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A Reliable Rosenbrock Integrator for Stiff Differential Equations

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Abstract — Zusammenfassung

A Reliable Rosenbrock Integrator for Stiff Differential Equations. This note points out that the reliability of step-by-step integrators for ordinary differential equations can be increased considerably by a simple trick. We incorporated this idea into a program based on an A-stable Rosenbrock formula. This program comprises about 100 statements only and gives good numerical results.

Ein verläßliches Rosenbrock-Programm für steife Differentialgleichungen. Es wird gezeigt, daß die Sicherheit eines Programmes für gewöhnliche Differentialgleichungen durch einen einfachen Trick wesentlich erhöht werden kann. Mit Hilfe dieser Idee und einer A-stabilen Rosenbrock-Formel haben wir ein kleines Programm geschrieben, welches gute numerische Resultate liefert.

1. Introduction

In [5], Kaps and Rentrop tested their Rosenbrock program on the 25 stiff test problems of Enright, Hull, and Lindberg [2] and observed for problem "*D* 5" accepted steps which missed satisfying the tolerance by two digits. We found out that this can easily be avoided by what may be called the "back-step algorithm", which with a little extra work increases the reliability of a program for many other equations too.

We consider the system of differential equations

$$y' = f(y), \quad y(t_0) = y_0, \quad \text{for } t_0 \le t \le t_{end}.$$

Suppose we integrate this equation step-by-step with the method of [5] as described in section 2 below. For the step from t to $t+h$ this method uses the derivative f and the Jacobian f' evaluated in t and also two more derivative evaluations in $t+\alpha_i h$, where $\alpha_2 = 0.438$ and $\alpha_3 = 0.87$ (see [5]). Based on these

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evaluations, the method then computes an approximation for $y(t+h)$ and an estimation for the local error which is used for the error control and the automatic adjustment of the step size h. However, when the integration arrives at a quasi-discontinuity of the solution, i.e., a region where the solutions change suddenly from a smooth behaviour to rapid movement which happens quite frequently in stiff problems, the above procedure may detect this change of the error function too late only, namely in the subsequent step.

We therefore have adopted the following procedure:

i) after a failure of the error test we estimate a step size h_{new} which will succeed. If $h_{new} \geq h_{old}$, we just recompute the step as is customary. If $h_{new} < h_{old}$, we back up one step and start from there with h_{new};

ii) after a backing up, the step size h_{new} is not allowed to increase in the following step;

iii) when the final point t_{end} has been reached, the solution for $t = t_{end}$ is computed only if one additional step beyond t_{end} has been accepted.

This last point needs the existence of $f(y)$ in a small interval outside the integration interval. Whenever this is not the case, $f(y)$ can be extended arbitrarily, since these values are only used for an eventual error control and do not enter into the computations for the values for $t = t_{end}$.

2. The Basic Formula

The integration formula used for the computation of the next solution point and an estimation of the local error for a given initial value y and step size h is essentially equivalent to the formula "GRK4A" of Kaps and Rentrop [5]; we have, however, redefined the meaning of the k-values. Therefore the coefficients have changed and the computations become simpler (see [6] for more details). The method has good stability properties, i.e. it is A-stable as defined in [1], and of order 4. The estimation of the local error is done with the help of an imbedded method of order 3. It usually overestimates the error and leads to very accurate numerical results (see section 4). Many people have contributed to the development of this kind of methods (H. H. Rosenbrock 1963, D. A. Calahan, P. van der Houven, S. P. Nørsett, A. Wolfbrandt [7], [9]) over a long time.

1. Compute $g_1 = f(y)$;
2. Compute the matrix $f' = \left(\dfrac{\partial f_i(y)}{\partial y_j}\right)$ by finite differences or analytically;
3. Compute the matrix $E = I - h\gamma f'$ and its LU-factorization;
4. Solve the linear system $E k_1 = h g_1$;
5. Compute $g_2 = f(y + a_{21} k_1)$;
6. Solve the linear system $E k_2 = h g_2 + c_{21} k_1$;

7. Compute $g_3 = f(y + a_{31} k_1 + a_{32} k_2)$;
8. Solve the linear system $E k_3 = h g_3 + c_{31} k_1 + c_{32} k_2$;
9. Solve the linear system $E k_4 = h g_3 + c_{41} k_1 + c_{42} k_2 + c_{43} k_3$;
10. New solution $y_{new} = y + b_1 k_1 + b_2 k_2 + b_3 k_3 + b_4 k_4$;
11. Error estimator:

$$EST = \text{Max}\left(U_{round}, \operatorname*{Max}_{i=1,n}\left(\left|\sum_{j=1}^{4} e_j k_j(i)\right| \Big/ \text{Max}\left(1, |y_i|, |y_{new}(i)|\right)\right)\right)$$

with the coefficients

$\gamma = .395$

$a_{21} = .438$	$c_{21} = -1.94347441894707$
$a_{31} = .938948678483428$	$c_{31} = .416957530989189$
$a_{32} = .0730795420615381$	$c_{32} = 1.32396782072923$
$b_1 = .729044879960308$	$c_{41} = 1.51951325778448$
$b_2 = .0541069773272405$	$c_{42} = 1.35370815030093$
$b_3 = .281599362440017$	$c_{43} = -.854151495257539$
$b_4 = e_4 = .25$	$e_1 = -.0190858871999474$
$e_2 = .255608791716455$	$e_3 = -.0863816280897592$

3. Numerical Results

The algorithm described has been coded in FORTRAN (Subroutine ROW4A) and SIMULA. Copies of these codes can be obtained from the authors. We have tested this program for the 25 stiff test problems of [2] and for the five additional problems $F\,1, \ldots, F\,5$ below. In Fig. 1 we have plotted the maximal errors for the three given tolerances $\text{TOL} = 10^{-2}$, 10^{-3}, 10^{-4} and compared them with those of the GEAR code of A. C. Hindmarsh. The errors are taken relative to $|y_i|$ for $|y_i| > 1$ and in an absolute sense for $|y_1| \leq 1$. The maximum over the whole integration interval and all components, divided by TOL, is plotted on a logarithmic scale.

It can be seen that the results of ROW4A are one or two digits more accurate than those of GEAR, and that the "back-step" clause can lead to a substantial increase of accuracy. The additional problems treated, which are harder and more complex, are the following:

$F\,1$: $y_1' = y_2$ $\qquad y_1(0) = 2$
$y_2' = 50(1 - y_1^2)\, y_2 - y_1$ $\qquad y_2(0) = 0$
$x_0 = 0$, $x_{end} = 40$, $h_0 = 10^{-3}$

(Van der Pol equation with a large stiffness parameter and long integration interval. The solution possesses a sharp peak at $t \sim 41$. In order for the maximal error to be meaningful, we have chosen x_{end} before this peak and treat the peak itself in $F\,2$).

$F\,2$: Equation as in $F\,1$, $y_1(0) = .6583$, $y_2(0) = -5.733$,
$x_0 = 40.9$, $x_{end} = 41.5$, $h_0 = 10^{-3}$.

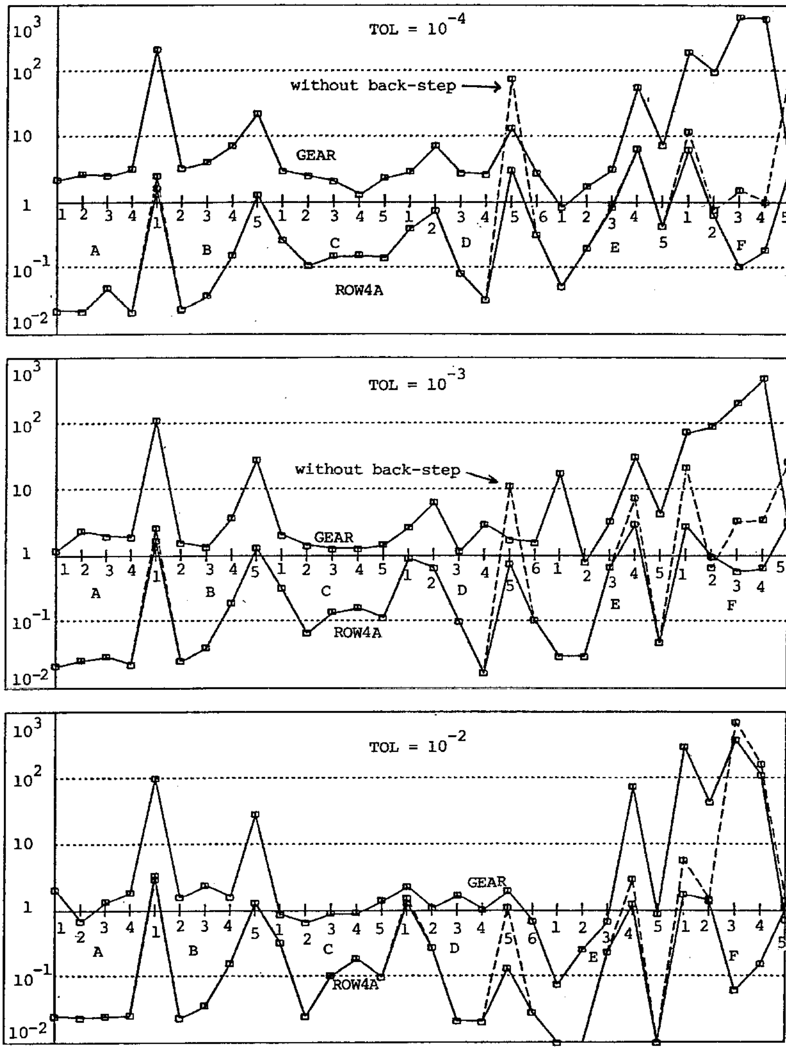


Fig. 1. Maximal global error of the computed solution, over the whole integration interval and all components, divided by TOL. (Results for $D4$ are multiplied by 10, results for $E5$ are multiplied by 1000, results for $F3$ and $F4$ are divided by 100.) In broken lines: The results of ROW4A without the back-step idea

$F3$:
$$y_1' = 77.27\,(y_2 + y_1\,(1 - 8.375 \cdot 10^{-6} \cdot y_1 - y_2)) \qquad y_1(0) = 3$$
$$y_2' = (y_3 - (1 + y_1)\,y_2)/77.27 \qquad y_2(0) = 1$$
$$y_3' = 0.161 \cdot (y_1 - y_3) \qquad y_3(0) = 2$$
$$x_0 = 0,\ x_{end} = 300,\ h_0 = 10^{-3}$$

(the Oregonator [3]; as $F1$, the solutions possess a sharp peak which again is treated separately in $F4$).

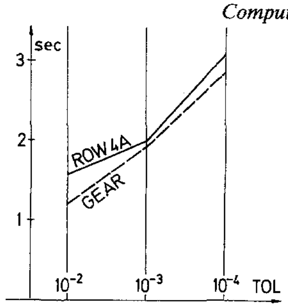
$F4$: Equation as in $F3$, $y_1(0) = 349.8765$, $y_2(0) = 0.72112$, $y_3(0) = 9.37206$, $x_0 = 303.35$, $x_{end} = 307$, $h_0 = 10^{-3}$.

$$
\begin{aligned}
F\,5\colon\quad & y_1' = -1.71\, y_1 + 0.43\, y_2 + 8.32\, y_3 + 7\cdot 10^{-4} & y_1(0)&=1\\
& y_2' = 1.71\, y_1 - 8.75\, y_2 & y_2(0)&=0\\
& y_3' = -10.03\, y_3 + 0.43\, y_4 + 0.035\, y_5 & y_3(0)&=0\\
& y_4' = 8.32\, y_2 + 1.71\, y_3 - 1.12\, y_4 & y_4(0)&=0\\
& y_5' = -1.745\, y_5 + 0.43\, y_6 + 0.43\, y_7 & y_5(0)&=0\\
& y_6' = -280\, y_6\, y_8 + 0.69\, y_4 + 1.71\, y_5 - 0.43\, y_6 + 0.69\, y_7 & y_6(0)&=0\\
& y_7' = 280\, y_6\, y_8 - 1.81\, y_7 & y_7(0)&=0\\
& y_8' = -y_7' & y_8(0)&=0.0057\\
& x_0 = 0,\; x_{end} = 400,\; h_0 = 10^{-2}
\end{aligned}
$$

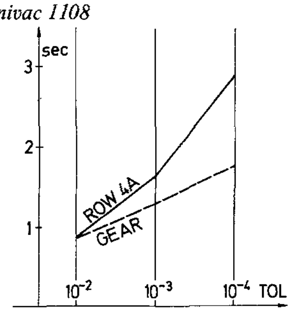
(the HIRES problem [8]).

In the following graphs are sketched the computing times for the FORTRAN version on the Univac 1108 accumulated over the five different classes of problems of [2]. ROW4A is usually slightly slower than GEAR and uses more function evaluations. GEAR runs very efficiently on problems of class *D* and fails on example *B* 5, which is the example with fast oscillating solutions. On the other hand, ROW4A is slow on example *F* 3 (but much more precise). The code (not including the linear equation solver and data) requires 595 words of memory for ROW4A and 2078 words for GEAR.

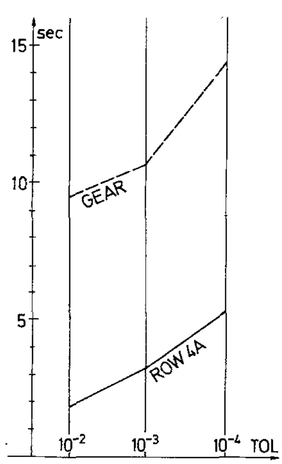
Computing Times for Univac 1108



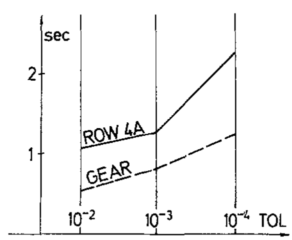
Class A
linear with real eigenvalues



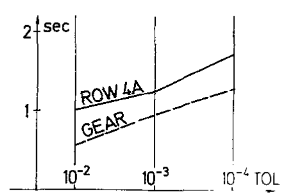
Class C
nonlinear coupling



Class B
linear with complex eigenvalues



Class D
nonlinear with real eigenvalues



Class E
nonlinear with complex eigenvalues

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