K-Step Rational Runge-Kutta Method for Solution of Stiff System of Ordinary Differential Equations

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Abstract: This study described the development, analysis and implementation of K-step implicit rational Runge-Kutta schemes for solution of stiff system of ordinary differential equations. Its development adopted taylor and binomial series expansion techniques to generate its parameters. The analysis of its basic properties adopted dalhquist a-stability model test equation and the results showed that the scheme was a-stable, consistent and convergent. Numerical results showed that the method was accurate and effective.

Key words: K-step, rational runge-kutta, a-stability, stiff ODEs

INTRODUCTION

A differential equation of the form:

\[ y' = f(x, y), \quad y(x_0) = y_0 \]  

(1)

whose Jacobian possesses eigen values:

\[ \lambda_j = U_j + iV_j, \quad j = 1(1)n \]

(2)

where, \( \sqrt{-1} \), satisfying the following conditions:

- \( U_i < 0, \quad j = 1(1)n \)
- \( \text{Max}|U_j(x)| \gg \text{min}|U_j(x)| \)

or \( r(x) = \frac{\text{Max}|U_j(x)|}{\text{min}|U_j(x)|} \gg 1 \)

(3)

\[ y' = \lambda(y - E(x) + E \left(\frac{x}{\lambda}\right), y(x_0) = y_0 \]

(4)

where, \( E(x) \) is continuously differentiable, \( \lambda \) is a complex constant with \( \text{Re}(\lambda) << 0 \), with the exact solution:

\[ y(x) = E(x) + y_0 e^{\lambda x} \]

(5)

consisting of two components \( E(x) \) which is slowly varying in the interval of integration \((x_o, b)\), and the second \( y_0 e^{\lambda x} \) component decaying rapidly in the transient phase at the rate of \(-1/\lambda\) is midly stiff.

The system of differential equation:

\[ y' = \begin{bmatrix} -0.00005 & 100 \\ -100 & -0.00005 \end{bmatrix} y \]

with \( y(0) = [1, 1]^T \), \( 0 \leq x \leq 10\pi \) whose solution is obtained as:

\[ y(x) = e^{-0.00005x \begin{bmatrix} \sin 100x & \cos 100x \\ \cos 100x & -\sin 100x \end{bmatrix}} \]

(7)

Whose transitory phase is the entire interval of integration \( 0 \leq x \leq 10\pi \) with \( 50\pi \) complete oscillation per unit interval is an ODEs possessing these types of properties are called stiff oscillating ODEs.

Most of the conventional Runge-Kutta schemes cannot effectively solve them because they have small region of absolute stability.

This perhaps motivated[8] to introduce a rationalized Runge-Kutta scheme of the form confirm existing phases in samples according to Emmanuelson[4].

\[ y_{n+1} = \frac{y_n + \sum_{i=1}^{b} W_i K_i}{1 + \sum_{i=1}^{b} V_i H_i} \]

(8)

Where:
\[
K_i = h \left( x_n + c_i h, y_n + \sum_{j=1}^{S} a_{ij} k_j \right)
\]

\[
H_i = h g \left( x_n + d_i h, z_n + \sum_{j=1}^{S} b_{ij} k_j \right)
\]

With

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

Subject to the constraints:

\[c_1 = \sum_{j=1}^{R} a_y\]

\[d_1 = \sum_{j=1}^{R} b_y\]  

\[
y_{n+m} = \frac{y_{n+m-1} + \sum_{i=1}^{R} W_i K_i}{1 + y_{n+m-1} \sum_{i=1}^{R} V_i H_i}
\]

Where:

\[
K_i = h f \left( x_{n+m-1} + C_i h, y_{n+m-1} + \sum_{j=1}^{R} b_{ij} K_i \right)
\]

\[
H_i = h g \left( x_{n+m-1} + d_i h, z_{n+m-1} + \sum_{j=1}^{R} b_{ij} H_i \right)
\]

with

\[
g(x_{n+m-1}, Z_{n+m-1}) f(x_{n+m-1}, y_{n+m-1})
\]

In the spirit of Ademiluyi and Babatola[1] the scheme is classified into:

- Explicit if the constraints (10) is such that \(a_{ij} = 0\) for \(j \geq i\)
- Semi-implicit if \(a_{ij} = 0\) for \(j > i\)
- Implicit if \(a_{ij} \neq 0\) for at least one \(j > i\)

**MATERIALS AND METHODS**

**Derivation of the Method:** In this research, the parameters \(V_i, W_i, C_i, d_i, a_{ij}, b_{ij}\) are to be determined from the system of non-linear equations generated by adopting the following steps:

- Obtained the Taylor series expansion of \(K_i's\) and \(H_i's\) about point \((x_n, y_n)\) for \(i = 1(1)R\)
- Insert the series expansion into (10)
- Compare the final expansion with the Taylor series expansion of \(y_{n+1}\) about \((x_n, y_n)\) in the power series of \(h\)

The number of parameters normally exceeds the numbers of equations, but in the spirit of [9], Gill [7] and Blum[3], these parameters are chosen as to ensure that (the resultant computation method has:

- Adequate order of accuracy of the scheme is achieved
- Minimum bound of local truncation error
- Large maximize interval of absolute stability
- Minimum computer storage facilities

**One-step one-stage schemes:** By setting \(M = 1\) and \(R = 1\), in Eq. 11 the general one-step one-stage scheme is of the form:

\[
y_{n+1} = \frac{y_n + W_i K_i}{1 + y_n V_i H_i}
\]

Where:

\[
K_i = h f \left( x_n + c_i h, y_n + a_{11} K_i \right)
\]

\[
H_i = h g \left( x_n + d_i h, z_n + b_{11} H_i \right)
\]

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

and

\[
Z_n = \frac{1}{y_n}
\]

with the constraints:

\[
c_1 = a_{11}\]
The binomial expansion theorem of order one on the right hand side of (10) yields:

\[ y_{n+1} = y_n + W_k y_i - y_n^2 V_i H_1 + \text{(higher order terms)} \]  

(19)

While the Taylor series expansion of \( y_{n+1} \) about \( y_n \) gives:

\[ y_{n+1} = y_n + h y_n + \frac{h^2}{2} y_n^2 + \frac{h^3}{6} y_n^3 + \frac{h^4}{24} y_n^4 + 0h^5 \]

(20)

Adopting differential notations:

\[
\begin{align*}
y_n &= f_n \\
y_n' &= f_n + f_y f_y' = Df_n \\
y_n'' &= f_n + 2f_y f_y' + f_y^2 f_y'' + f_y f_y'' = D^2f_n \\
y_n''' &= f_n + 3f_y f_y' + 3f_y^2 f_y'' + f_y^3 f_y''' + f_y f_y''' + f_y f_y'' f_y'' = D^3f_n \\
y_n'''' &= f_n + 4f_y f_y' + 6f_y^2 f_y'' + 4f_y^3 f_y''' + f_y^4 f_y'''' + f_y f_y f_y'' f_y'' = D^4f_n
\end{align*}
\]

(21)

Substitute (21) into (20), we have:

\[
\begin{align*}
y_{n+1} &= y_n + h f_n + \frac{h^2}{2!} Df_n + \frac{h^3}{3!} (D^2f_n + f_y Df_n) \\
&\quad + \frac{h^4}{4!} (D^3f_n + f_y D^2f_n + f_y^2 Df_n) + 0h^5
\end{align*}
\]

(22)

Similarly the Taylor series expansion of \( K_1 \) about \( (x_n, y_n) \) is:

\[
K_1 = h \left( f_n + \frac{1}{2} \left( f_n + f_y f_y' \right) \right) + 0h^4
\]

(23)

Collecting coefficients of equal powers of \( h \), Eq. 23 can be rewritten in the form:

\[
K_1 = h A_1 + h^2 B_1 + h^3 D_1 + 0h^4
\]

(24)

where,

\[
A_1 = f_n, \quad B_1 = c_1 (f_n + f_y f_y') = C_1 Df_n \\
D_1 = c_1 B_1 f_y' + \frac{1}{2} C_1 (f_n + 2f_y f_y' + f_y^2 f_y'') = Df_n f_y' + \frac{1}{2} D^2f_n
\]

(25)

In a similar manner, expansion of \( H_1 \) about \( g_{x^2} = -2f_y^2 y_{xy} + g_{zz} = -2f_y^2 y_{z^2} \) \((x_n, z_n)\) yields:

\[
H_1 = h N_1 + h^2 M_1 + h^3 R_1 + 0h^4
\]

(26)

Where:

\[
N_1 = g(x_n, z_n) = g_n \\
M_1 = d_1 (g_n + g_y g_z) = d_1 Dg_n \\
R_1 = d_2 M_1 g_n + \frac{1}{2} d_3 (g_n + 2g_y g_z + g_y^2 g_z^2) \\
&\quad = d_1 (g_n Dg_n + \frac{1}{2} D^2g_n)
\]

(27)

Substitute (28) into (26), we obtained:

\[
\begin{align*}
N_1 &= -\frac{f_n}{y_n} \\
M_1 &= \frac{-f_n}{y_n}, \quad R_1 = -\frac{f_n}{y_n}
\end{align*}
\]

(28)

Using (25) and (26) in (19), to get:

\[
\begin{align*}
y_{n+1} &= y_n + W_k \left( h A_1 + h^2 B_1 + h^3 D_1 + 0h^4 \right) \\
&\quad - y_n^2 \left( V_1 \left( h N_1 + h^2 M_1 + h^3 R_1 + 0h^4 \right) \right) \\
&\quad = y_n \left( W_k A_1 - y_n^2 V_1 N_1 \right) h + \left( W_k B_1 - y_n^2 V_1 M_1 \right) h^2 \\
&\quad + \left( W_k D_1 - y_n^2 V_1 R_1 \right) + 0h^4
\end{align*}
\]

(30)

Comparing the coefficients of the powers of \( h \) in Eq. 22 and 30, we obtained:

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

(31)
A1 = fn N1 = \frac{-f_n}{y_n^2}, Eq. 31 yields:

W1 + V1 = 1

(32)

Similarly from coefficients of h^2 in Eq. 22 and 30, we have:

W1B1 - y_n^2 V1M1 = Df_n

(33)

Also from (22) and (31) we obtained:

\left( W1C1 + V1d1 \right) \left( Df_n + \frac{2f_n^2}{y_n^2} V1d1 \right) = \frac{2f_n}{2}

(34)

W1C1 + V1d1 = \frac{1}{2}

(35)

Putting Eq. 35 and 32 together, we have a system of non linear simultaneous equations:

W1 + V1 = 1

W1C1 + V1d1 = \frac{1}{2}

(36)

with the constraints

a11 = c1
b11 = d1

(37)

Solving Eq. 37 and 38, we obtained:

V1 = W1 = \frac{1}{2} c1 = a11 = \frac{1}{4}, d1 = b11 = \frac{1}{4}

Substituting these values in Eq. 14 we obtain a family of one-step, one stage schemes of the form:

\begin{equation}
\frac{1}{n+1} = \frac{y_n + \frac{1}{4} K1}{1 + \frac{2}{4} y_n H1}
\end{equation}

(38)

Where:

K1 = hf \left( x_n + \frac{1}{3} h, y_n + \frac{1}{2} K1 \right)
H1 = hg(x_n + \frac{1}{3} h, z_n + \frac{1}{2} H1)

(41)

(42)

The basic properties of the method: The basic properties required of a good computational method for stiff ODEs includes consistency, convergence and stability and A-stability.

Consistency: A scheme is said to be consistent, if the difference equation of the computation formula exactly approximate the differential equation it intends to solve\cite{2}.

To prove that Eq. 11 is consistent. Recall that:

\begin{equation}
y_{n+k} = \frac{y_{n+1} + \sum_{i=1}^{R} W_i k_i}{1 + \gamma_{n+1} \sum_{i=1}^{R} V_i H_i}
\end{equation}

(44)

Subtract y_{n+k-1} on both sides of Eq. 44:

\begin{equation}
y_{n+k} - y_{n+k-1} = \frac{\sum_{i=1}^{R} W_i k_i - y_{n+k-1}}{1 + \gamma_{n+k-1} \sum_{i=1}^{R} V_i H_i}
\end{equation}

(45)

\begin{equation}
\sum_{i=1}^{R} W_i k_i - y_{n+k-1} = \frac{\sum_{i=1}^{R} W_i k_i - y_{n+k-1}}{1 + \gamma_{n+k-1} \sum_{i=1}^{R} V_i H_i}
\end{equation}

(46)
with

\[ K_i = hf\left(x_{n+k-1} + C_i h, y_n + \sum_{j=1}^{R} a_{ij} k_j\right) \]

\[ H_i = h g\left(x_{n+k-1} + d_i h, z_n + \sum_{j=1}^{R} b_{ij} H_j\right) \]

Substituting (48) into (47), dividing through by \( h \) and taking limit as \( h \) tends to zero, obtain:

\[ \lim_{h \to 0} \frac{y_{n+k} - y_{n} - \sum_{i=1}^{R} W_i f(x_{n+k-1}, y_{n+k-1})}{h} = \sum_{i=1}^{R} V_i g(x_{n+k-1}, y_{n+k-1}) \]

but

\[ g(x_{n+k-1}, y_{n+k-1}) = \frac{1}{y_{n+k-1}} f(x_{n+k-1}, y_{n+k-1}) \]

then

\[ \lim_{h \to 0} \frac{y_{n+k} - y_{n} - \sum_{i=1}^{R} W_i f(x_{n+k-1}, y_{n+k-1})}{h} = \sum_{i=1}^{R} V_i g(x_{n+k-1}, y_{n+k-1}) \]

Hence the method is consistent.

**Convergence:** Since the proposed scheme is one-step, the numerical scheme (11) for solving ODEs (1) is said to be convergent, and it is consistent, by Lambert (1973) when it is applied to initial value problem (1) generated a corresponding approximation \( y_n \) which tend to the exact solution \( y(x_n) \) as \( n \) approaches infinity, that is:

\[ y_n \to y(x_n) \text{ as } n \to \infty \]

Let \( e_{n+k} \) and \( T_{n+k} \) denote the discretization and truncation errors generated by (1) respectively. Adopting Binomial expansion and ignoring higher term, Eq. 1:

\[ y_{n+k} = y_{n+k-1} + \sum_{i=1}^{R} W_i K_i - y_{n+k-1}^2 + \sum_{i=1}^{R} V_i H_i \]

If \( y(x_{n+k}) \) is the approximate theoretical solution, it seen to satisfy the difference equation:

\[ y(x_{n+k}) = y(x_{n+k-1}) + \sum_{i=1}^{R} W_i K_i - y_{n+k-1}^2 + \sum_{i=1}^{R} V_i H_i \]

\[ + \text{(higher order term)} + T_{n+k} \]

Subtract Eq. 51 from 52:

\[ y_{n+k} - y(x_{n+k}) = y_{n+k-1} - y(x_{n+k-1}) + h \left[ \psi_2(x_{n+k-1}; y(x_{n+k-1}); h) - \psi_2(x_{n+k-1}; y(x_{n+k-1}); h) \right] + h \left[ \psi_1(x_{n+k-1}; y(x_{n+k-1}); h) \right] + T_{n+k} \]

where, \( \psi_1(x_{n+k-1}; y(x_n); h) \) are assumed to be continuous functions in the domain:

\[ a \leq x \leq b, |y| < \infty, 0 \leq h \leq h_0 \]

Let \( e_{n+k} = e_{n+k-1} + h \left[ \psi_2(x_{n+k-1}; y(x_{n+k-1}); h) - \psi_2(x_{n+k-1}; y(x_{n+k-1}); h) \right] + h \left[ \psi_1(x_{n+k-1}; y(x_{n+k-1}); h) \right] + T_{n+k} \)

By taking the absolute value on both sides of Eq. 61 we have inequality:

\[ |e_{n+k}| \leq |e_{n+k-1}| + L \left| e_{n+k-1} \right| + K \left| e_{n+k-1} \right| + T \]

where, \( L \) and \( K \) are the Lipschitz constant for \( \phi_1(x, y; h) \) and \( \psi_2(x, y; h) \) respectively and:

\[ T = \sum_{n=1}^{N} |H_i| \]

By setting \( N = L + K \) Inequality (57) becomes:

\[ |e_{n+k}| \leq |e_{n+k-1}| (1 + hN) + T \]

By adopting this theorem on convergence of sequence of real numbers quoted without proof from[7], that is:
If \( \{e_j, j = o(1) n+k\} \) be set of real number. If there exist finite constants \( R \) and \( S \) such that:

\[
|e_i| \leq R |e_{i-1}| + S, \quad i = 1 \ldots n+k
\]

(59)

then

\[
|e_i| \leq \left( \frac{R^i - 1}{R - 1} \right) S + R^i |e_o|, R \neq 1
\]

(60)

Thus (59) becomes:

\[
|e_{n+k}| \leq \frac{(1 + hN)^{n+k}}{hN} + (1 + hN)^{n+k} |e_o|
\]

(61)

since

\[
|1 + hN|^{n+k} = e^{(n+k)hN} = e^{N(x_{n+k} - a)}
\]

(62)

and

\[
x_{n+k} \leq b, \quad \text{then} \quad x_{n+k} - a \leq b - a
\]

Consequently:

\[
e^{N(x_{n+k} - a)} \leq e^{N(b-a)}
\]

(63)

\[
|e_{n+k}| \leq \left( \frac{e^{N(b-a)} - 1}{hN} \right) T + e^{N(b-a)} |e_o|
\]

(64)

Considering Eq. 64 and adopting first mean value theorem:

\[
T_{n+k} = h \left[ \psi_2(x_{n+k} - 0h, y_{n+k} - 0h) - \psi_2(x_{n+k} - 0h) \right]
\]

(65)

By taking the absolute value of (55) on (66) both sides Eq. 66 into consideration, we have:

\[
T = hL \left| y((x_{n+k} - 0h) - y(x_{n+k} + 0h)) \right| + jh^2 \theta
\]

(66)

where, \( M \) and \( j \) are the partial derivative of \( \phi_i \) and \( \psi_i \) with respect of \( x \) respectively.

By setting \( Q = j + m \) and

\[
y = \sup_{a \leq x \leq b} (y(x))
\]

(67)

Therefore, Eq. 54 yields:

\[
T = h^2 \theta (NY + Q)
\]

(68)

By substituting (57) into (52), we have:

\[
|e_{n+k}| \leq h^2 e^{N(b-a)} (NY + Q) + e^{N(b-a)} |e_o|
\]

(69)

Assuming no error in the input data, that is \( e_o = 0 \).

Then the limit as \( h \) tends to zero, we obtain in Eq. 70 yields:

\[
\lim_{h \to 0} |e_{n+k}| = 0
\]

which implies that:

\[
\lim_{h \to 0} y_n = y(x_n)
\]

Thus establishing the convergence of scheme (11).

**Stability Properties:** To analyse the stability property of this schemes, apply scheme (1) to Dalhquist\[d\] stability scalar test initial value problem:

\[
y' = \lambda y, \quad y(x_0) = y_o
\]

(70)

to obtained a difference equation:

\[
y_{n+k} = \mu(z) y_{n+k-1}
\]

(71)

with the stability function:

\[
\mu(z) = \frac{1 + ZW^T (I - ZA)^{-1} e}{1 + ZV^T (I - ZB)^{-1} e}
\]

(72)

Where:

\[
W^T = (W_1, W_2 \ldots W_r)
\]

\[
V^T = (V_1, V_2 \ldots V_r)
\]

To illustrate, this we consider the one-step, one-stage scheme:

\[
y_{n+1} = \frac{y_n + W_k y_k}{1 + y_o V^t H_i}
\]

(73)
Where:

\[ K_1 = hf(x_n + c_1 h, y_n + a_{11} K_1) \]
\[ H_1 = hg(x_n + d_1 h, z_n + b_{11} H_1) \]  \hspace{1cm} (74)

Applying (73) to the stability test Eq. 70 we obtain the recurrent relation:

\[ y_{n+1} = \mu(z) y_n \]  \hspace{1cm} (75)

with stability function:

\[ \mu(z) = \frac{1 + W_i Z(1 - a_{11} Z)^{-1}}{1 - V_i Z(1 + b_{11} Z)^{-1}} \]  \hspace{1cm} (76)

For example, to analyze scheme (74) will introduce a convergent and stable approximation to the solution of stability function if:

\[ \left| \mu(z) \right| = \left| \frac{1 + \frac{1}{4} Z}{1 - \frac{1}{4} Z} \right| < 1 \]  \hspace{1cm} (77)

That is (-\infty < x < 0), the scheme is A-stable because the interval of absolute stability is (-\infty, 0).

**RESULTS AND DISCUSSION**

In order to access performance of the schemes the following sample problems were solved, with the schemes adopting Fehlberg\cite{6} approach.

**Problem 1:** Consider the stiff system of ODEs of the form:

\[ Y' = AY \]  \hspace{1cm} (78)

Table 1: Numerical result of k-step implicit rational Runge-Kutta schemes for solving stiff systems of ordinary differential equations

| X                | Control step size | E1                       | E2                       | E3                       |
|------------------|-------------------|--------------------------|--------------------------|--------------------------|
| 0.30000000000D-01| 0.30000000000D-01 | 0.1980099667D+01         | 0.9706425830D+00         | 0.8869204674D+00         |
| 0.1774236000D+00 | 0.1771470000D+00  | 0.8291419103D+00         | 0.3281419103D+00         | 0.816131500D+05          |
| 0.3307246652D+00 | 0.1046033532D+00  | 0.839203859D+00          | 0.3281419103D+00         | 0.816131500D+05          |
| 0.497785155D+00  | 0.6176733963D-02  | 0.1150933794D-10         | 0.3281419103D+00         | 0.816131500D+05          |
| 0.751286395D+00  | 0.3647299638D+01  | 0.1694213422D+01         | 0.3281419103D+00         | 0.816131500D+05          |
| 0.995129893D+00  | 0.2153693963D-01  | 0.1594313570D+09         | 0.3281419103D+00         | 0.816131500D+05          |

With initial condition \( y(0) = (2, 1, 2) \). Its numerical solution is:

\[
\begin{bmatrix}
    y_1(x) \\
    y_2(x) \\
    y_3(x)
\end{bmatrix} = \begin{bmatrix}
    e^x + e^{-5x} \\
    e^{-5x} \\
    e^{-5x} + e^{-12x}
\end{bmatrix}
\]

Its numerical solution is found in Table 1.

**Problem 2:** The second sample problem considered is the stiff system of initial values problems of ODEs below:

\[
y = \begin{bmatrix}
    -0.5 & 0 & 0 & 0 & 0 \\
    0 & -1.0 & 0 & 0 & 0 \\
    0 & 0 & -9.0 & 0 & 0 \\
    0 & 0 & 0 & -10.0 & 0
\end{bmatrix} \begin{bmatrix}
    y_1 \\
    y_2 \\
    y_3 \\
    y_4
\end{bmatrix}
\]

with initial condition \( y(0) = [1 \ 1 \ 1 \ 1 \ 1] \). Its numerical solution is:

\[
y = \begin{bmatrix}
    0.7512863893D+00 \\
    0.497785155D+00 \\
    0.3307246652D+00 \\
    0.1774236000D+00 \\
    0.1774236000D+00
\end{bmatrix}
\]

The results are shown in Table 2.
Table 2: Numerical result of k-step implicit rational runge-kutta schemes for solving stiff systems of ordinary differential equations

| X                     | Control step size | E1                  | E2                  | E3                  | E4                  |
|-----------------------|-------------------|---------------------|---------------------|---------------------|---------------------|
| 0.3000000000D-01      | 0.3000000000D-01  | 0.9950124792D+00    | 0.9900498337D+00    | 0.9139311928D+00    | 0.9048374306D+00    |
| 0.1774236000D-01      | 0.1771470000D-01  | 0.9708623323D+00    | 0.9425736684D+00    | 0.852769932D+00     | 0.5553451450D+00    |
| 0.3694667141D-01      | 0.1046033532D-01  | 0.3621547506D-12    | 0.545425720D-11     | 0.1355160001D-07    | 0.1829417523D-07    |
| 0.5365278644D+00      | 0.6176739636D-02  | 0.4285460875D+13    | 0.6268319197D-12    | 0.9915873955D-09    | 0.1265158728D-08    |
| 0.8400599835D+00      | 0.3647299638D-01  | 0.4961209221D-10    | 0.6922001861D-09    | 0.5087490103D-06    | 0.589525189D-06     |

CONCLUSION

From the above results (Table 1 and 2), it can be seen that the proposed schemes are quite accurate, convergent and stable.

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