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A Moderate Order Numerical Integrator for Stiff Differential Systems

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Abstract

In this paper we derived a new moderate order numerical integrator for the solution of initial value problems in ordinary differential systems that are stiff, singular or oscillatory.

We compared our integrator with certain Maximum order second derivative hybrid multi – step methods. Our results show good improvement over the Maximum order second derivative hybrid multi – step methods.

Key words: Rational Integrator, Initial Value Problems, Convergence, Consistency, Stability

1. Introduction

Solutions to Initial Value Problems in Ordinary Differential equations that are either Stiff, Singular or Oscillatory resulting from real life problems, some from physical situations, chemical kinetics, engineering work, population models, electrical networks, biological simulations, mechanical oscillations, process control have been discussed and examined by many researcher see [1], [2], [3], [6] and [9].

The pressing need have been to have efficient, stable and consistent methods that will yield accurate results. In this paper, the initial value problem (ivp),

$$\mathbf{y}^1 = \mathbf{f}(x,\mathbf{y}), \quad \mathbf{y}(x_0) = \mathbf{y}_0, \; a \le x \le b \tag{1.1}$$

is considered, where $f(x,y)$ is defined and continuous in $D \subset C[a,b]$. The ivp may be oscillatorily Singulo – Stiff.

The desire is to have a moderate order numerical rational integrator for the solution of initial value problems in ordinary differential equations and compared with the results obtain with the Maximum order second derivative hybrid multi – step methods of [4]. We found that our rational integrator is a better method for obtaining numerical results to initial value problems of the problems considered.

Our next section, namely section 2 of this paper will be on derivation of the integrator. In section 3 we will examine the Stability of the new integrator. Section 4 will be on convergence and Consistency while section 5 will be devoted to numerical examples. The remarks and conclusions will be on section 6.

2. Construction of the moderate order numerical integrator

Let the operator:

$U : R \rightarrow C^{m+2}$ (x) be defined by

$$U(x) \; \left[1 + q_1 x + q_2 x^2 + q_3 x^3\right] \equiv p_0 + p_1 x + p_2 x^2 + p_3 x^3 \tag{2.1}$$

where,

U(x) has at least 1^{st}, 2^{nd}, 3^{rd} . . . $(m + 2)^{th}$ derivatives

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$$U(x_{n+i}) = \begin{cases} y(x_{n+i}) & \text{for } i=0 \\ y_{n+i} & \text{for } i=0,1,2 \end{cases} \quad (2.2)$$

Comparing equations (2.1) and (2.2) for a case m = 3 we obtain

$$q_1 = \frac{c_6c_2^2 - c_6c_3c_1 + c_5c_4c_1 - c_4^2c_2 - c_5c_3c_2 + c_4c_3^2}{c_5c_3c_1 - c_5c_2^2 - c_4^2c_1 + 2c_4c_3c_2 - c_3^3} \quad (2.3)$$

$$q_2 = \frac{c_5c_4c_2 - c_5^2c_1 - c_6c_4c_1 - c_6c_3c_2 - c_4^2c_3 + c_3^2c_5}{c_5c_3c_1 - c_5c_2^2 - c_4^2c_1 + 2c_4c_3c_2 - c_3^3} \quad (2.4)$$

$$q_3 = \frac{c_5^2c_2 - 2c_5c_4c_3 + c_4^3 - c_6c_4c_2 + c_6c_3^2}{c_5c_3c_1 - c_5c_2^2 - c_4^2c_1 + 2c_4c_3c_2 - c_3^3} \quad (2.5)$$

where $c_r = \dfrac{h^r y_n^{(r)}}{r!\,x_{n+1}^r}$ (2.6)

Employing (2.3) – (2.6) we obtain values for our q_1x_{n+1}, $q_2x_{n+1}^2$ *and* $q_3x_{n+1}^3$ as

$$q_1x_{n+1} = \frac{h\left[6y_n^{(6)}{y_n^{(2)}}^2 - 4y_n^{(6)}y_n^{(3)}y_n^{(1)} + 6y_n^{(5)}y_n^{(4)}y_n^{(1)} - 15{y_n^{(4)}}^2y_n^{(2)} - 12y_n^{(5)}y_n^{(3)}y_n^{(2)} + 20y_n^{(4)}{y_n^{(3)}}^2\right]}{2\left[12y_n^{(5)}y_n^{(3)}y_n^{(1)} - 18y_n^{(5)}{y_n^{(2)}}^2 - 15{y_n^{(4)}}^2y_n^{(1)} + 60y_n^{(4)}y_n^{(3)}y_n^{(2)} - 40{y_n^{(3)}}^3\right]} = A \quad (2.7)$$

$$q_2x_{n+1}^2 = \frac{h^2\left[15y_n^{(5)}y_n^{(4)}y_n^{(2)} - 6{y_n^{(5)}}^2y_n^{(1)} + 5y_n^{(6)}y_n^{(4)}y_n^{(1)} - 10y_n^{(6)}y_n^{(3)}y_n^{(2)} - 25{y_n^{(4)}}^2y_n^{(3)} + 20{y_n^{(3)}}^2y_n^{(5)}\right]}{10\left[12y_n^{(5)}y_n^{(3)}y_n^{(1)} - 18y_n^{(5)}{y_n^{(2)}}^2 - 15{y_n^{(4)}}^2y_n^{(1)} + 60y_n^{(4)}y_n^{(3)}y_n^{(2)} - 40{y_n^{(3)}}^3\right]} = B \quad (2.8)$$

$$q_3x_{n+1}^3 = \frac{h^3\left[36{y_n^{(5)}}^2y_n^{(2)} - 120y_n^{(5)}y_n^{(4)}y_n^{(3)} + 75{y_n^{(4)}}^3 - 30y_n^{(6)}y_n^{(4)}y_n^{(2)} + 40y_n^{(6)}{y_n^{(3)}}^2\right]}{120\left[12y_n^{(5)}y_n^{(3)}y_n^{(1)} - 18y_n^{(5)}{y_n^{(2)}}^2 - 15{y_n^{(4)}}^2y_n^{(1)} + 60y_n^{(4)}y_n^{(3)}y_n^{(2)} - 40{y_n^{(3)}}^3\right]} = C \quad (2.9)$$

Our integrator from equation (2.1) is then given as

$$y_{n+1} = \frac{p_0 + p_1x_{n+1} + p_2x_{n+1}^2 + p_3x_{n+1}^3}{1 + q_1x_{n+1} + q_2x_{n+1}^2 + q_3x_{n+1}^3} \quad (2.10)$$

where $p_0 = y_n$ (2.11)

$$p_1 = c_0q_1 + c_1 \quad (2.12)$$

which becomes

$$p_1 = y_nq_1 + \frac{hy_n^{(1)}}{x_{n+1}} \quad (2.13)$$

$$p_1x_{n+1} = y_nq_1x_{n+1} + hy_n^{(1)} \quad (2.14)$$

Similarly,

$$p_2 = c_0q_2 + c_1q_1 + c_2 = y_nq_2 + \frac{hy_n^{(1)}q_1}{x_{n+1}} + \frac{h^2y_n^{(2)}}{x_{n+1}^2}$$

leading us to

$$p_2x_{n+1}^2 = y_nq_2x_{n+1}^2 + hy_n^{(1)}q_1x_{n+1} + \frac{h^2y_n^{(2)}}{2!} \quad (2.15)$$

and

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$$p_3 = c_0 q_3 + c_1 q_2 + c_2 q_1 + c_3 = y_n q_3 + \frac{h y_n^{(1)} q_2}{x_{n+1}} + \frac{h^2 y_n^{(2)} q_1}{x_{n+1}^2} + \frac{h^3 y_n^{(3)}}{3!}$$

which implies that

$$p_3 x_{n+1}^3 = y_n q_3 x_{n+1}^3 + h y_n^{(1)} q_2 x_{n+1}^2 + \frac{h^2 y_n^{(2)} q_1 x_{n+1}}{2!} + \frac{h^3 y_n^{(3)}}{3!} \tag{2.16}$$

Substituting (2.7) – (2.9), (2.11) and (2.14) – (2.16) into equation (2.10) our integrator becomes

$$y_{n+1} = \frac{\sum_{r=0}^{3} \frac{h^r y_n^{(r)}}{r!} + A \sum_{r=0}^{2} \frac{h^r y_n^{(r)}}{r!} + B \sum_{r=0}^{1} \frac{h^r y_n^{(r)}}{r!} + C y_n}{1 + A + B + C} \tag{2.17}$$

where A, B, C are specified by (2.7), (2.8) and (2.9) respectively.

3. Stability Considerations

To effectively solve ivp in ordinary differential equations which are stiff problems we need numerical integrators that possess special stability properties such as A – Stability.

Definition [Dahlquist (1963)] :

A numerical method is said to be A – Stable if its Region of Absolute Stability contains the whole of the left – hand half of the complex plane ie $\mathrm{Re}(h) < 0$.

We employ the usual linear test equation

$$y^1 = \lambda y \tag{3.1}$$

which gives $y^{(r)} = \lambda^r y$ by induction.

Employing it on equations (2.7) – (2.9), (2.11) and (2.14) – (2.16), we have

$$A(\bar{h}) = \quad q_1 x_{n+1} = -\frac{\bar{h}}{2} \tag{3.2}$$

$$B(\bar{h}) = \quad q_2 x_{n+1}^2 = \frac{\bar{h}^2}{10} \tag{3.3}$$

$$C(\bar{h}) = \quad q_3 x_{n+1}^3 = -\frac{\bar{h}^3}{120} \tag{3.4}$$

$$p_1 x_{n+1}(\bar{h}) = \frac{\bar{h} y_n}{2} \tag{3.5}$$

$$p_2 x_{n+1}^2 \ (\bar{h}) = \frac{\bar{h}^2 y_n}{10} \tag{3.6}$$

$$p_3 x_{n+1}^3 \ (\bar{h}) = \frac{\bar{h}^3 y_n}{120} \tag{3.7}$$

Substituting (2.11), (3.2) – (3.7) into (2.10) we obtain our Stability function as

$$\zeta(\bar{h}) = \frac{120 + 60\bar{h} + 12\bar{h}^2 + \bar{h}^3}{120 - 60\bar{h} + 12\bar{h}^2 - \bar{h}^3} \tag{3.8}$$

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By setting $\overline{h} = u + iv,\ i^2 = -1$, we get

$$\left| \zeta\left(\overline{h}\right) \right| \leq 1 \Leftrightarrow \tag{3.9}$$

$$\left| 120 + 60(u+iv) + 12(u+iv)^2 + (u+iv)^3 \right| \leq \left| 120 - 60(u+iv) + 12(u+iv)^2 - (u+iv)^3 \right| \tag{3.10}$$

Now then

$$120 + 60(u+iv) + 12(u+iv)^2 + (u+iv)^3 = A(u,v) + i\,B(u,v)$$

$$where$$

$$A(u,v) = 120 + 60u + 12u^2 - 12v^2 + u^3 - 3uv^2$$

$$B(u.v) = 60v + 24uv + 3u^2v - v^3$$

$$and$$

$$120 - 60(u+iv) + 12(u+iv)^2 - (u+iv)^3 = C(u,v) + i\,D(u,v)$$

$$where$$

$$C(u,v) = 120 - 60u + 12u^2 - 12v^2 - u^3 + 3uv^2$$

$$D(u,v) = -60v + 24uv - 3u^2v + v^3$$

Hence our inequality above becomes,

$$\left| \zeta\left(\overline{h}\right) \right| \leq 1 \Leftrightarrow \left| A(u,v) + i\,B(u,v) \right| \leq \left| C(u,v) + i\ D(u,v) \right|$$

$$ie \ \Leftrightarrow A(u,v)^2 + B(u,v)^2 \leq C(u,v)^2 + D(u,v)^2$$

which holds after expansion $\Leftrightarrow$

$$\begin{aligned} &14400 + 14400u + 6480u^2 + 720v^2 + 1680u^3 + 720uv^2 + 264u^4 + 288u^2v^2 + 24u^5 + 48u^3v^2 + 24v^4 \\ &+ 24uv^4 + u^6 + 3u^4v^2 + 3u^2v^4 + v^6 \leq 14400 - 14400u + 6480u^2 + 720v^2 - 1680u^3 - 720uv^2 + 264u^4 \\ &+ 288u^2v^2 - 24u^5 - 48u^3v^2 + 24v^4 + 24uv^4 + u^6 + 3u^4v^2 + 3u^2v^4 + v^6 \end{aligned}$$

which in turn holds $\Leftrightarrow$

$$28800u + 3360u^3 + 1440uv^2 + 48u^5 + 96u^3v^2 + 48uv^4 \leq 0 \tag{3.11}$$

$$\Leftrightarrow$$

$$48u\left(600 + 70u^2 + 30v^2 + u^4 + 2u^2v^2 + v^4\right) \leq 0 \tag{3.12}$$

Observe that :

$$600 > 0,\ 70u^2 > 0\ \forall\ u \neq 0,\ 30v^2 > 0\ \forall v \neq 0,\ \ u^4 > 0\ \forall\ u \neq 0,\ \ 2u^2v^2 > 0\ \forall\ u \neq 0, v \neq 0,$$

$$v^4 > 0\ \forall\ v \neq 0,$$

$$\therefore\ \ 600 + 70u^2 + 30v^2 + u^4 + 2u^2v^2 + v^4 > 0\ \forall\ u,v \tag{3.13}$$

Consequently, the inequality

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$$48u\left(600+70u^2+30v^2+u^4+2u^2v^2+v^4\right)<0 \Leftrightarrow u<0$$

and

$$48u\left(600+70u^2+30v^2+u^4+2u^2v^2+v^4\right)=0 \Leftrightarrow u=0$$

$$ie\ \mathrm{Re}\{u+iv\}<0\ \ \forall\ u<0$$

Hence the integrator is A – stable and so the Region of Absolute Stability of the integrator is the entire left – half of the complex plane.

4. Convergence and Consistency

One-step methods are normally described symbolically by

$$y_{n+1}=y_n+h\Phi(x_n,y_n;h) \qquad (3.1)$$

where

$\Phi(x_n,y_n;h)$ is called the increment function, x_n the mesh point and h the mesh size. Fatunla (1988) states that a rational integrator is said to be consistent if the increment function is consistent with the initial value problem, that is if

$$\Phi(x,y,0)=f(x,y)$$

Lambert (1973) described Convergence as a minimal property to expect of a numerical method, as there is no practical use to which we can put methods which are not convergent even though there are some convergent methods that are not suitable for practical computation. As reported in Hall and Watt (1976) by Lambert (1976) a one – step numerical integrator is said to be convergent if and only if the one step method is consistent. Hence we state and prove the convergence and consistency of our moderate order rational integrator.

THEOREM

The moderate order rational integrator (2.17) is consistent and convergent.

Proof

By 2.17,

$$y_{n+1}-y_n=\frac{\sum_{r=1}^{3}\frac{h^r y_n^{(r)}}{r!}+A\left(hy_n^{(1)}+\frac{h^2y_n^{(2)}}{2!}\right)+Bhy_n^{(1)}}{1+A+B+C}$$

which gives

$$\frac{y_{n+1}-y_n}{h}=\frac{y_n^{(1)}(1+A+B)+\frac{hy_n^{(2)}}{2!}+\frac{h^2y_n^{(3)}}{3!}+\frac{Ahy_n^{(2)}}{2!}}{1+A+B+C}$$

Note that by (2.7), (2.8), (2.9)

$$\underset{h\to 0}{Limit}\quad A=0$$

$$\underset{h\to 0}{Limit}\quad B=0$$

$$\underset{h\to 0}{Limit}\quad C=0$$

Hence $\underset{h\to 0}{Limit}\left(\frac{y_{n+1}-y_n}{h}\right)=\frac{y_n^{(1)}(1+0+0)+0+0+0}{1+0+0+0}$

$$=y_n^{(1)}$$

$$\therefore \underset{h\to 0}{Limit}\left(\frac{y_{n+1}-y_n}{h}\right)=y_n^{(1)}=f(x_n,y_n) \text{ as required.}$$

Therefore the one step integrator is consistent. Hence, our integrator is convergent [10].

5. Numerical Examples

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We illustrate the performance of our new integrator over the Maximum order second derivative hybrid multi – step methods of [4] in the following examples.

Example 1: [4]

$$y^{(1)} = -100\,y, \quad y(x_0) = 1, \quad x \in [0,1]$$

The exact solution to is

$y(x) = \ell^{-100x}$ and the time constant is 0.01.

A variable step size was used starting with h = 0.10

Example 2: Ademiluyi and Kayode (2001)

$${}^{1}y^{1} = -2000\ {}^{1}y + 999.75\ {}^{2}y + 1000.25$$

$${}^{2}y^{1} = {}^{1}y - {}^{2}y$$

with initial condition.

$$\begin{matrix} {}^{1}y(0) = 0 \\ {}^{2}y(0) = -2 \end{matrix} \qquad x \in [0,10];\ h = 0.50$$

The exact solutions are

$${}^{1}y = -1.499875\ \exp(-0.5x) + 0.499875\ \exp(-2000.5x) + 1$$

$${}^{2}y = -2.99975\ \exp(-0.5x) - 0.00025\ \exp(-2000.5x) + 1$$

Table 1a: Numerical Integration Solutions to Example 1

h	Value of x	Analytic solution	Ademiluyi, and Kayode (2001)	Moderately Order Rational [integrator
1.00000D-01	1.00000D-01	4.53999D-05	-0.188083D1	-1.68748D+02
5.00000D-02	1.50000D-01	3.05902D-07	-0.657766D0	-5.09314D-04
2.50000D-02	1.75000D-01	2.51100D-08	-0.122095D0	-1.01713D-07
1.25000D-02	1.87500D-01	7.19412D-09	0.261286D00	6.97190D-09
6.25000D-03	1.93750D-01	3.85074D-09	0.535235D00	3.84976D-09
3.12500D-03	1.96875D-01	2.81726D-09	0.731615D00	2.81725D-09
1.56250D-03	1.98438D-01	2.40973D-09	0.855345D00	2.40973D-09
7.81250D-04	1.99219D-01	2.22864D-09	0.92449D00	2.22864D-09
3.90625D-04	1.99609D-01	2.14326D-09	0.961691D00	2.14326D-09
1.95313D-04	1.99805D-01	2.10180D-09	0.980658D00	2.10180D-09
9.76563D-05	1.99902D-01	2.08138D-09	**Not Stated**	2.08138D-09
4.88281D-05	1.99951D-01	2.07124D-09	0.995129D00	2.07124D-09

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Table 1b: Errors in Numerical Integration of Example 1

H	Value of x	Analytic solution	Ademiluyi, and Kayode (2001)	Moderately Order Rational [integrator
1.00000D-01	1.00000D-01	4.53999D-05	2.14454D-02	1.68748D+02
5.00000D-02	1.50000D-01	3.05902D-07	2.00536D-02	5.09620D-04
2.50000D-02	1.75000D-01	2.51100D-08	1.97436D-02	1.26823D-07
1.25000D-02	1.87500D-01	7.19412D-09	1.68208D-02	2.22223D-10
6.25000D-03	1.93750D-01	3.85074D-09	1.24074D-02	9.79550D-13
3.12500D-03	1.96875D-01	2.81726D-09	7.84083D-03	7.59669D-15
1.56250D-03	1.98438D-01	2.40973D-09	4.43528D-03	-1.52056D-15
7.81250D-04	1.99219D-01	2.22864D-09	2.36270D-03	-8.87885D-16
3.90625D-04	1.99609D-01	2.14326D-09	1.21590D-03	1.33227D-15
1.95313D-04	1.99805D-01	2.10180D-09	6.19892D-04	6.66134D-16
9.76563D-05	1.99902D-01	2.08138D-09	**Not Stated**	-1.33227D-15
4.88281D-05	1.99951D-01	2.07124D-09	1.55871D-04	-6.66134D-16

Table 2a: Numerical Integration Solutions to Example 2 [First component]

Value of x	Analytic solution	Numerical result of Ademiluyi, and Kayode (2001)	Numerical result of Moderately Order Rational [integrator	Error in Ademiluyi, and Kayode (2001)	Error in Moderately Order Rational [integrator
0.5	-1.6810382451D-	-0.638918D-7	4.179101D+08	0.62546D-10	-4.1791014417D+08
1.0	9.0279826764D-02	-0.168268D00	-2.309493D+02	-0.164725D-4	2.3103955961D+02
1.5	2.9150921671D-01	0.903685D-1	1.709019D+02	0.884654D-5	-1.7061034625D+02
2.0	4.4822682317D-01	0.291795D0	4.482273D-01	0.285650D-4	-4.9296814553D-07
2.5	5.7027861781D-01	0.44856D0	-1.885015D+02	0.439218D-4	1.8907180450D+02
3.0	6.6533265105D-01	0.570838D0	-1.883998D+03	0.558816D-4	1.8846633795D+03
3.5	7.3936080657D-01	0.665985D0	-8.617518D+02	0.951960D-4	8.6249113083D+02
4.0	7.9701399206D-01	0.640085D0	7.970142D-01	0.724500D-4	-2.4439470969D-07
4.5	8.4191433806D-01	0.797795D0	8.419145D-01	0.780994D-4	-1.9650851280D-07

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Table 2b: Errors in Numerical Integration in Example 2 [Second component]

Value of x	Analytic solution	Numerical result of Ademiluyi, and Kayode (2001)	Numerical result of Moderately Order Rational [integrator	Error in Ademiluyi, and Kayode (2001)	Error in Moderately Order Rational [integrator
0.5	-1.3362076490D+00	-0.20096D1	-2.079698D+05	-0.195980D-3	2.0796841379D+05
1.0	-8.1944034647D-01	-0.133752D1	-6.707376D-01	-0.130935D-3	-1.4870278191D-01
1.5	-4.1698156658D-01	-0.320243D0	-4.854549D-01	-0.802970D-4	6.8473320567D-02
2.0	-1.0354635365D-01	-0.417390D0	-1.035454D-01	-0.406600D-4	-9.0397990449D-07
2.5	1.4055723562D-01	-0.103645D0	2.866786D-01	-0.101465D-4	-1.4612137661D-01
3.0	3.3066530209D-01	0.140695D0	4.456838D-02	0.137732D-4	2.8609691989D-01
3.5	4.7872161313D-01	0.330990D0	1.922764D-01	0.32401D-4	2.8644518002D-01
4.0	5.9402798411D-01	0.479191D0	5.940284D-01	0.46910D-4	-3.695801299D-07
4.5	6.8382867612D-01	0.594610D0	6.838289D-01	0.58208D-4	-2.1420309138D-07

6. Remarks and Conclusion

We have derived a moderate order rational integrator for solving stiff, singular and oscillatory initial value problems in ordinary differential equations that is consistent and stable. Examining closely the tables 1a, 1b, 2a, and 2b we observe that
the new integrator gives a better approximation when compared with the Maximum order second derivative hybrid multi –
step methods of [4], since the resulting solutions of the new integrator are closer to the analytic solutions.

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step methods of [4], since the resulting solutions of the new integrator are closer to the analytic solutions.

The use of numerical integrators in solving first order initial value problem have been demonstrated using the moderate order rational integrators and have proved more attractive. Tables 1b shows that our moderate order rational integrator converges quickly to the analytic solution at each mesh point than the Maximum order second derivative hybrid multi – step methods. Tables 2a and 2b shows encouraging results as convergence rate is quick at some mesh point. The oscillatory nature of its convergence is allowed for further research. This makes the moderate order rational numerical integrator more efficient than the Maximum order second derivative hybrid multi – step methods.

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