IN COMPARISON OF SOME NUMERICAL METHODS FOR SOLVING STIFF INITIAL VALUE PROBLEMS FOR ORDINARY DIFFERENTIAL EQUATIONS

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Abstract:

This paper presents comparison of Some Numerical methods for solving Initial Value Problems (IVPs) in Ordinary differential equations. Rational one step methods are considered against Linear Multistep methods of the BDF type as implemented in ODE15s. The superiority of the Rational one step methods is illustrated in the solution of some stiff problems.

1 Introduction

In this research paper work, we shall consider the numerical solution of Initial value problems (IVP) for systems of ordinary differential equations (ODEs)

$$\frac{dy}{dt} = f(t,y), 0 < t \leq T, y(0) = y_0, f: R \times R^m \to R^m (1)$$

In literature most of the methods for solving (1) are based on polynomial interpolation in h, according to [1, 2, 3, 4] and these methods are said to perform poorly when the IVP is stiff or when its solution possesses singularities. The aim of the paper is to compare Van Nierkerk's [2] rational one-step method with the linear multistep methods of the BDF type for Initial value problems with singular solutions and the one that are considered to be stiff.

Some Definitions to consider

Stiffness

An ordinary differential equation problem is **stiff** if the solution being sought is varying slowly, but there are nearby solutions that vary rapidly, so the numerical method must take small steps to obtain satisfactory results.

Singularity

A **singular solution**$y_s(x)$of an ordinary differential equation is a solution that is singular or one for which the Initial Value problem fails to have a unique solution at some point on the solution. The set on which a solution is singular may be as small as single point or as large as the full real line.

The term singular solution could also mean a solution at which there is a failure of uniqueness to the IVP at every point on the curve, Hence a singular solution in this form is often given as tangent to every solution from a family of solutions. This means that there is a point $y_s(x) = y_c(x)$and $y'_s(x) = y'_c(x)$where $y_c$is a solution in a family of solutions parameterized by c, which implies that the singular solution is the envelope of the family of solutions.

2 Linear Multistep Methods

Let us consider the Initial value problem

$$y'(t) = f(t,y), y(t_0) = y_0 \qquad (2)$$

where $t \in [t_{0,} t_0 + Nh]$ where N is a natural number and h a constant time step,$y: [t_{0,} t_0 + Nh] \to R^m$, y' stands for the first derivative, and $f: R^m \to R^m$is continuous and differentiable. The general multistep method can be written in the from (Ascher and Petzold,1998)

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

where α_i, β_i are parameters to be determined,$y_n = y(t_0 + nh)$. A multistep method is said to be of order p if and only if (Butcher 2003)

$$\sum_{i=0}^{k} \alpha_i\, i^q = q \sum_{i=0}^{k} \beta_i i^{q-1} + O(h^p) \qquad (4)$$

Where $0 \leq q \leq p$.

The linear multistep in consideration for our paper is the Backward Differentiation formula given by

$$\sum_{i=0}^{k} \alpha_i y_{n-i} = h\beta_0 f(y_n) \qquad (5)$$

This scheme is a class of k-step formula of order k. In practice the implementation of BDF methods is carried out through varying the step size h_n and/or order k [10, 11, 12]. At each integration step t_n we must solve the nonlinear equation

$$F(y_n) \equiv y_n + \varphi_n - h_n\beta_0 f(y_n) = 0, \qquad (6)$$

where, $\varphi_n = \sum_{i=1}^{k} \alpha_i\, y_{n-i}$ is known value. In solving for y_n, practical codes use the Newton Iterative methods. The use of Newton method and its variants is to overcome the issue of stiffness.

In carrying out our experiments our results are obtained using a Matlab code from MATLAB ode suite [11] known as ode15s[12]. This code is a variable step variable order code which integrates stiff Initial value problems. The code has an option to use either modified BDF's or use the standard BDF's. The iteration is started with a predicted value

$$y_n^{(0)} = \sum_{m=0}^{k} \nabla^m\, y_{n-1}$$

where ∇ denotes the backward difference operator. This represents the backward difference form of the interpolating polynomial that matches the back values, $y_{n-1}, y_{n-2}, \dots, y_{n-k-1}$ and then is evaluated att_n.

3 Rational one-step method by Van Nierkerk

In his paper, Van Nierkerk, [1] developed a numerical one step method for solving Initial Value problems, where the theoretical solution of$y' = f(t, y(t))$ is approximated by

$$y_n = a_n + \frac{b_n t_n}{1 + c_n t_n} \qquad (7)$$

where a_n, b_n, c_n are real constants to be determined.

The method produced use an interpolation function which is expressed in the form of a continued fraction. The theoretical solution is approximated by

$$T_k(t) = a_0 + \cfrac{a_1 t}{1 + \cfrac{a_2 t}{1 + \cfrac{a_3 t}{1 + \ddots \cfrac{a_k t}{1 + a_{k+1} t}}}}$$

where $T_k(t)$ is a finite continued fraction and $k$denotes the order of the fraction.

$$T_1(t) = y_n = a_n + \frac{b_n t_n}{1 + c_n t_n} \qquad (8)$$

andy_n denotes the approximate value of $y(nh)$ and $t_n = nh$.

Expanding $y(t_n + 1)$ by Taylor's expansion, we get the following expression

$$y(t_n + 1) = y(t_n) + hy'(t_n) + \frac{h^2}{2} y''(t_n) + \frac{h^3}{3!} y'''(t_n) + \cdots\cdots\cdots + \frac{h^m}{m!} y^m(t_n)$$

which can be generalized as

$$y(t_n + 1) = \sum_{m \in N} \frac{h^m}{m!} y^m(t_n) \approx \sum_{m \in N} \frac{h^m}{m!} y^m \qquad (9)$$

where$y^{(m)} = \frac{d^m y}{dt^m}$.

For y_{n+1}, equation (7) yields

$$y_{n+1} = a_{n+1} + b_{n+1}(n+1)h \sum_{m \in N} (-1)^m c_{n+1}^m (n+1)^m h^m \quad (10)$$

since $y_{n+1} \approx y(t_n + 1)$, it follows from equations (9) and (10) that ,

$$a_{n+1} + b_{n+1}(n+1)h + b_{n+1}(n+1)h[(-1)c_{n+1}(n+1)h] = y(t_n) + hy'(t_n) + \frac{h^2}{2}y''(t_n)$$

Comparing the coefficients of h^mwe find that

$$a_{n+1} = y(t_n) = y_n \quad (11)$$

$$b_{n+1} = \frac{y'(t_n)}{n+1} \quad (12)$$

and

$$c_{n+1} = -\frac{y''(t_n)}{2(n+1)^2 b_{n+1}}$$

Substituting the value b_{n+1},we get

$$c_{n+1} = -\frac{y''(t_n)}{2y'(t_n)(n+1)} \quad (13)$$

Substituting (11), (12), (13) in equation (7), the following first order one-step method is given by, we have

$$y_{n+1} = y_n + \frac{2h(y'_n)^2}{2y'_n - hy''_n} \quad (14)$$

$$T_2(t_n) = y_n = a_n + \frac{b_n t_n}{1 + \frac{c_n t_n}{1 + d_n t_n}} = a_n + b_n(1 + d_n)t_n(1 + (c_n + d_n)t_n)^{-1}$$

The following coefficients are the same as for $k = 1$, $a_{n+1}, b_{n+1}, c_{n+1}$ and this requreires determination of d_{n+1}, which is given by

$$d_{n+1} = \frac{3(y''_n)^2 - 2y'''_n y'_n}{6y'_n y''_n (n+1)} \qquad (15)$$

We find that when the order of fraction is increased, it is only necessary to calculate the new constant as all constants previously obtained stays exactly the same, hence the second order one step method is represented by

$$y_{n+1} = y_n + \frac{h(6y'_n y''_n + 3(y''_n)^2 - 2y'_n y'''_n h)}{2(3y''_n - y'''_n h)} \qquad (16)$$

which is derived from

$$y_{n+1} = a_{n+1} + \frac{b_{n+1}t_{n+1}}{1 + \frac{c_{n+1}t_{n+1}}{1+d_{n+1}t_{n+1}}}$$

4 Numerical Results

In order to confirm the applicability and suitability of the methods for solution of initial value problem, a solution near a singularity and one stiff problem was solved and results displayed on table and graph. The rational method considered was of order one, which is given by equation (14).

Problem 1 (Singular Problem)

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

a. In the first case problem 1 was solved with initial condition $y(0) = 0$ and time interval of $t \in [0,1.55]$, for both Ode15s and the rational method. The problem was integrated with step size $h = 0.01$, 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(a)

t	Analytical	Ode15s	Rational (y_n)
0.1	0.1003	0.1003	0.1003
0.2	0.2027	0.2027	0.2027
0.3	0.3093	0.3093	0.3093
0.4	0.4228	0.4228	0.4228
0.5	0.5463	0.5463	0.5463

0.6	0.6841	0.6842	0.6841
0.7	0.8423	0.8423	0.8422
0.8	1.0296	1.0297	1.0296
0.9	1.2602	1.2602	1.2601
1.0	1.5574	1.5575	1.5573
1.5	14.1014	14.1068	14.0914
1.55	48.0785	48.1421	47.9593

Table 1(b)

Results for problem 1(a) were computed with a precision of 10 decimals and are shown in the table 1b with their absolute errors

t	Analytical	Ode15s	Rational (y(nh))	Error(Ode15s)	Error(Rational)
0.1	0.1003346721	0.1003433112	0.1003313054	8.63910E-06	3.36670E-06
0.2	0.2027100355	0.2027194054	0.2027030953	9.36990E-06	6.94020E-06
0.3	0.3093362496	0.3093493393	0.3093252934	1.30897E-05	1.09562E-05
0.4	0.4227932187	0.4228091925	0.4227775030	1.59738E-05	1.57157E-05
0.5	0.5463024898	0.5463230977	0.5462808506	2.06079E-05	2.16392E-05
0.6	0.6841368083	0.6841608247	0.6841074496	2.40164E-05	2.93587E-05
0.7	0.8422883805	0.8423180874	0.8422484965	2.97069E-05	3.98840E-05
0.8	1.0296385571	1.0296755513	1.0295836244	3.69942E-05	5.49327E-05
0.9	1.2601582176	1.2602075926	1.26008005852	4.93750E-05	7.815908E-05
1.0	1.5574077247	1.5574764626	1.5572935535	6.87379E-05	1.141712E-04
1.5	14.1014199472	14.1067725941	14.0914350841	5.35264690E-03	9.98486310E-03
1.55	48.0784824792	48.1421426705	47.9593044166	6.36601913E-02	1.19178063E-01

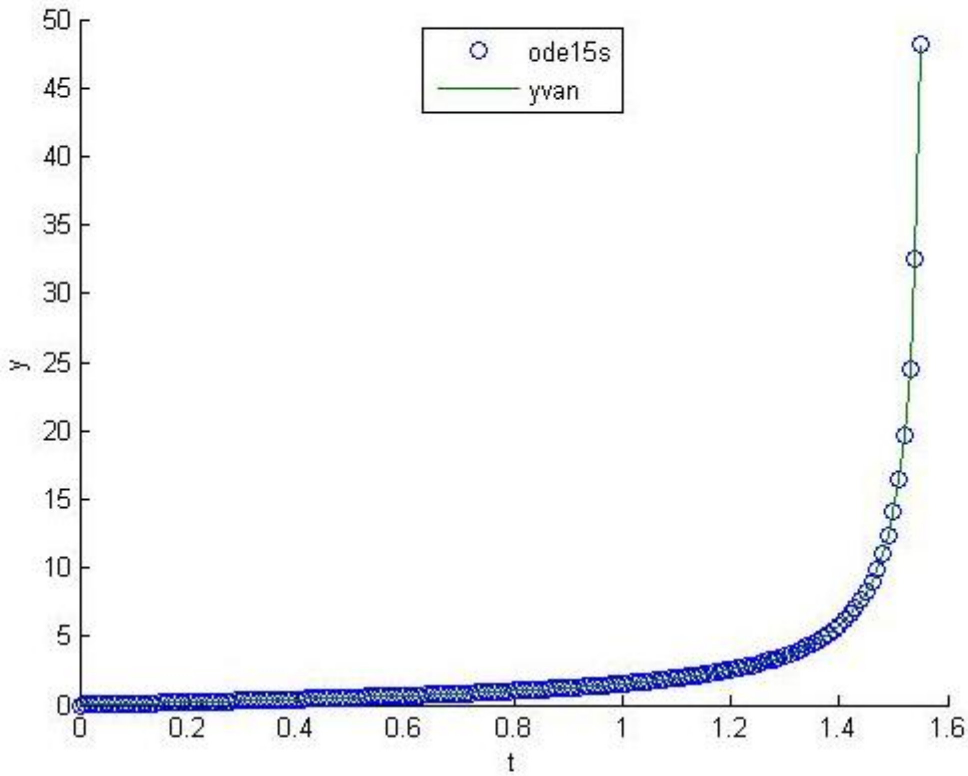

Figure 1

b. For the second part, problem 1 was solved with initial condition $y(0) = 1$ and time interval of $t \in [0,1.55]$. The integration step considered was a fixed step $h = 0.05$, the analytic solution of problem 1 within this interval is given by $y = \tan\left(t + \frac{\pi}{4}\right)$, the results obtained are displayed as per Table 2 and plotted as in figure 2.

Table 2

t	Analytical	Ode15s	Rational (y_n)
0.1	1.2230	1.2231	1.2228
0.2	1.5085	1.5085	1.5080
0.3	1.8958	1.8958	1.8946
0.4	2.4650	2.4650	2.4626
0.5	3.4082	3.4083	3.4030
0.6	5.3319	5.3321	5.3172
0.65	7.3404	7.3409	7.3109
0.7	11.6814	11.6827	11.6019
0.75	28.2383	28.2463	27.7486

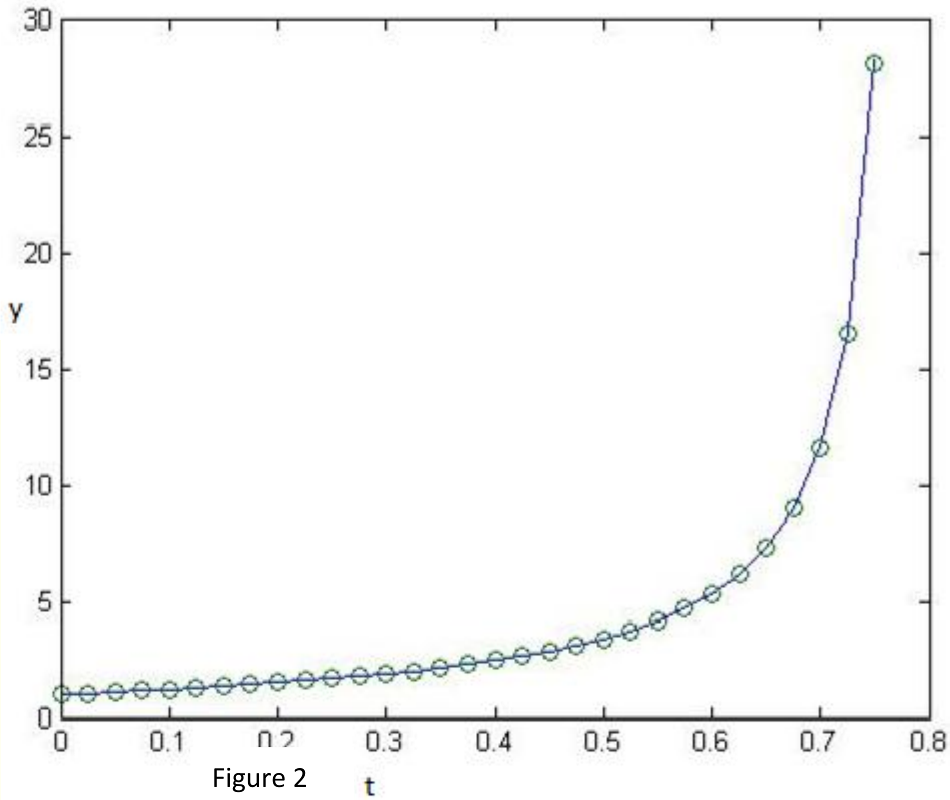

Figure 2

c. Problem 1 was also considered with initial condition as in (a), by the time interval taken as $t \in [0, \pi/2]$, with fixed step size of $h = 0.01$, the results are as given in table 3 and the plotted as per figure 3.

Table 3

t	Analytical	Ode15s	Rational (y_n)
0.1	0.1003	0.1003	0.1003
0.2	0.2027	0.2027	0.2027
0.3	0.3093	0.3093	0.3093
0.4	0.4228	0.4228	0.4228
0.5	0.5463	0.5463	0.5463
0.6	0.6841	0.6842	0.6841
0.7	0.8423	0.8423	0.8422
0.8	1.0296	1.0297	1.0296
0.9	1.2602	1.2602	1.2601
1.0	1.5574	1.5575	1.5573
1.5	14.1014	14.1058	14.0914
1.55	48.0785	48.1313	47.9593
1.56	92.858	92.858	92.616
1.57	1255.766	1301.151	1254.941
1.58	-108.6490	-	-108.8652

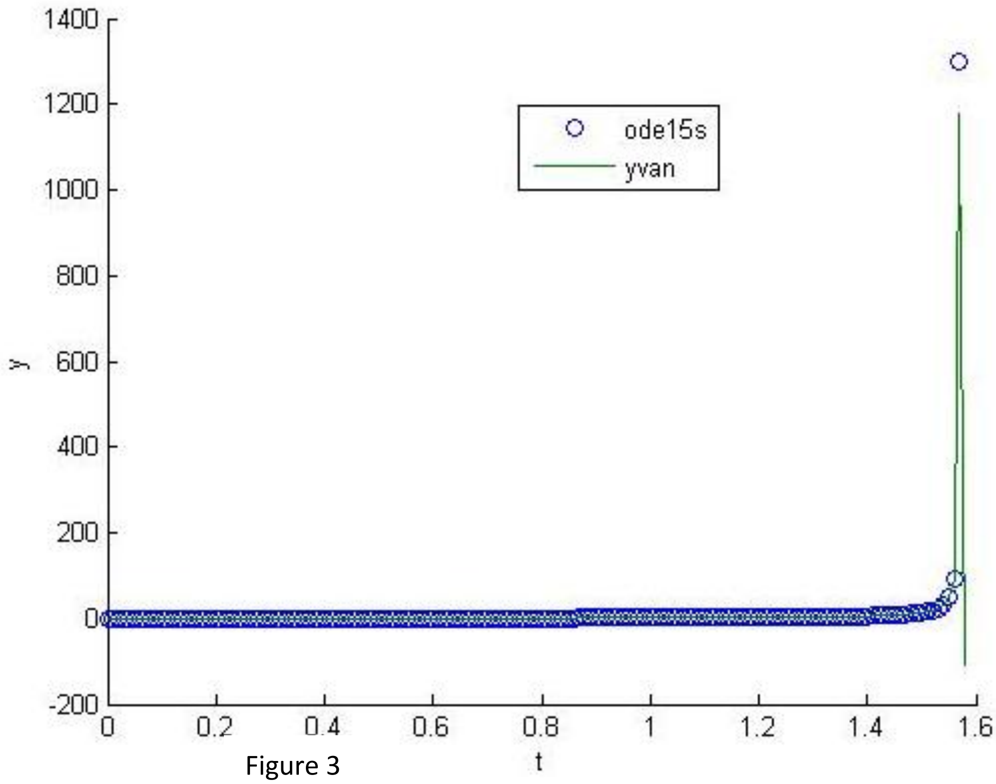
1400
1200
1000
800
600
400
200
0
-200
y
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
t
ode15s
yvan

Figure 3

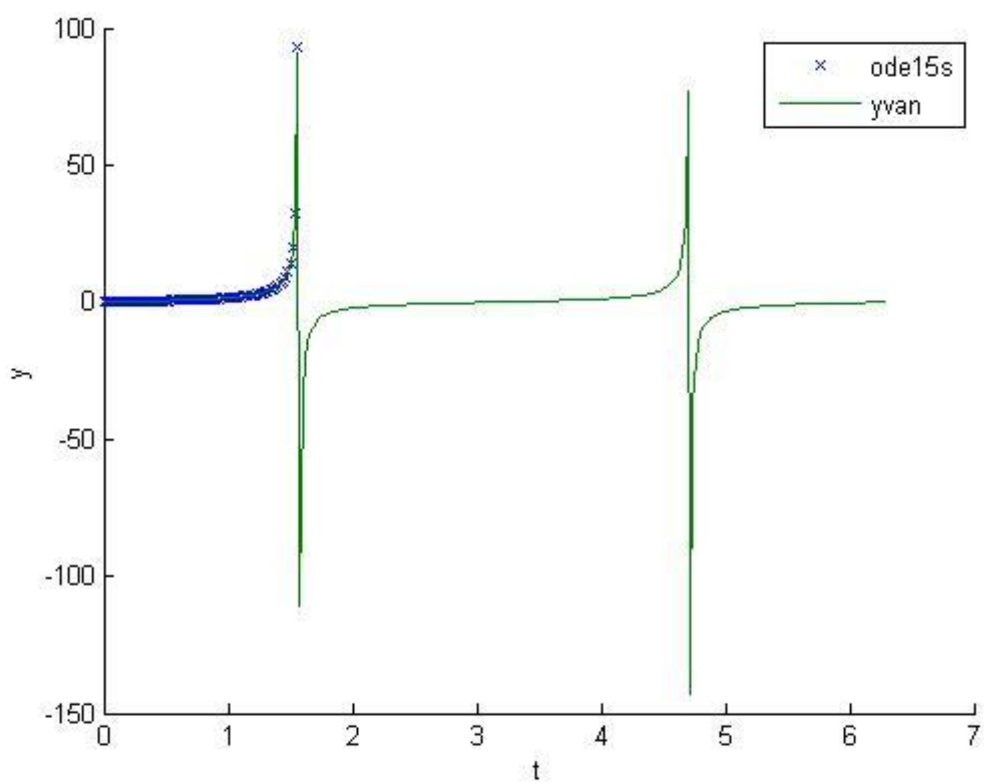
100
50
0
-50
-100
-150
y
0
1
2
3
4
5
6
7
t
ode15s
yvan

Figure 3a Shows problem 1 solved in the interval 0 to 2π for both methods, ODE15s fails at the first point of singularity.

Problem 2 (Stiff problem)

The second problem considered is a stiff differential equation given by

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

$$g(0) = 3, g(t) = \sin(0.1t) + 2 \; and \; g'(t) = \cos\,(0.1t) \times 0.1$$

Table 4, λ= -10

Table 4

t	Analytical	Ode15s	Rational (y_n)
0.1	2.37788	2.37788	2.376955
0.2	2.15533	2.15533	2.154263
0.3	2.07978	2.07978	2.078728
0.4	2.05830	2.05831	2.058202
0.5	2.05672	2.05672	2.056533
0.6	2.06244	2.06244	2.062253
0.7	2.07085	2.07086	2.070813
0.8	2.08025	2.08025	2.080262
0.9	2.0900	2.0900	2.09003
1.0	2.09988	2.09988	2.09827

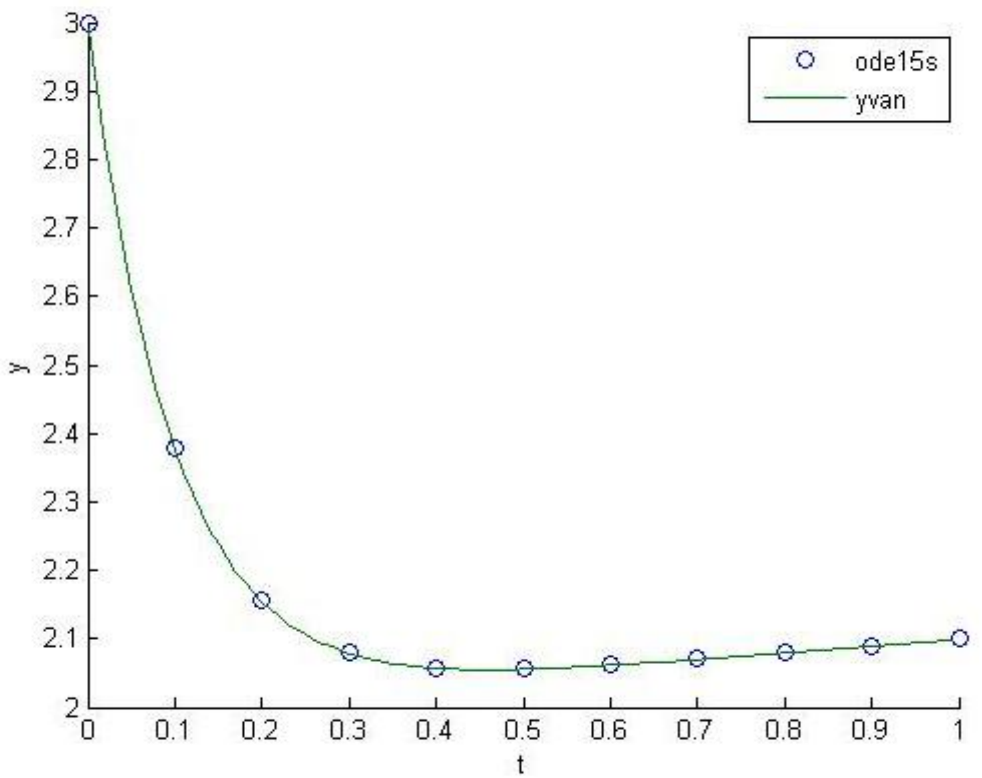

Figure 4

Table 5, λ = -1000

t	Theoretical Solution	Ode15s	Rational (y_n)
0.01	2.001045	2.001046	2.001000
0.02	2.002000	2.002000	2.002000
0.03	2.003000	2.003000	2.003000
0.04	2.004000	2.004000	2.004012
0.10	2.010000	2.010000	2.008864
0.30	2.029996	2.029995	2.029596
0.50	2.049979	2.049979	2.049580
0.70	2.069943	2.069943	2.069544
0.90	2.089879	2.089879	2.089480
1.00	2.099833	2.099833	2.099435

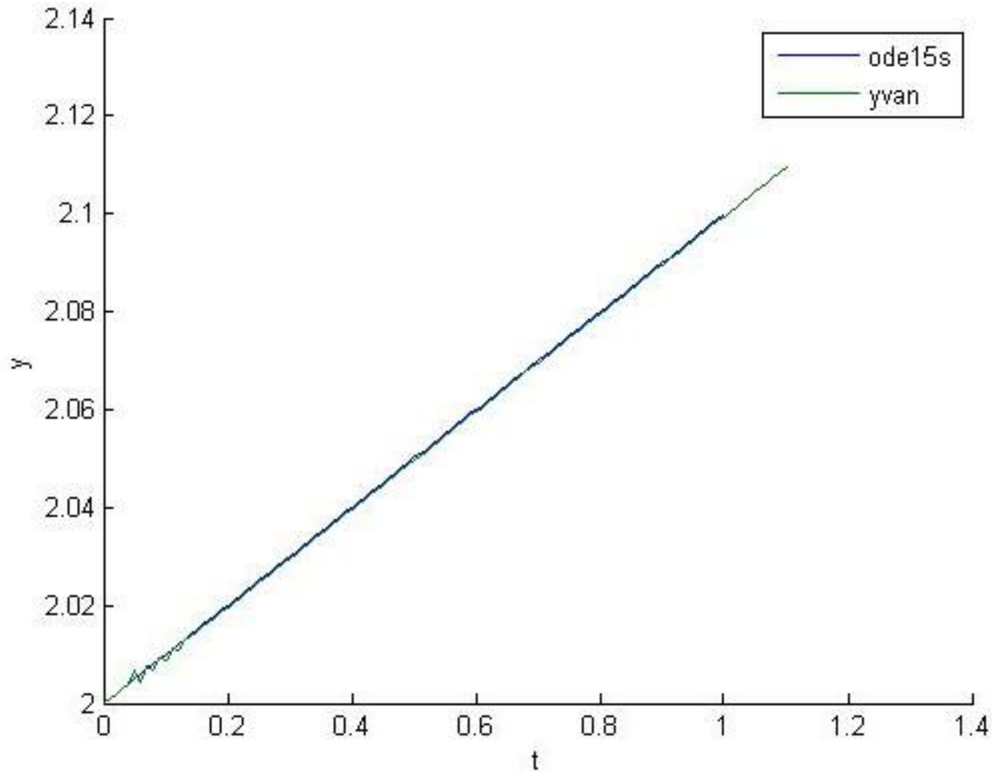

Figure 5

5 Conclusion

We have to our disposal two numerical methods for solving stiff Initial value problems in ordinary differential equations. Figure 1 and 2 which show that both the ode15s and the rational one step scheme produce identical results. The absolute errors for the two methods presented in Table 1b show the Ode15s and the rational method produce results with similar accuracy. The major disadvantage that one would pick is the use of higher derivatives for high order rational one step scheme which can prove to be tiresome and often difficult for some Initial Value problems. When both methods are integrated between the interval of $[0,\frac{\pi}{2}]$, the ode15s fails at t=1.570769, as it is unable to meet Integration tolerance without reducing the step size below the smallest value allowed which is 3.552714e-015, but its counterpart does pass through the same point and produces results which are relatively close to the analytical solution. The rational step method considered could pose to be a better advantage since it is an explicit method which does not required LU decompositions or the solution through the use of Jacobian matrix. Computing the Jacobian matrix is one of the most expensive part when using multistep methods. The CPU time in solving problem 1(a) for the rational fraction method is 0.0178 seconds compared to ODE15s of 1.0253 seconds.For stiff problem 2, the two methods give relatively the same results as per table 5 and Figure 5.

We conclude that, in this regard, the Rational Fraction Method is superior to the Linear Multistep Method based ODE15s in view of the results and observation above for the examples here considered. Further experiments on more examples can be performed to further elaborate or disprove our statement. Meanwhile we continue to explore the Rational Fraction Method. We are also investigating why ODE15s failed and how we can advance it to cope with such scenarios.

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]S.O. FANTULA, Non Linear Multistep Methods for Initial Value Problems},Compt.Math. Application.,8(3) (1982) 231-239

[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]K.O. Okosun and R.A. Ademiluyi, A Three Step Rational Methods for Integration of Differential Equations with Singularities,Research Journal of Applied Sciences 2(1):(2007) 84-88

[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,Southern Africa Journal of Pure and Applied Mathematics 4 (2009) 13-27

[11]Lawrence F. Shampine and Mark 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