Scheme for solving ordinary differential equations with derivative discontinuities: A new class of semi-implicit rational, Runge-Kutta

Bolarinwa Bolaji¹*, Ademiluyi R. A.¹, Oluwagunwa A. P.¹ and Awomuse B. O.²

¹Department of Mathematics and Statistics, Rufus Giwa Polytechnic, Owo, Nigeria.
²Department of Mathematical Sciences, Federal University of Technology, Akure, Nigeria.

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In this paper, a class of semi-implicit Rational Runge–Kutta scheme is proposed for the integration of differential equations with derivative discontinuities. The method is motivated by varieties of application areas of this class of ordinary differential equations such as electrical transmission network, nuclear reactions, delay problems computer aided designs, economy affected by inflation as well as perturbation problems and dynamic processes in industries and technology fields, and the need to cater for the deficiencies identified in the adoption of the existing methods of solving this class of differential equations. For the development of the scheme, we adopted power series (Taylor and Binomial) expansion, while its analysis and implementation on a micro computer adopts Pade approximation technique and FORTRAN programming respectively. The convergence and stability properties were investigated; it was discovered that the scheme converge and were stable. Numerical result of the adoption of the scheme on some sample problems shows that it is effective and efficient. It compares favourably with modified Euler’s scheme.

Key words: Rational Runge-Kutta, derivative discontinuities, semi-implicit, differential equations.

INTRODUCTION

The mathematical models of a large variety of science, engineering and technological problems leads to initial value problems of the form:

\[ y' = f(x, y) \quad y(x_0) = y_0 \quad a < x < b \quad (1.1) \]

in which \( f \) has some points that is not smooth, or of discontinuities. The derivative in the ordinary differential equation contains some finite jumps otherwise referred to as discontinuities in the region of \( x - y \) plane defined by: \( D = \{(x, y) \text{such that } a = x = b, -\infty < y < \infty \} \) at initial point \((x_0, y_0)\). When \( f(x,y) \) is infinite or unbounded and the partial derivatives \( f_x, f_y \) are large and unbounded, then we say that \( f(x,y) \) has low order derivative discontinuities. The state of economy of some third world countries infected by inflation and large foreign debts will lead to equations of this form, when modeled.

At this points where there is derivative discontinuities in the differential equation of the form (1.1), a numerical method adopted for their solution may become either inaccurate, inefficient or both in this region of discontinuities identified. This is due to the fact that these class of differential equations does not satisfy the existence and uniqueness theorem, that is \( f(x, y) \) and its partial derivatives \( f_x, f_y \) are non-continuous and unbounded in the region of integration; consequently, conventional algorithm that are based on polynomial representation which pre – assumes that the solution to an ordinary differential equation and its derivatives are sufficiently continuous throughout the region of integration will be deficient in solving initial value problem that violates the uniqueness theorem, because they give rise to a solution whose derivatives explodes in the
neighbourhood of this discontinuities (Carver, 1978). The existing methods of solving this class of ODEs evolved from researchers who were motivated to work in this area, after having discovered that the accuracy and efficiency of the methods varies with the location of points of discontinuities, which is state dependent (Paul, 1999). Such methods include: fraction step method proposed by Fatunla and Evans (1975), the switching function technique proposed by Fatunla and Evans (1974), use of discontinuity tracking equation proposed by Paul (1999), use of defect error control method proposed by Paul (1999). The computational algorithm resulting from some of the aforementioned methods are only valid in the neighbourhood of derivative discontinuities or transient region as long as the mesh points are carefully chosen so as to sandwich the points of discontinuities. There are some other deficiencies of these methods. In this work, we propose a class of semi-implicit one-step scheme which is absolutely stable and capable of handling, effectively, the differential equations of this type (that is, differential equations with derivatives discontinuities).

DERIVATION OF THE SCHEME

By setting R = 1 in equation (1.2), the general one stage semi-implicit scheme, is of the form:

\[ y_{n+1} = \frac{y_n + \sum_{i=1}^{k} w_i k_i}{1 + y_n \sum_{i=1}^{k} v_i k_i} \] (2.1)

Where \( k_i = hf\left(x_n + c_i h, y_n + \sum_{j=1}^{k} a_{ij} k_j\right) \) \( i = 1(1)r \) \( (2.2) \)

\[ H_i = hg\left(x_n + d_i h, Z_n + b_{1i} h_i\right) \] \( i = 1(1)s \) (2.3)

\[ g(x_n, y_n) = -z_n^2 f(x_n, y_n) \] (2.4)

And \( Z_n = \frac{1}{y_n} \) (2.5)

With the constraints

\[ c_i = \sum_{j=1}^{k} a_{ij} \] \( i = 1(1) \) (2.6)

To determine the unknown parameter \( a_{11}, b_{11}, c_1 \) and \( d_1 \) we shall adopt the following steps:

1. Obtain the binomial series expansion of the r.h.s of (2.1) ignoring terms of order higher than one and obtain:

\[ y_{n+1} = y_n + w_i k_i - y_n v_i H_i \] (2.7)

2. Obtain the Taylor series expansion of \( y_{n+1}, H_i \) and \( k_i \) so as to obtain the following results:
\[ y_{n+1} = y_n + hf_n + \frac{h^2}{2} Df_n + \frac{h^3}{6} \left( D^2f_n + f_n Df_n \right) + \frac{h^4}{24} \left( D^3f_n + f_n D^2f_n + 3DFf_n + f_n Df_n \right) + O(h^5) \]  

(2.8)

\[ H_1 = hN_1 + h^2 M_1 + h^3 R_1 + O(h^4) \]  

(2.9)

\[ K_1 = hA_1 + h^2 B_1 + h^3 D_1 + O(h^4) \]  

(2.10)

Where:

\[ Df_n = f_x + f_n f_y \]

\[ A_1 = f_n \]

\[ B_1 = c_1 \left( f_n + f_n f_y \right) = c_1 Df_n \]

\[ D_1 = c_1^2 \left( Df_n f_y + \frac{1}{2} D^2 f_n \right) \]

\[ N_1 = \frac{f_y}{y_n^2} \]

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\[ M_1 = -\frac{d^2}{y_n^2} \left( Df_n + 2 f_n^2 \right) / y_n \]

\[ R_1 = \frac{d^3}{y_n^2} \left( c - Df_n f_y / y_n \right) / y_n \]

\[ \frac{h^3}{2} D^2 f_n - 2 f_n^2 / y_n \left( f_n^2 + f_n \right) \]

By inserting (2.9) and (2.10) into (2.8) we have:

\[ y_{n+1} = y_n + \left( W_1 A_1 - y_n^2 V_1 N_1 \right) h + h^2 + \left( W_1 A_1 - y_n^2 V_1 R_1 \right) h^3 + O(h^4) \]  

(2.11)

By comparing the coefficients of equal powers of \( h \) in equations (2.8) and (2.11), we obtain:

\[ W_1 A_1 - y_n^2 V_1 N_1 = f_n \]  

(2.12)

\[ W_1 B_1 - y_n^2 V_1 M_1 = Df_n / 2 \]  

(2.13)

By using the expression for \( N, M \) and \( B \) in equation (2.12) and (2.13) we obtain the set of linear equations:

\[ W_1 + V_1 = 1 \]

\[ W_1 C_1 + V_1 D_1 = 1 / 2 \]  

(2.14)

With \( a_{11} = c_1 \) and \( b_{11} = d_1 \)

This set of linear equations is solved by imposing condition:

\[ V_1 = W_1 = \frac{1}{2} \]

Then, \( c_1 = a_{11} = \frac{3}{4} \) and \( d_1 = b_{11} = \frac{1}{4} \)

By adopting these values in (2.1) we obtain one stage formula of order 2:

\[ y_{n+1} = y_n + \frac{1}{2} K_1 + \frac{1}{1+4/5 \ h^2} \]

(2.15)

where \( K_1 = hf_n + \frac{3}{4} h, y_n + \frac{3}{4} k_1 \)

\[ H_1 = hg \left( x_n + \frac{1}{4} h, Z_n + \frac{1}{4} H_1 \right) \]

By imposing condition \( W_1 = \frac{1}{5} \) on equation (2.14) and then set:

\[ V_1 = \frac{4}{5}, \text{which implies that } c_1 = d_1 = \frac{1}{2} \text{ and } a_{11} = b_{11} = \frac{1}{2} \]

When these values of the parameters from the set of linear equations (2.14) are adopted in equation (2.1), we obtain one stage formula:

\[ y_{n+1} = \frac{y_n + \frac{1}{2} K_1}{1 + \frac{4}{5} \ h} \]

where \( K_1 = hf_n + \frac{1}{2} h, y_n + \frac{1}{2} k_1 \)

\[ H_1 = h g \left( x_n + \frac{1}{2} h, Z_n + \frac{1}{2} H_1 \right) \]  

(2.16)

These proposed formulae (2.15) and (2.16) are based on a current value \( y_n \) of \( y_{n+1} \), its derivative \( f_n \) and the step size \( h \). These values are used to compute the next approximation \( y_{n+1} \) to \( y \) at the point \( x = x_{n+1} \) . The truncation error \( T_{n+1} \) associated with these families of one stage method is of the form:

\[ T_{n+1} = y(x_{n+1}) - y_n + w_1 k_1 + 0(h^{p+1}) \]

This truncation error is the amount by which the exact solution \( y(x_{n+1}) \) fails to satisfy the numerical formula (2.1)

**PROPERTIES OF THE NEW SCHEME**

In the process of the development of the computational
scheme, errors occur, it is therefore important to analyze these errors, convergence and stability properties of the new schemes so that we can examine and know if the method is capable, adequate and efficient towards solving differential equation of our interest, that is, ordinary differential equations with derivative discontinuities. All these are investigated in this section.

**Error analysis**

Numerical approximation involves iteration process, due to this, there will be propagation of errors from step to step when iterating with the scheme. These propagated errors can grow to the extent of distorting the accuracy of the numerical results. The main feature of an adequate method is adopted in this work because its procedure is such error so that the quality of the integration could be guaranteed. Of the two methods of error estimation techniques namely: Richardson extrapolation method and Felhberg error estimation techniques that are relevant to one step schemes, Richardson extrapolation method is adopted in this work because its procedure is less cumbersome, less time and energy consuming relatively, when compared with Felhberg error estimation techniques. By Richardson extrapolation techniques, if we designate the solution by one method, using single step size $h$ by $y(x_{n+1})$, then local error can be estimated from:

$$e_{n+1} = y(x_{n+1}) - y_{n+1} = \Psi(x_n, y(x_n))h^{p+1} + 0(h^{p+2}) \quad (3.1)$$

Similarly, by adopting single step size $h/2$, the local error of the method is given by:

$$y(x_{n+1}) - l_{n+1} = \Psi(x_n, y(x_n))h/2h^{p+1} + 0(h^{p+2}) \quad (3.2)$$

Where $l_{n+1}$ is the computed solution by the method using step size $h/2$, by subtracting (3.1) from (3.2) and simplifying, we have:

$$\Psi(x_n, y(x_n))h^{p+1} = (y_{n+1} - l_{n+1}) \left(1 - \frac{1}{2^{p+1}}\right) \quad (3.3)$$

The accuracy of the scheme is estimated from:

$$D = \left| (y_{n+1} - l_{n+1}) \left(1 - \frac{1}{2^{p+1}}\right) \right| \quad (3.4)$$

Thus $D = |\Psi(x_n, y(x_n))h| h^{p+1} \quad (3.5)$

Therefore the, discretization error of the scheme is estimated from:

$$e_{n+1} = [y_{n+1} - l_{n+1}] \left[ \frac{2^p}{1 - 2^p} \right] \quad (3.6)$$

Thus, the approximation from the scheme is accepted as a good approximation to the exact solution if:

$$|e_{n+1}| < \text{Tolerance}$$

That is, the global error is less than error tolerance; which implies that the scheme is accurate. The truncation error is the error introduced into the scheme as a result of ignoring higher terms of the power series expansion (by either Taylor or Binomial algorithm). Mathematically, this is defined as the amount by which the actual solution of differential equation (1.1) fails to satisfy the difference equation (2.1), that is:

$$y_{n+1} = (y_{n+1}) - \frac{y(x_n) + w_{1} K_1}{1 + y(x_n) v_1 H_1}$$

where $K_1 = hf(x_n + c_1 h, y_n + a_{11} k_1)$

$$H_1 = hg(x_n + d_1 h, Z_n + b_{11} h_1)$$

$$g(x_n, y_n) = -z_n f(x_n, y_n).$$

By adopting Taylor’s series expansion for $y(x_{n+1})$, $H_1$ and $K_1$ about $(x_n, y(x_n))$ in equation (3.7) term by term and simplifying, the truncation error associated with our one stage method of order 2 is found to be:

$$T_{n+1} = C_0 y_n + C_1 h + C_2 h^2 + C_3 h^3 + 0(h^4) \quad (3.8)$$

Where

$$C_0 = 0, \quad C_1 = f_n - w_{1} f_n - y(x_n)^3 V_1 g_n$$

$$C_2 = \frac{Df}{2} - w_{1} c_1 Df + y(x_n)^3 V_1 d_1 Dg_n$$

$$C_3 = \frac{D^2 f}{2} - w_{1} c_1 Df + y(x_n)^3 V_1 d_1 Dg_n$$

By imposing accuracy of order 2 on $T_{n+1}$, we have $C_0 = 0$, $C_1 = 0$, and $C_2 \neq 0$; so as to have:

$$T_{n+1} = \left(\frac{D^2 f}{2} - w_{1} c_1 Df + y(x_n)^3 V_1 d_1 Dg_n\right) h.$$
The bound of the principal local truncation error $T_{n+1}$ can be found by adopting Lotkin (1951) definition:

$$\left| \frac{d^{i+j} f(x, y)}{dx^i dy^j} \right| < \frac{N^{i+j}}{M^{j-i}}$$

$x \in [a, b]$ \hspace{1cm} $y \in (-\infty, \infty)$

For bound of $f$ and its partial derivatives. Thus, the bound of $T_{n+1}$ is given by

$$|T_{n+1}| < \left[ N_1 |P_1| + M |P_2| \right] h^j$$

Where

$$P_1 = \frac{1}{c_1} - \frac{1}{2} w_1 c_1 - \frac{1}{2} y_1 V_1 d_1^2$$
$$P_2 = \frac{1}{c_1} - \frac{1}{2} w_1 c_1 - y_1^2 V_1 d_1^2$$

This shows that the bound of the truncation error of one stage method exists. This implies that the error cannot grow as the scheme is used for the integration of ordinary differential equations, thus, showing that the method has some degree of accuracy.

**Stability properties of the scheme**

Stability analysis of the scheme is important since it form the basis by which the suitability of the scheme is assessed. Here, Dalquist (1956) and Dalquist (1959) stability scalar test initial value problem:

$$y' = \lambda y, \quad y(x_0) = y_0.$$  \hspace{1cm} (3.9)

This becomes a readily important tool. Consequently, we apply scheme (2.1) to the scalar initial value problem (3.9), under the assumption that Re ($\lambda$) << 0; $\lambda$ being a complex constant with negative real part. We then obtain the recurrent relation:

$$y_{n+1} = \left( 1 + w_i \alpha (1 - a_{1i} \alpha) \right)^{-1} y_n.$$  \hspace{1cm} (3.10)

For the approximation to the solution and for its convergence, we consider the function:

$$u(\alpha) = \frac{1 + w_i \alpha (1 - a_{1i} \alpha)}{1 - v_i \alpha (1 + b_{1i} \alpha)}.$$  \hspace{1cm} (3.11)

This can be shown to satisfy Pade's approximation to $e^\alpha$ and can be expressed in the form:

$$u(\alpha) = \sum_{i=1}^{\infty} a_i \alpha^i + O(\alpha^3).$$  \hspace{1cm} (3.12)

For example, the associated stability function $u(\alpha)$ is given by:

$$u(\alpha) = \frac{1 + \frac{1}{2} \alpha}{1 - \frac{1}{2} \alpha}.$$  \hspace{1cm} (3.13)

Which is (1,1) Pade's approximation to $e^\alpha$ since:

$$u(\alpha) = 1 + \alpha + \frac{1}{4} \alpha^2 + \ldots.$$  \hspace{1cm} (3.14)

The stability functions (3.13) satisfy the condition for the Pade's approximation with (-0,0) as the corresponding interval of absolute stability. This implies that the scheme is A – stable which stimulate the usage of the scheme for integration of ordinary differential equations with derivative discontinuities and stiff ODEs. Also, since any method that is stable is convergent, then the new scheme that is proposed is convergent.

**IMPLEMENTATION OF THE SCHEME WITH SAMPLE PROBLEMS**

To confirm the applicability of the new scheme and its suitability to integration of ordinary differential equations, we rewrite formula (2.14) in algorithm form and translate it into computer code using FORTRAN programming language and implement with sample problem on a digital computer. These sample problems were solved with the new scheme and the results are shown in Tables 1 to 3. In order to assess the performance of our scheme, the results of our scheme was compared with the result obtained from the other existing method, that is, the modified Euler scheme of the same order, and the results are shown in Table 4.

**Problem 1**

We consider the initial value problem:

$$y' = -\frac{y}{x} \quad ; \quad x_0 = -1, \quad y_0 = 1 \quad -1 \leq x < 1$$

Whose theoretical solution: $y(x) = \sqrt{2 - x^2}$ is a family of a circle centre $(0, 0)$. This differential equation is with derivative discontinuities at $(\sqrt{2}, 0)$.

This problem was solved numerically using the one-step formula (2.15) and the result is as shown in Table 1.

**Problem 2**

We consider the initial value problem: $y' = \frac{y}{x}$. 


Table 1. Result of one stage scheme for problem 1.

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Table 2. Result of one stage scheme for problem 2.

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<td>1.06816500D+01</td>
</tr>
<tr>
<td>0.24000000D+01</td>
<td>0.18754690D+01</td>
<td>0.69835240D+00</td>
<td>1.14145600D+01</td>
</tr>
</tbody>
</table>
y(1) = -1 whose theoretical solution is y = -x. The equation has derivative discontinuity at x = 0. It was solved with the one stage formula (2.15) and the result shown in Table 2.

### Problem 3

The third problem considered is:  
\[ y' = \frac{1}{x}, \quad x_0 = 1, \quad y_0 = -1 \]  
whose theoretical solution is:  
\[ y = \ln x. \]  
The differential equation has discontinuities at x = 0. The numerical solution of this problem is as shown in Table 3. From the results of the solution to the sample problems 1 to 3 as displayed in Tables 1, 2 and 3, it was observed that the discretization error obtained from the solution are sufficiently small, showing that the scheme were accurate, stable and convergent. By considering Table 4 where results obtained from our method was compared with modified Euler’s method of the same order, it can be seen that the new method compared well with the said existing method.

### Conclusion

Babatola (2000) and Bolarinwa (2005) proposed semi-implicit Rational Runge-Kutta schemes for the numerical integration of ordinary differential equations. The work was motivated by Rational Runge-Kutta scheme proposed by Hong (1982) and a variety of application areas of this class of ODEs and the need to cater for the deficiencies identified in the adoption of the existing methods of solving this class of differential equations. The new scheme was derived using power series expansion technique; it was analyzed, and implemented with sample problems on a micro computer. The results showed that the scheme is absolutely stable, convergent, efficient and effective towards solving ordinary differential equations with derivative discontinuities.

### REFERENCES


