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NUMERICAL TREATMENT OF SINGULAR INITIAL VALUE PROBLEMS†

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Abstract—An efficient extrapolation scheme whose basic integrator is the inverse Euler scheme (cf. Fatunla, 1982) is proposed for nonlinear singular initial value problems $y' = f(x, y)$, $y(0) = y_0$. The automatic (polynomial/rational) extrapolation code DIFEX1 (Deuflhard 1983, 1985) is modified to accommodate the basic integrator. The new algorithm was implemented in variable step, variable order mode and compares favourably with the earlier works.

1. INTRODUCTION

The mathematical formulation of physical situations in simulation and control often leads to initial value problems (ivps) in ordinary differential equations (ODEs)

$$y' = f(x,y), \quad y(0) = y_0 \tag{1.1}$$

($x \in [0, b], y \in R^m$), whose solutions contain singularities. For nonlinear differential systems, the theory of ODEs offers no clue as regards the location and nature of the singularities. Besides the conventional numerical integrators (i.e. the Runge Kutta processes and the linear multistep formulas) whose derivation is based on polynomial interpolation perform very poorly in the neighbourhood of such singularities. This is clearly illustrated in Table 1 where the Gragg–Bulirsch–Stoer rational extrapolation scheme (Gragg, 1965; Bulirsch and Stoer, 1966), and the Gragg–Neville–Aitken polynomial extrapolation (Gragg, 1965; Neville, 1934; Aitken, 1932) are both inefficient in the neighbourhood of the singularity. On the other hand the rational interpolation schemes of Luke *et al.* (1975) can be observed in Table 2 to be effective in the neighbourhood of the singularity and even beyond. The new algorithm is not only more effective but more accurate and more efficient than the existing algorithms.

2. EXISTING ALGORITHMS FOR SINGULAR INITIAL VALUE PROBLEMS

Several noteworthy algorithms have been proposed for singular ivps (1.1).

Lambert and Shaw (1965, 1966) were the first to develop quadrature formulas based on rational interpolating functions

$$F(x) = P_n(x)/(b + x) \tag{2.1}$$

and

$$F(x) = P_n(x) + a\,|A + x|^N, \quad N \notin \{0, 1, \ldots, n\} \tag{2.2a}$$

or

$$F(x) = P_n(x) + a\,|A + x|^N \ln|A + x|, \quad N \in \{0, 1, \ldots, n\} \tag{2.2b}$$

where $P_n(x)$ is a polynomial of degree n.

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Table 1. Performance of a non-stiff extrapolation code on the singular ivp. $y' = 1 + y^2$, $y(0) = 1$ $0 \leqslant x \leqslant 1$ $h_0 = 0.25$, $h_{max} = 1.0$, maximum extrapolation 6

	Modified midpoint (+) rational extrapolation Gragg–Bulirsch–Stoer–DIFEX1 Deuflhard (1983)			Modified midpoint (+) polynomial extrapolation Gragg–Neville–Aitken–DIFEX1 Deuflhard (1983)		
$\epsilon = 10^{-q}$ q	Termination point x	No. of steps	No. of Fn evaluation	Termination point x	No. of steps	No. of Fn evaluation
1	0.904585413	17	299	0.785492433	132	1710
2	0.786585246	88	880	0.786472360	88	880
3	0.785412676	97	1843	0.785399251	103	1975
4	0.785399984	203	5057	0.785398887	208	5182
5	0.785398693	166	3190	0.785399861	164	3140
6	0.785398201	179	2843	0.785398171	153	5045
7	0.785398166	289	4471	0.785398170	180	5936

The resultant integration formulas are very unwieldy and besides require analytic generation of first and higher order derivatives of f. Shaw (1967) developed perturbed linear multistep methods based on (2.2) which required the solution of nonlinear transcendental equations for the singularity parameters A and N at every integration step.

Luke *et al.* (1975) further developed the idea of Lambert and Shaw (1965) by replacing (2.1) with a general rational function

$$F(x) = P_m(x)/Q_n(x) \tag{2.3}$$

where $P_m(x)$ and $Q_n(x)$ are respectively polynomials of degree m and n

$$P_m(x) = \sum_{i=0}^{m} a_i x^i, \quad Q_n(x) = 1 + \sum_{i=1}^{n} b_i x^i. \tag{2.4}$$

With the representation

$$L_{m,n}(x) = Q_n(x)y(x) - P_m(x), \tag{2.5}$$

and its derivative w.r.t.x

$$L'_{m,n}(x) = Q'_n(x)y(x) + Q_n(x)y'(x) - P'_m(x), \tag{2.6}$$

Luke *et al.* (1975) derived two sets of predictor corrector formulas by substituting $x = x_0 + th$ after imposing the following constraints on (2.5) and (2.6).

(*i*) $m + n = 2k$

Predictor: (error order $p = 2k$)

$$\begin{aligned} L_{m,n}(x_i) &= 0, \quad i = 0(1)k + 1 \\ L'_{m,n}(x_i) &= 0, \quad i = 1(1)k \end{aligned} \tag{2.7}$$

Corrector: (error order $p \geqslant 2k$)

$$\begin{aligned} L_{m,n}(x_i) &= 0, \quad i = 1(1)k + 1 \\ L'_{m,n}(x_i) &= 0, \quad i = 1(1)k \end{aligned} \tag{2.8}$$

Table 2. Performance of Luke *et al.* (1975) on the singular ivp. $y' = 1 + y^2$, $y(0) = 1$, $0 \leqslant x \leqslant 1$, $m = 1$, $n = 2$, $p = 4$

X	Theoretical solution	Predicted (Uniform $h = 0.05$)	Corrected (Uniform $h = 0.05$)	Predicted (Uniform $h = 0.01$)	Corrected (Uniform $h = 0.01$)
0.1	1.22305	1.22304	1.22305	1.22305	1.22305
0.2	1.50850	1.50848	1.50850	1.50850	1.50850
0.3	1.89577	1.89574	1.89577	1.89577	1.89577
0.4	2.46496	2.46493	2.46498	2.46496	2.46496
0.5	3.40822	3.40815	3.40826	3.40822	3.40822
0.6	5.33186	5.33165	5.33186	5.33186	5.33186
0.7	11.68137	11.68998	11.68153	11.68138	11.68139
0.8	−68.47967	−68.59667	−68.66273	−68.48685	−68.49443
0.9	−8.68763	−8.73393	−8.68629	−8.69860	−8.69493
1.0	−4.58804	−4.62137	−4.64804	−4.56120	−4.56121

(*ii*) $m + n = 2k - 1$ (error order $p = 2k - 1$)
Predictor: (error order $p = 2k - 1$)

$$\begin{aligned} L_{m,n}(x_i) &= 0, \quad i = 0(1)k \\ L'_{m,n}(x_i) &= 0, \quad i = 0(1)k - 1 \end{aligned} \tag{2.9}$$

Corrector: (error order $p \geqslant 2k - 1$)

$$\begin{aligned} L_{m,n}(x_i) &= 0, \quad i = 0(1)k \\ L'_{m,n}(x_i) &= 0, \quad 1 = 1(1)k. \end{aligned} \tag{2.10}$$

The simplest of the resultant integration formulas is obtained from $m = n = 1$, yielding the predictor

$$y_{n+2} = \frac{2y_n y_{n+1} - 2y_{n+1}^2 + hy'_{n+1}y_n}{2y_n - 2y_{n+1} + hy_{n+1}} \tag{2.11a}$$

and the corresponding corrector

$$y_{n+2} = \frac{y_{n+1}^2 - h^2 y'_{n+1} y'_{n+2}}{2y_{n+1} - y_{n+2}}. \tag{2.11b}$$

Higher order formulas are quite unwieldy and can be found in Luke *et al.* (1975).

In an attempt to derive more easily generalizable numerical integrators, Fatunla (1982) replaced the interpolating function (2.3) with

$$F(x) = \frac{A}{Q_k(x)}, \quad k \geqslant 1. \tag{2.12}$$

On setting

$$L_k(x) = Q_k(x)y(x) - A \tag{2.13}$$

and imposing the constraints

$$\begin{aligned} L_k(x_i) &= 0, \quad i = 1(1)k \\ L'_k(x_i) &= 0, \quad i = 0(1)k - 1 \end{aligned} \tag{2.14}$$

we obtained the explicit nonlinear integration formula

$$y_{n+k} = \frac{y_n}{1 + \sum_{r=1}^{k} k^r a_r}, \quad k > 1, \quad n \geqslant 0 \tag{2.15}$$

which is of error order $p = k$, whose coefficients can be obtained from the linear system

$$R\underline{a} = \underline{b} \tag{2.16}$$

$$R_{ij} = hi^j y'_i + ji^{j-1} y_i$$

$$b_i = -hy'_i$$

for

$$i = 0(1)k - 1, \quad j = 1(1)k. \tag{2.17}$$

Both the methods proposed by Luke *et al.* (1975) and Fatunla (1982) require the solution of m sets of linear systems at every integration step. In the next section, we attempt to eliminate the linear algebra involved by way of extrapolation process.

3. EXTRAPOLATION PROCESS

Hull *et al.* (1973) concluded that the Gragg–Bulirsch–Stoer (GBS) rational extrapolation scheme is very competitive with the Adam's code for non-stiff ivps particularly when function evaluation is inexpensive or high accuracy is desired, and output is demanded infrequently. Deuflhard (1985) argued that the Gragg modified midpoint rule combined with the polynomial extrapolation is more efficient that the GBS. Deuflhard (1983) proposed a new order and stepsize control for extrapolation methods which culminates in the automatic codes DIFEX1 (cf. Deuflhard, 1985) for non-stiff ivps and METAN1 (cf. Bader and Deuflhard, 1983) for stiff ivps.

In this section, we shall adopt (2.15)–(2.17) for $k = 1$ as the basic integrator which possesses an asymptotic error expansion in h and of the form

$$y(x, h) = y(x) + \sum_{r=1}^{\infty} e_r(x)h^r \tag{3.2}$$

unlike the Gragg modified midpoint rule (Gragg, 1965) which has asymptotic expansion in h^2, i.e.

$$\bar{y}(x, h) = y(x) + \sum_{r=1}^{\infty} \bar{e}_r(x)h^{2r}. \tag{3.3}$$

With $H > 0$ as the basic integration step and the integer sequence

$$I = \{n_r\} = \{2, 4, 6, 10, 12, 14, 16, 18, 20\} \tag{3.4}$$

we define a decreasing stepsize sequence

$$\left\{h_r : h_r = \frac{H}{n_r}, \quad r = 1, 2, \ldots\right\}. \tag{3.5}$$

Adopting the one-step integration formula given by (2.15), we generate the first column of the extrapolation table (3.6) as follows

$$\begin{array}{llll} T_{11} & & & \\ T_{21} & T_{12} & & \\ T_{31} & T_{22} & T_{13} & \\ \vdots & \vdots & \vdots & \ddots \\ T_{m1} & T_{m-12} & \cdots & T_{1m} \end{array}$$

$$t_s = x_n + sh_r, \quad s = 1(1)n_r, \quad r = \leqslant m \tag{3.6}$$

and generate

$$z_0 = y_n,$$

$$z_{s+1} = z_s + \frac{h_r z_s' z_s}{z_s - hz_s'} \tag{3.7}$$

for

$$s = 0(1)n_r - 1 \quad \text{and} \quad T_{r,1} = y(x_{n+1}, h_r), \quad r \leqslant m \tag{3.8}$$

where m is the maximum allowable extrapolation.

The subsequent columns can be generated with the polynomial extrapolation scheme (Neville, 1934; Aitken, 1932) using the triangle rule as

$$T_{r,s} = T_{r,s-1} + \frac{T_{r,s-1} - T_{r-1,s-1}}{\left(\dfrac{n_r}{n_{r-s+1}}\right)^{\gamma} - 1} \tag{3.9}$$

where

$$\gamma = \begin{cases} 1, & \text{for (3.7)} \\ 2, & \text{for Gragg modified midpoint rule} \end{cases} \tag{3.10}$$

Table 3. Performance of Fatunla (1982) on the singular ivp $y' = 1 + y^2$, $y(0) = 1$, $0 \leqslant x \leqslant 1$ order $p = k$ for $1 \leqslant k \leqslant 9$. Uniform mesh-size $h = 0.05$

	Theoretical	Errors in nonlinear multistep methods								
X	solution	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$	$k=7$	$k=8$	$k=9$
0.00	1.000,000,000									
0.10	1.223,048,880	1.228(−2)	−8.277(−4)							
0.20	1.508,497,647	2.9.9(−2)	−1.894(−3)	2.298(−4)	−5.953(−5)					
0.30	1.895,765,123	5.580(−2)	−3.520(−3)	5.507(−4)	−5.434(−5)	2.303(−5)	−7.863(−6)			
0.40	2.464,962,757	1.045(−1)	−6.473(−3)	6.726(−4)	−1.685(−4)	2.408(−5)	−4.912(−6)	4.267(−6)	−1.622(−6)	
0.50	3.408,223,442	2.134(−1)	−1.312(−2)	1.754(−3)	−2.238(−4)	7.234(−5)	−1.308(−5)	6.867(−6)	7.931(−8)	1.337(−6)
0.60	5.331,855,223	5.562(−1)	−3.405(−2)	4.206(−3)	−7.541(−4)	1.272(−4)	−4.788(−5)	−7.639(−6)	−7.579(−6)	4.552(−6)
0.65	1.340,436,575	1.106(0)	−6.664(−2)	8.379(−3)	−1.509(−3)	2.338(−4)	−1.270(−4)	2.714(−5)	2.540(−5)	1.104(−5)
0.70	11.681,373,800	3.092(0)	−1.762(−1)	2.016(−2)	−3.322(−3)	7.849(−4)	−8.941(−5)	1.871(−4)	−4.133(−5)	−7.349(−5)
0.75	28.238,252,850	2.903(1)	−1.074(0)	1.181(−1)	−1.893(−2)	4.902(−3)	−3.262(−5)	−1.947(−4)	−1.505(−3)	−1.019(−4)
0.80	68.479,668,346	3.776(1)	−8.284(0)	7.037(−1)	−1.282(−1)	2.622(−2)	−1.003(−2)	−1.730(−2)	−4.723(−3)	1.585(−2)
0.90	8.687,629,546	1.166(0)	1.952(−1)	−6.093(−3)	−2.108(−2)	6.158(−3)	3.739(−2)	8.639(−2)	−7.082(−2)	−4.204(−1)
1.00	4.588,037,825	3.421(−1)	2.340(−1)	9.291(−3)	1.610(−2)	1.054(−2)	6.934(−2)	2.033(−1)	−2.145(−1)	−2.127(0)

Index: $a(-b) = a.10^{-b}$.

Table 4. Performance of new extrapolation codes on the singular ivp, $y' = 1 + y^2$, $y(0) = 1$, $0 \leqslant x \leqslant 1$. $h_0 = 0.25$, $h_{max} = 1.0$, maximum extrapolation 6. Theoretical solution: $y(x) = \tan(x + \pi/4)$. Exact solution: −4.588037825

	Inverse Euler (+) rational extrapolation			Inverse Euler (+) polynomial extrapolation		
$\epsilon = 10^{-9}$ q	Y	No. of steps	No. of Fn evaluation	Y	No. of steps	No. of Fn evaluation
1	−4.69169062	5	41	−4.66101122	5	41
2	−4.58611369	5	65	−4.58357207	3	47
3	−4.58834175	4	72	−4.58788415	3	55
4	−4.58804399	4	108	−4.58800517	3	63
5	−4.58802489	4	126	−4.58803957	3	105
6	−4.58803927	4	162	−4.58803846	3	105
7	−4.58803780	4	188	−4.58803822	691	5107

Numerical solution to ivp $y' = 1 + y^2$, $y(0) = 1$, $0 \leqslant x \leqslant 1$.

An alternative to (3.9) is the Bulirsch and Stoer (1966) rational extrapolation scheme which adopts the rhombus rule

$$T_{r,-1} = 0,$$

$$T_{r,s} = T_{r+1,s-1} + \frac{T_{r+1,s-1} - T_{r,s-1}}{\left(\dfrac{n_r}{n_{r-s+1}}\right)^{\gamma}\left[1 - \dfrac{T_{r+1,s-1} - T_{r,s-1}}{T_{r+1,s-1} - T_{r+1,s-2}}\right] - 1} \tag{3.11}$$

with γ specified by (3.10).

Deuflhard (1985) favoured the polynomial extrapolation (3.9) to rational extrapolation (3.11) for both theoretical and practical reasons:

(i) rational extrapolation lacks translation invariance,
(ii) in special cases, rational extrapolation may impose additional restrictions on the basic stepsize, and that
(iii) the polynomial extrapolation is slightly more efficient in the variable step, variable order implementation.

We however observed from Table 4 that for the singular ivps, the rational extrapolation scheme is more efficient and more accurate than the polynomial extrapolation scheme particularly when high degree of accuracy is desired.

4. NUMERICAL EXPERIMENT

The new algorithm was incorporated into the automatic code DIFEX1 (cf. Deuflhard, 1983) and called DIFEX2 implemented in double precision arithmetic on Prime 750 computer located at the Computer Centre, University of Benin, Benin City, Nigeria.

The essential amendments to the original code DIFEX1 are as follows:

(a) the inclusion of the new integrator (3.7) using the indicator ITYPE i.e.

$$\text{ITYPE} = \begin{cases} 0, & \text{Gragg modified midpoint rule} \\ 1, & \text{inverse Euler (3.7)} \end{cases} \tag{4.1}$$

(b) the extrapolation procedure is coded to accommodate the difference in the asymptotic error expansion for the two basic integrators:

(i) the Gragg modified midpoint rule (in h^2)
(ii) the inverse Euler (in h) as indicated by (3.2), (3.3) and (3.10).

Deuflhard (1985) approximated the local error with the subdiagonal error criterion

$$e_{s+1,s} = \| T_{2s} - T_{1,s+1} \| \leqslant \text{TOL} \tag{4.2}$$

and adopted the local extrapolation by setting

$$y(x_{n+1}, H) = T_{1,s+1}. \tag{4.3}$$

The stepsize for the next integration step is taken as

$$H_{\text{new}} = \left\{\frac{\text{TOL}}{e_{1,s}}\right\}^{1/p_s} H_{\text{old}}, \tag{4.4}$$

where TOL is the allowable error tolerance, and the error order

$$p_s = \begin{cases} s, & \text{for inverse Euler integrator} \\ 2s, & \text{for midpoint integrator} \end{cases}. \tag{4.5}$$

We consider the scalar ivp of Luke *et al.* (1975)

$$y' = 1 + y^2, \quad y(0) = 1, \quad 0 \leqslant x \leqslant 1, \quad h_0 = 0.25, \quad h_{\max} = 1 \tag{4.6}$$

for tolerances

$$\text{TOL} = 10^{-q}, \quad q = 1(1)7. \tag{4.7}$$

(4.6) has a theoretical solution $y(x) = \tan(x + \pi/4)$ which has a singularity at $x = \pi/4$. The details of numerical experiments are given in Tables 1–4.

From Table 1, it can be observed that both the Gagg–Bulirsch–Stoer rational extrapolation scheme and the Gragg–Neville–Aitken polynomial extrapolation scheme were halted in the neighbourhood of the singularity $x = \pi/4 \simeq 0.785398$. This is simply because the basic integrator (Gragg modified midpoint rule) is based on polynomial interpolation and require more than the allowable maximum number of stepsize reduction which is set to 5 in the code.

Tables 2–4 show that the proposed scheme as well as those of Luke *et al.* (1975) and Fatunla (1982) can adequately and efficiently cope with singular ivps.

The new scheme has the advantage of being implemented in variable order, variable step mode and besides does not require the solution of linear systems at every integration step as Luke *et al.* (1975) and Fatunla (1982).

REFERENCES

1. A. C. Aitken, On interpolation by iteration of proportional parts. *Proc. Edinburgh Math. Soc.* **2**, 56–76 (1932).
2. G. Bader and P. Deuflhard, A semi-implicit midpoint rule for stiff systems of ordinary differential equations. *Numer. Math.* **41**, 373–398 (1983).
3. R. Bulirsch and J. Stoer, Numerical treatment of ODES by extrapolation methods. *Numer. Math.* **8**, 1–13 (1966).
4. P. Deuflhard, Order and stepsize control in extrapolation methods. *Numer. Math.* **41**, 399–422 (1983).
5. P. Deuflhard, Recent progress in extrapolation methods for ODEs. *SIAM Rev.* **27**, 505–536 (1985).
6. W. Fair and Y. L. Luke, Rational approximations to the solution of the second order Riccati equation. *Math. Comp.* **20**, 602–606 (1966).
7. S. O. Fatunla, Nonlinear multistep methods for ivps. *Comp. Maths Applic.* **8**, 231–239 (1982).
8. W. B. Gragg, On extrapolation algorithms for ordinary initial value problems. *SIAM J. Numer. Anal.* **2**, 384–404 (1965).
9. T. E. Hull, W. H. Enright, B. M. Fellen and A. E. Sedgwick, Comparing numerical methods for ODES. *SIAM J. Numer. Anal.* **9**, 603–637 (1973).
10. J. D. Lambert and B. Shaw, On the numerical solution of $y' = f(x, y)$ by a class of formulae based on rational approximation. *Maths. Comp.* **19**, 456–462 (1965).
11. J. D. Lambert and B. Shaw, A method for the numerical solution of $y' = f(x, y)$ based on a self-adjusting non-polynomial interpolant. *Maths Comp.* **20**, 11–20 (1966).
12. Y. L. Luke, W. Fair and J. Wimp, Predictor-corrector formulas based on rational interpolants. *Comp. Maths Applic* **1**, 3–12 (1975).
13. E. H. Neville, Iterative Interpolation. *J. Ind. Math. Soc.* **20**, 87–120 (1934).
14. B. Shaw, Modified multistep methods based on a non-polynomial interpolant. *J. assoc. Comput. Mach.* **14**, 143–154 (1967).