 + (\frac{1}{6} - \frac{3}{2}\beta + 3\beta^2 - \beta^3)z^3}{(1-\beta z)^3}.$$

This rational function is A-acceptable for all $\beta \in [\frac{1}{3}, 1.06858]$ and can be made L-acceptable by requiring $\beta^3 - 3\beta^2 + \frac{3}{2}\beta - \frac{1}{6} = 0$ (see [3], table 1 and 2). The internal stability function $R^{(2)}$ reads

$$(3.7) \quad R^{(2)}(z) = \frac{1 + (\gamma_2 - \beta)z}{1 - \beta z}.$$

This function is A-acceptable if $\gamma_2 \in [0, 2\beta]$.

In section 5 we shall present numerical results of the scheme defined by the parameter solution (3.5), where

$$(3.8) \quad \gamma_2 = \frac{2}{3}, \quad \beta = 0.4358665216.$$

Solution (3.8) yields parameters independent of η . Further, the resulting scheme is L-stable and its internal stability function $R^{(2)}$ is strongly A-acceptable. A third order scheme which is closely related to the scheme presented here, has been given in [17].

4. METHODS OF ORDER $p = 4$

To begin with we prove the following theorem:

THEOREM 4.1. Let in (2.1) the order $p \geq 4$. A necessary condition for boundedness of the integration parameters with respect to η and ξ is then $\beta = \frac{1}{2}$.

PROOF. Consider equation 7 in table 2.1. By making use of equations 2 and 3 of the same table, equation 7 can be rewritten as

$$\sum_{i,j} \tilde{v}_{ij} \gamma_j^2 - \beta \sum_i \tilde{v}_i \gamma_i^2 + \beta \sum_i v_i \gamma_i^2 = \frac{1}{12} - \frac{1}{3} \beta + (2\beta^2 - \beta) \eta.$$

As η does not appear in the left-hand side, η has to vanish in the right-hand side in order to obtain bounded parameters \square

This theorem has two consequences. The first is that the order q of the stability function is always smaller than or equal to the degree s of its denominator. The second is that, to a certain extent, the boundedness requirement is the determining factor for the A-stability of methods of order $p \geq 4$.

Let us proceed with the construction of a 3-stage, 4-th order method. We then have $q = s = 4$, while $\beta = \frac{1}{2}$ lies in the A-acceptability range (cf.[3], table 1). For $m = 3$ and $\beta = \frac{1}{2}$ the consistency conditions can be simplified to

$$(4.1) \quad \sum_{i=1}^3 \tilde{v}_i = 1,$$

$$(4.2) \quad \sum_{i=1}^3 \tilde{v}_i \gamma_i + \frac{1}{2} \sum_{i=1}^3 v_i = 0,$$

$$(4.3) \quad \sum_{i=1}^3 \tilde{v}_i \gamma_i^2 + \eta \sum_{i=1}^3 v_i = \frac{1}{3} - \eta,$$

$$(4.4) \quad \frac{1}{2} \sum_{i=1}^3 v_i \gamma_i + \tilde{v}_3 \gamma_{32} \gamma_{21} = -\frac{1}{12},$$

$$(4.5) \quad \sum_{i=1}^3 \tilde{v}_i \gamma_i^3 + \frac{3}{2} \eta^2 \sum_{i=1}^3 v_i = \frac{1}{4} - \frac{3}{2} \eta^2,$$

$$(4.6) \quad \frac{1}{2} \eta \sum_{i=1}^3 v_i \gamma_i + \frac{1}{2} \xi \sum_{i=1}^3 v_i + \tilde{v}_3 \gamma_3 \gamma_{32} \gamma_2 = -\frac{1}{24} - \frac{1}{2} \xi + \frac{1}{4} \eta,$$

$$(4.7) \quad \frac{1}{2} \sum_{i=1}^3 v_i \gamma_i^2 + \tilde{v}_3 \gamma_{32} \gamma_2^2 = -\frac{1}{12},$$

$$(4.8) \quad \gamma_2 v_3 \gamma_{32} = \frac{1}{12}.$$

We have 9 unknowns and 8 conditions. By a tedious calculation, which is otherwise elementary and thus not reproduced here, it can be shown that for any solution of (4.1) - (4.8), the parameters γ_2 and γ_3 have to satisfy the relation

$$(4.9) \quad \gamma_3 \left[\left(\frac{1}{3} \xi - \frac{1}{6} \eta^2 - \frac{1}{6} \eta \right) + \gamma_2 \left(-\frac{5}{6} \xi - \frac{1}{12} \eta^2 + \frac{1}{4} \eta + \frac{1}{12} \right) + \gamma_2^2 \left(\frac{1}{2} \xi + \frac{1}{6} \eta - \frac{1}{8} \right) \right] = \\ \left(\frac{1}{4} \xi - \frac{1}{8} \eta^2 - \frac{1}{2} \eta^3 \right) + \gamma_2 \left(-\frac{7}{12} \xi + \frac{1}{24} \eta + \frac{13}{24} \eta^2 + \frac{1}{4} \eta^3 \right) + \gamma_2^2 \left(\frac{1}{3} \xi - \frac{1}{12} \eta - \frac{1}{6} \eta^2 \right).$$

However using the asymptotic relation $\xi \sim \frac{1}{2} \eta^2$, as $\eta \rightarrow -\infty$, we must conclude from (4.9) that equations (4.1) - (4.8) do not possess a solution which is bounded with respect to η and ξ . In the foregoing we thus proved the following negative result:

THEOREM 4.2. Any 3-stage, 4-th order method belonging to class (2.1) possesses integration parameters which are unbounded with respect to η and ξ \square

No attempt has been made to construct 4-th order methods from class (2.1) where the number of stages is larger than 3. Because in our opinion, if one succeeds in finding bounded integration parameters for $m > 3$, it is doubtful whether such a method will be significantly more efficient than the 2-stage, 3-rd order schemes (3.5). Of course, it remains of interest to think about other types of Rosenbrock methods than class (2.1). In this respect it is of importance to remark that the 3-stage, 4-th order scheme developed in [17] also possesses unbounded parameters.

5. SOME NUMERICAL EXAMPLES

To get insight into the practical use of time-lagged Jacobian matrices for Rosenbrock-type integration methods, we applied the third order method defined by (3.5), (3.8) to problem class D of the test set given by Enright, Hull & Lindberg [5]. Altogether 72 integrations have been carried out, each integration with a prescribed step size sequence $\{h_n\}$ defined by

$$(5.1) \quad h_n = \begin{cases} h_{\max}/2^N, & n = 0, \\ h_{\max}/2^{N+1-n}, & n = 1, 2, \dots, N, \\ h_{\max}, & n = N+1, N+2, \dots, \end{cases}$$

where h_{\max} is a constant which may differ per integration. Thus apart from the initial phase, all integrations have been performed with a constant stepsize h_{\max} . Note that we used $N+1$ steps for the initial interval $[x_0, x_0 + h_{\max}]$. The integer N will be specified at the examples.

To get insight into the behaviour of the integration formula when using a time-lagged Jacobian, we added to each step size sequence $\{h_n\}$ a parameter STEPS. This parameter defines the number of integration steps with constant step size $h = h_{\max}$ per Jacobian evaluation. During the initial phase, i.e. $n \leq N$, the Jacobian was always evaluated. All evaluations of $J(y)$ were performed at step points ($\bar{\eta} = \bar{\xi} = 0$, see (2.2')).

In the tables of results we give $SD = -10 \log$ (maximum error of the solution components at the end of the given interval), FEV = the number of $f(y)$ -evaluations, and JEV = the number of $J(y)$ -evaluations. Note that if STEPS = 1, the number of Jacobian evaluations is equal to the number of integration steps. All computations were performed on a CDC Cyber 73/28 computer which has an arithmetic precision of approximately 14 decimals.

Problem D1: $N = 10$

$$\begin{aligned} y_1' &= 0.2(y_2 - y_1), & y_1(0) &= 0, \quad y_1(400) = 22.242211, \\ y_2' &= 10y_1 - (60 - y_3/8)y_2 + y_3/8, & y_2(0) &= 0, \quad y_2(400) = 27.110701, \\ y_3' &= 1, & y_3(0) &= 0, \quad y_3(400) = 400. \end{aligned}$$

STEPS		1		5		10		20	
h_{\max}	FEV	SD	JEV	SD	JEV	SD	JEV	SD	JEV
0.5	1620	3.88	810	2.45	171	2.12	91	2.01	51
1.0	820	3.40	410	1.75	91	1.56	51	1.46	31
2.0	420	2.78	210	1.26	51	1.14	31	0.58	21

Problem D2: N = 10

$$y_1' = -0.04y_1 + 0.01y_2y_3,$$

$$y_1(0) = 1, y_1(40) = 0.7158271,$$

$$y_2' = 400y_1 - 100y_2y_3 - 3000y_2^2,$$

$$y_2(0) = 0, y_2(40) = 0.09186,$$

$$y_3' = 30y_2^2,$$

$$y_3(0) = 0, y_3(40) = 28.41637.$$

STEPS		1		5		10		20	
h_{\max}	FEV	SD	JEV	SD	JEV	SD	JEV	SD	JEV
0.25	340	4.82	170	3.44	43	2.80	27	2.16	19
0.5	180	4.10	90	2.59	27	1.94	19	1.26	15
1.0	100	3.31	50	1.79	19	1.11	15	0.27	13

Problem D3: N = 20

$$y_1' = y_3 - 100y_1y_2,$$

$$y_1(0)=1, y_1(20)=0.639760447,$$

$$y_2' = y_3 + 2y_4 - 100y_1y_2 - 20000y_2^2,$$

$$y_2(0)=1, y_2(20)=0.5630850708_{10}^{-2},$$

$$y_3' = -y_3 + 100y_1y_2,$$

$$y_3(0)=0, y_3(20)=0.3602395553,$$

$$y_4' = -y_4 + 10000y_2^2,$$

$$y_4(0)=0, y_4(20)=0.3170647970.$$

STEPS		1		5		10		20	
h_{\max}	FEV	SD	JEV	SD	JEV	SD	JEV	SD	JEV
0.5	120	>10.0	60	>10.0	29	>10.0	25	>10.0	23
1.0	80	>10.0	40	>10.0	25	>10.0	23	>10.0	22
2.0	60	>10.0	30	>10.0	23	>10.0	22	>10.0	22

Problem D4: N = 10

$$\begin{aligned}
 y_1' &= -0.013y_1 - 1000y_1y_3, & y_1(0)=1, y_1(50) &= -0.189338654 \cdot 10^{-5}, \\
 y_2' &= -2500y_2y_3, & y_2(0)=1, y_2(50) &= 0.597654698, \\
 y_3' &= -0.013y_1 - 1000y_1y_3 - 2500y_2y_3, & y_3(0)=0, y_3(50) &= 1.402343409.
 \end{aligned}$$

STEPS		1		5		10		20	
h_{\max}	FEV	SD	JEV	SD	JEV	SD	JEV	SD	JEV
0.25	420	>8.0	210	>8.0	51	7.53	31	6.89	21
0.5	220	>8.0	110	7.23	31	6.60	21	5.97	16
1.0	120	>8.0	60	6.32	21	5.68	16	5.05	14

Problem D5: N = 10

$$\begin{aligned}
 y_1' &= 0.01 - [1 + (y_1 + 1000)(y_1 + 1)] * \\
 &\quad (0.01 + y_1 + y_2), & y_1(0)=0, y_1(100) &= -0.99164207, \\
 y_2' &= 0.01 - (1 + y_2^2)(0.01 + y_1 + y_2), & y_2(0)=0, y_2(100) &= 0.98333636.
 \end{aligned}$$

STEPS		1		5		10		20	
h_{\max}	FEV	SD	JEV	SD	JEV	SD	JEV	SD	JEV
0.25	820	5.76	410	4.81	91	4.12	51	3.62	31
0.5	420	4.29	210	3.86	51	3.35	31	2.99	21
1.0	220	4.10	110	3.15	31	2.79	21	2.56	16

Problem D6: N = 10

$$y_1' = -y_1 + 10^8 y_3 (1 - y_1),$$

$$y_1(0)=1, y_1(1) = 0.8523997,$$

$$y_2' = -10y_2 + 3 \times 10^7 y_3 (1 - y_2),$$

$$y_2(0)=0, y_2(1) = 0.1476001,$$

$$y_3' = -y_1' - y_2',$$

$$y_3(0)=0, y_3(1) = 0.577308_{10}^{-7}.$$

STEPS		1		5		10		20	
h_{\max}	FEV	SD	JEV	SD	JEV	SD	JEV	SD	JEV
0.025	100	4.93	50	4.94	19	4.94	15	4.96	13
0.05	60	4.56	30	4.57	15	4.58	13	4.60	12
0.1	40	4.12	20	4.14	13	4.16	12	4.16	12

The results of the numerical experiments lead us to the following observations:

- (i) In the present section 72 numerical integrations are reported. In all integrations the algorithm delivers a stable result, which, once more, illustrates the excellent stability behaviour of Rosenbrock-type Runge-Kutta methods.
- (ii) Generally, as to be expected, the accuracy decreases as soon as the Jacobian is kept fixed. For problems D1 and D2 this decrease is significant. On the other hand, the results obtained for problems D3-D6 justify the conclusion that with respect to computational efficiency the application of time-lagged Jacobians is of use in connection with a certain class of practical problems, viz. problems for which the costs of $J(y)$ -evaluations + LU-decompositions are dominating.
- (iii) In practice Rosenbrock algorithms are usually provided with step-size and local error control [2,4,6,7,9,10,16]. To implement time-lagged Jacobians in such algorithms in a successful way, it is necessary to have some detailed understanding of the non-linearity of the problem and of the "non-linear behaviour" of the integration formulas being used for step continuation and error

estimation. In the near future we intend to carry on our research in this direction.

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