Towards a Derivative Free Rational one step Method for Solving Stiff Initial Value Problems

Ronald Tshelametse[#1], Thuso Nkatse[*2]

[#1]Department of Mathematics ,University of Botswana
P. O. Box UB 70111, Gaborone, Botswana

[#2]Department of Mathematics,University of Botswana
P/Bag 0022,UB, Gaborone, Botswana

***Abstract*— We present a derivative free rational one step scheme of order two, capable of solving Ordinary differential equations which are stiff and others with singular solution. The scheme allows for the use of the state function alone and does not require calculation of higher derivatives of f(y$_n$), and the proposed strategy was compared to the scheme of Van-Niekerk of which almost similar results were obtained for stiff problems.**

***Keywords*— Rational Methods, Stiff problems, Singular solutions.**

I. Introduction

Our interest is on the numerical solution of the Initial value Problem (IVP).

$$y' = f(t, y), \qquad (1)$$

$$y(t_0) \in R^n, t \in [t_0, t_k], y(t) \in R^n$$

which may be stiff or possess singularities in a given interval. The conventional one step scheme is given by

$$y_{n+1} = y_n + h\varphi(t_n, y_n, h) \qquad (2)$$

where $\varphi(t_n, y_n, h)$ is the increment function and the conventional Linear Multistep methods(LMM) is described by

$$\sum_{i=0}^{k} \alpha_i y_{n-i} = h\sum_{i=0}^{k} \beta_i f(y_{n-i}) \qquad (3)$$

where α_i, β_i are real constants. When $\beta_0 = 0$, the method is said to be explicit otherwise it is implicit. In literature explicit methods are said to be performing poorly when solving stiff problems, hence this require the use of Implicit methods for which Backward Differentiation formula (BDF's) is one of them. Some commonly used codes like Matlab Ode15s [9,10,11], which were proposed by [11] apply the BDF's for solving stiff ordinary differential equations. The conventional explicit and implicit methods are said to fail when solving ODE with singularities because they are based of polynomial interpolation which focuses on existence and uniqueness of the solution within a specified interval. According to Ikhile [6], singularities arises from unbounded Jacobians,

$$J = \left[\frac{\partial f_i}{\partial y_j}\right]_{i, j=1,\ldots,m}$$

also this singularities are said to arise in

a) Components of $f(t, y(t))$
b) Derivatives of $f(t, y(t))$
c) Components of the solution vector $y(t)$

II. Rational methods

Most rational schemes found in [1],[2],[4],[5],[6],[7],[8] use higher derivatives of the state function. Therefore this has been picked as a major disadvantage as it can be tiresome or difficult for some Initial Value problems to reach those higher derivatives; hence a need to approximate the higher derivatives is proposed. This paper seeks to extend Van Niekerk's rational scheme [2], to the one with free derivative of $f(t, y)$. The methods proposed by these different authors were presented in a fixed step size approach and managed to pass through singular points. In [6] Ikhile indicates that the normal step size selection strategies does not work when implementing the methods in variable step mode, as in most cases the next step will be very large compared to the last step hence, reducing the step sizes to a desirable one will not be easy. The paper goes on to indicate that the way to pass through these singular points the use of extrapolation methods proves to be very useful.

III. DEVELOPMENT OF DERIVATIVE FREE SCHEME

The rational one step scheme proposed by Van Niekerk is given below

$$y_{n+1} = y_n + \frac{2h(y'_n)^2}{2y'_n - hy''_n} \quad (4)$$

Where $y' = f(t, y)$ and

$$y''_n = f'(t_n, y_n) = f_t(t_n, y_n) + f_y(t_n, y_n) f(t_n, y_n)$$

the denominator in (4) can be represented as

$$2f(t_n, y_n) - hf'(t_n, y_n) = 2f(t_n, y_n) - h(f_t(t_n, y_n) + f_y(t_n, y_n) f(t_n, y_n))$$
$$= 2f(t_n, y_n) - hf_t(t_n, y_n) - hf_y(t_n, y_n) f(t_n, y_n)$$
$$= 2f(t_n, y_n) + f(t_n, y_n) - f(t_n, y_n) - hf_t(t_n, y_n) - hf_y(t_n, y_n) f(t_n, y_n)$$
$$= 3f(t_n, y_n) - (f(t_n, y_n) + hf_t(t_n, y_n) + hf_y(t_n, y_n) f(t_n, y_n)) \quad (5)$$

From multivariate Taylor expansion

$$f(x+a, y+b) = f(x, y) + af_x(x, y) + bf_y(x, y)$$

Assumption: From the above multivariate Taylor expansion b, can be taken as a function instead of a constant, as from [3], we see that the general Runge Kutta (RK) method is given by

$$y_{n+1} = y_n + h_n \varphi(y_n, h) = y_n + \sum_{i=1}^{s} b_i k_0, \text{ where}$$

$k_1 = h_n f(y_n)$ and

$$k_i = h_n f(y_n + \sum_{j=1}^{i-1} a_{ij} k_j), i = 2, 3, \ldots, \ldots, s$$

and usually $y_0 = y(t_0)$ Hence from (5)

$$f(t_n, y_n) + hf_t(t_n, y_n) + hf_y(t_n, y_n) f(t_n, y_n)$$
$$= f(t_n + h, y_n + hf(t_n, y_n))$$

Therefore (5) can be represented by

$$3f(t_n, y_n) - f(t_n + h, y_n + hf(t_n, y_n)) \quad (6)$$

Substituting these into (4) yields,

$$y_{n+1} = y_n + \frac{2h(f(t_n, y_n))^2}{3f(t_n, y_n) - f(t_n + h, y_n + hf(t_n, y_n))} \quad (7)$$

From this (4) can be implemented without finding the 2nd derivatives of the original function, hence the state function only would be sufficient and this method (7) could be presented in a variable step.

IV. LOCAL TRUNCATION ERROR

In order to test the performance of the proposed strategy, one needs to highlight how the local truncation error of the rational scheme (4). The idea used follows the definitions given on Lambert 1991.

The rational scheme (4) was derived from the continued fraction given by,

$$y_n = a_n + \frac{b_n t_n}{1 + c_n t_n} \quad (8)$$

Hence, the following definition follows,

Definition 1: The **Linear difference operator *L*** associated with the rational scheme (8) is defined by

$$L[y(t); h] = (y_{t+h} - a_n) \times (1 + c_n h) - b_n h \quad (9)$$

Where $y(t) \in C^1[a, b]$ is an arbitrary function. We choose the function $y(t)$ to be differentiable as often as we need. Expanding $y(t+h)$ in Taylor series and collecting the terms in (9) yields the following expression;

$$L[y(t); h] = C_0 h^0 + C_1 h^1 + \cdots + C_k h^k + C_{k+1} h^{k+1} + \cdots \quad (10)$$

Definition 2: The difference operator (9) on the associated rational scheme (8) are said to be of order $p = k+1$, if in (10)

$$C_0 = C_1 = C_2 = \cdots = C_K = 0, C_{K+1} = 0, C_{K+2} \neq 0.$$

Definition 3: (Lambert 1991) [12],The local truncation error or LTE of the method (8) at t_{n+k}, denoted by T_{n+k} is defined by

$$T_{n+k} = L[y(t_n); h],$$

Where ***L*** is the associated difference operator defined by (9) and y(t) is the exact solution of the initial value problem (1), the local truncation of rational method (8) is then

$$L[y(t); h] = C_{k+1} h^{k+1} + O(h^{k+2}) \quad (11)$$

From (9), If we expand $y(t+h)$ using Taylors method, we obtain

$$L[y(t); h] = (y(t) + hy'(t) + \frac{h^2}{2} y''(t) + \frac{h^3}{6} y'''(t) - a_n) \times (1 + c_n h) - b_n h$$
$$= -a_n + y(t) + h[-b_n - a_n c_n + c_n y(t) + y'(t)] + h^2 \left[\frac{y''(t)}{2} + c_n y'(t) \right] + h^3 \left[\frac{c_n y''(t)}{2} + \frac{y'''(t)}{6} \right]$$

We see that (9) and (10) implies that

$$C_0 = -a_n + y(t), \; C_1 = -b_n - a_n c_n + c_n y'(t)$$

$$C_2 = \frac{y''(t)}{2} + c_n y'(t) \text{ and } C_3 = \frac{c_n y''(t)}{2} + \frac{y'''(t)}{6}$$

The coefficients a_n, b_n, c_n are given from [2] as $a_n = y(t)$, $b_n = y'(t)$ and $c_n = \frac{y''(t)}{2y'(t)}$, hence C_3 is defined as;

$$C_3 = -\frac{(y''(t))^2}{4y'(t)} + \frac{y'''(t)}{6}$$

where $y(t)$ is taken as the theoretical solution of the initial value problem (1) at point t_n i.e $y(t) = y(t_n)$, hence the Local truncation error is given by

$$LTE = h^3\left(-\frac{\left((y_n'')^2\right)}{4y_n'} + \frac{y_n'''}{6}\right) + O(h^4) \qquad (12)$$

V. NUMERICAL RESULTS

We compare the current strategy (7) with Van-Niekerk's rational scheme (4) for problems 1 and 2.

Problem 1 (Singular Problem)

$$y' = 1 + y^2$$

In the first case problem 1 was solved with initial condition $y(0) = 0$ and time interval of $t \in [0,1.55]$, Van-Nierkerk's scheme and the proposed approach. The problem was integrated with step size *h=0.001*,for both schemes and the analytic solution of the problem is given by $y = \tan(t)$ the results obtained are displayed in Table 1 and plotted as per figure 1.

TABLE 1. $y' = 1 + y^2, y(0) = 0, h = 0.001$

t	Analytical	Error(Proposed Strategy)	Error (Van-Rational)
0.1	0.1003346721	1.79000E-08	3.36670E-06
0.2	0.2027100355	3.45000E-08	6.94020E-06
0.3	0.3093362496	6.04000E-08	1.09562E-05
0.4	0.4227932187	9.13000E-08	1.57157E-05
0.5	0.5463024898	1.40200E-07	2.16392E-05
0.6	0.6841368083	2.11700E-07	2.93587E-05
0.7	0.8422883805	3.19500E-07	3.98840E-05
0.8	1.0296385571	5.12900E-07	5.49327E-05
0.9	1.2601582176	8.52400E-07	7.815908E-05
1.0	1.5574077247	1.52530E-06	1.141712E-04
1.5	14.1014199472	1.29951E-03	9.984863E-03
1.55	48.0784824792	5.31986E-02	1.191786E-01

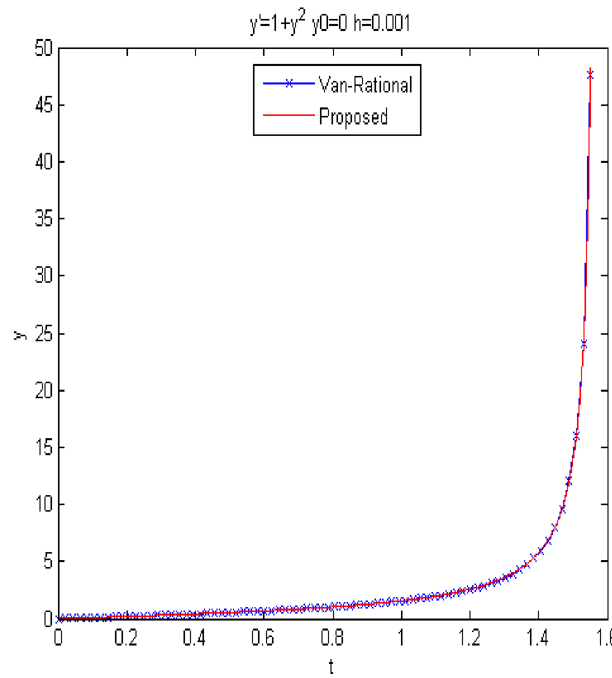

fig 1, Singular Problem y(0)=0

For the second part problem 1 was solved with initial condition $y(0) = 1$ and time interval of $t \in [0,0.75]$. The integration step considered was a fixed step *h=0.001* the analytic solution of problem 1 within this initial conditions is given by $y = \tan(t + \frac{\pi}{4})$, the results obtained are displayed as per Table 2 and plotted as in figure 2.

TABLE 2. $y' = 1 + y^2, y(0) = 1, h = 0.001$

t	Analytical	Error(Proposed Strategy)	Error (Van-Rational)
0.1	1.2230488804	1.9490E-07	2.0765E-04
0.2	1.5084976471	6.1340E-07	5.4497E-04

0.3	1.8957651229	1.5951E-06	1.1462E-03
0.4	2.4649627567	4.2307E-06	2.3532E-03
0.5	3.4082234423	1.3055E-05	5.2414E-03
0.6	5.3318552235	5.7655E-05	1.4653E-02
0.65	7.3404365750	1.6138E-04	2.9566E-02
0.7	11.6813738003	6.9748E-04	7.9521E-02
0.75	28.2382528501	1.0524E-02	4.8962E-01

Singular points- To check the behavior of the two schemes at singular points, problem 1 with condition y(0)=0 is extended up to 1.58 ,where its singular point is at π/2 and problem 1 with condition y(0)=1 was extended up to 0.8, where its singular point is at π/4. The results as displayed by table 3 and 4.

TABLE 3. $y' = 1 + y^2, y(0) = 0, h = 0.001$

t	Analytical	Error(Proposed Strategy)	Error (Van-Rational)
0.1	0.1003346721	1.79000E-08	3.36670E-06
0.2	0.2027100355	3.45000E-08	6.94020E-06
0.3	0.3093362496	6.04000E-08	1.09562E-05
0.4	0.4227932187	9.13000E-08	1.57157E-05
0.5	0.5463024898	1.40200E-07	2.16392E-05
0.6	0.6841368083	2.11700E-07	2.93587E-05
0.7	0.8422883805	3.19500E-07	3.98840E-05
0.8	1.0296385571	5.12900E-07	5.49327E-05
0.9	1.2601582176	8.52400E-07	7.815908E-05
1.0	1.5574077247	1.52530E-06	1.141712E-04
1.5	14.1014199472	1.29951E-03	9.984863E-03
1.55	48.0784824792	5.31986E-02	1.191786E-01
1.56	92.6204963162	3.780067E-01	4.461151E-03
1.57	1255.76559140	2.027084E+03	8.247270E-01
1.58	-108.649203606	4.156140E+02	6.217993E-03

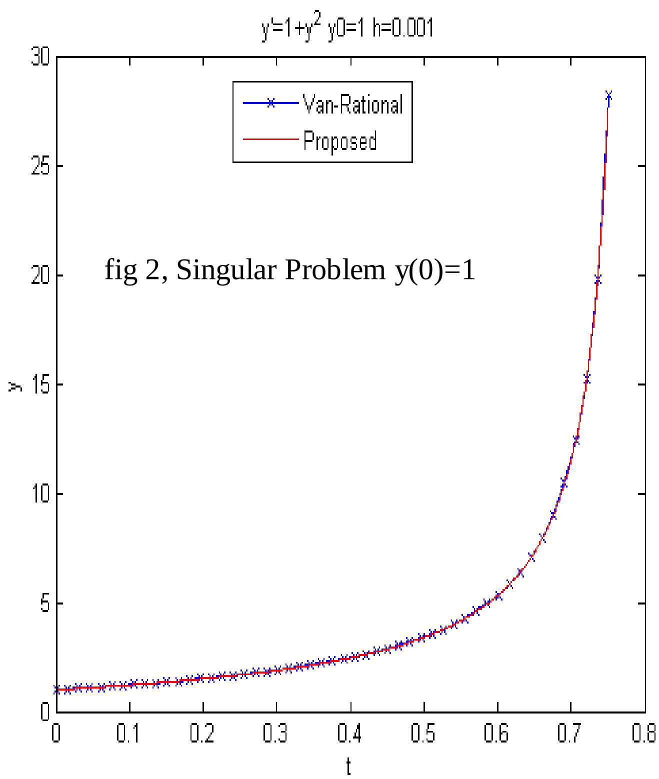

fig 2, Singular Problem y(0)=1

TABLE 4. $y' = 1 + y^2, y(0) = 1, h = 0.001$

t	Analytical	Error(Proposed Strategy)	Error (Van-Rational)
0.1	1.2230488804	1.9490E-07	2.0765E-04
0.2	1.5084976471	6.1340E-07	5.4497E-04
0.3	1.8957651229	1.5951E-06	1.1462E-03
0.4	2.4649627567	4.2307E-06	2.3532E-03
0.5	3.4082234423	1.3055E-05	5.2414E-03
0.6	5.3318552235	5.7655E-05	1.4653E-02
0.65	7.3404365750	1.6138E-04	2.9566E-02
0.7	11.6813738003	6.9748E-04	7.9521E-02
0.75	28.2382528501	1.0524E-02	4.8962E-01
0.76	39.3644592671	2.880027E-02	3.928045E-04
0.77	64.9376772062	1.299212E-01	1.082576E-03
0.78	185.246390849	2.963046e+00	8.922044E-03

Problem 2 (Stiff problem)

The second problem considered is a stiff differential equation given by

$y' = \lambda(y - g(t)) + g'(t)$

$g(0) = 3, g(t) = \sin(0.1t) + 2$ and

$g'(t) = 0.1\cos(0.1t)$ with $t \in [0,1]$

Where the exact solution is given by

$y(t) = \sin(0.1t) + 2 + e^{(-\lambda t)}$

TABLE 5. $\lambda = -10, h = 0.01$

t	Analytical	Error (Proposed Strategy)	Error (Van-Rational)
0.1	2.3778792745	3.2221E-04	3.2221E-04
0.2	2.1553339499	2.4712E-04	2.4711E-04
0.3	2.0797825686	1.4958E-04	1.4958E-04

0.4	2.0583049731	9.3454E-05	9.3445E-05
0.5	2.0567171163	5.7570E-05	5.7555E-05
0.6	2.0624427587	1.0152E-05	1.0134E-05
0.7	2.0708547293	1.06069E-06	1.5876E-06
0.8	2.0802501566	5.6800E-08	7.8200E-08
0.9	2.0900019590	2.3530E-07	2.5910E-07
1.0	2.0998788166	1.5270E-07	1.7900E-07

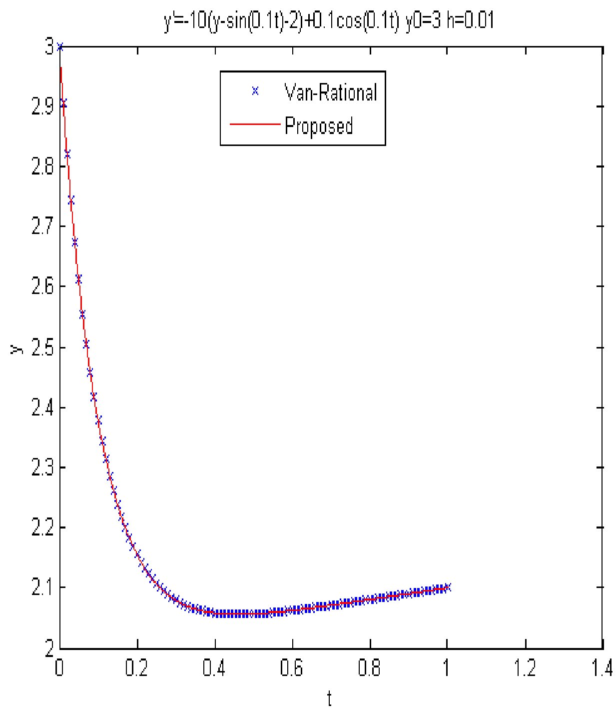

fig 3, Stiff Problem λ= -10

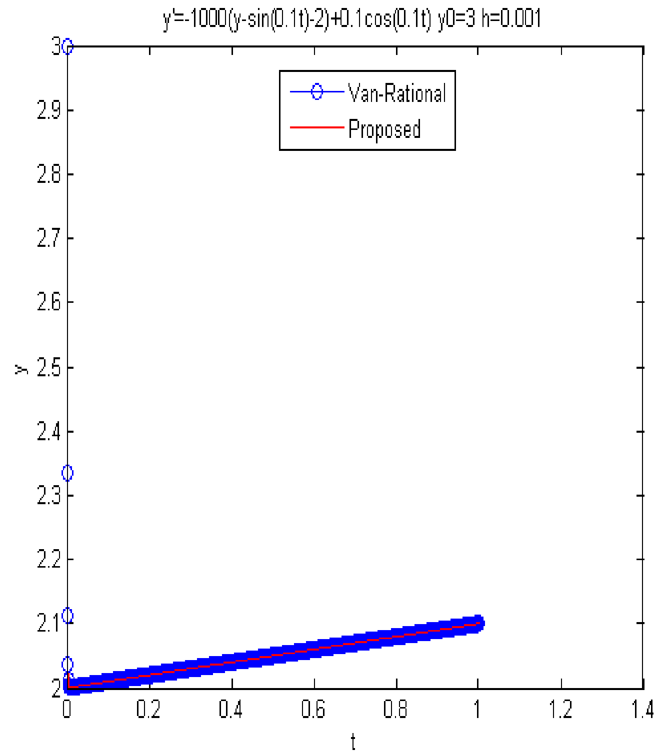

fig 4 ,Stiff Problem λ= -1000

TABLE 6. $\lambda = -10^3, h = 0.001$

t	Analytical	Error (Proposed Strategy)	Error (Van-Rational)
0.01	2.00104539976309	3.2359E-05	3.2359E-05
0.02	2.002000000727820	1.2796E-08	1.2805E-08
0.03	2.002999995500096	9.0150E-14	1.4760E-11
0.04	2.003999989333342	1.9320E-11	3.4017E-13
0.10	2.008999878500492	4.4340E-11	3.2996E-13
0.30	2.029995500202496	1.4931E-10	3.2996E-13
0.50	2.049979169270678	2.4922E-10	3.4017E-13
0.70	2.069942847337533	3.4904E-10	3.2996E-13
0.90	2.089878549198011	4.4872E-10	3.2996E-13
1.00	2.099833416646828	4.9848E-10	3.4017E-13

VI. CONCLUSIONS

In this article we have proposed an approach to one step explicit method based on rational functions proposed by Van-Niekerk. The method is derivative free requiring only state function and its Initial conditions. The formulation is given by (7) while the local truncation error for the rational method (4) is given by Definition 1 and 2. To test performance of the proposed strategy, two problems were solved with problem (1) being singular and tested over two different initial conditions. Problem (2) is a stiff problem given by Frank and Ueberhuber,[2], applied with λ= -10and λ= -10^3. Results obtained from table1, 2,5,6 shows performance of the two methods as yielding almost the same results which is confirmed by figures 1,2,3 and 4. For problem (1) the interval of integration was increased to allow for singular points and the proposed strategy though managed to cross the points, it is outclassed by Van-

Niekerk's method beyond the point of singularity. Future studies should discuss the extension of this approach for orders more than two and application of the method to non-linear and/or stiff systems of first order ordinary differential equations, also the approach has to be explored further especially after point of singularity.

REFERENCES

[1] F.D. Van Niekerk, "Non Linear One-Step Methods for Initial Value Problems", *Compt Math Application*,13 (4) (1987) 367-371

[2] F.D. Van Niekerk, "Rational-One Step Methods for Initial Value Problems", *Compt.Math. Application*.,16(12) (1988) 1035-1039

[3] J.R Dormand and P.J Prince , "A family of embedded Runge-Kutta formulae", *Journal of Computational and Applied Mathematics*, Vol. 6, No. 1, 1980.

[4] M.N.O. IKHILE, "Coefficients for Studying One step Rational Schemes for IVPs in ODEs:I, Computer and Mathematics with Applications 41(2001) 769-781

[5] M.N.O. IKHILE, Coefficients for Studying One step Rational Schemes for IVPs in ODEs:II, Computer and Mathematics with Applications 44(2002) 545-557

[6] M.N.O. IKHILE,, "Coefficients for Studying One step Rational Schemes for IVPs in ODEs:III Extrapolation Methods", *Computer and Mathematics with Applications* 47(2004) 1463-1475.

[7] Teh Yuan Ying, Nazeeruddin Yaacob and Norma Alias, "A New Class of Rational Multistep Methods for the Numerical Solution of First Order Initial Value Problems", *MATEMATIKA* 27(1) (2011) 59-78

[8] Teh Yuan Ying and Nazeeruddin Yaacob, "A New Class of Rational Multistep Methods for the Numerical Solution of First Order Initial Value Problems", *Malaysian Journal of* Mathematical Sciences 7(1) (2013) 31-57

[9] Teh Yuan Ying and Nazeeruddin Yaacob, "One-Step Exponential-rational Methods for the Numerical Solution of First Order Initial Value Problems", *MATEMATIKA* 27(1) (2011) 59-78

[10] R. Tshelametse., "The Milne error estimator for stiff problems", *Southrn Africa Journal of Pure and Applied Mathematics* 4 (2009) 13-27

[11] L.F. Shampine and M.W. Reichelt. "The MATLAB ODE suite". SIAM J. Sci Sta. Comput., 18, No. 1:1-22, January 1997.

[12] R. Tshelametse., "Terminating Simplified Newton Iterations: A Modified Strategy"

[13] J.D. Lambert, *Numerical Methods for Ordinary Differential Systems The Initial Value Problem*, 1991, John Wiley & Sons Ltd, Sussex.