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Stability Analysis on The Implicit Keller Box Method for Solving Time Fractional Diffusion Equation

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Abstract
One dimensional time fractional diffusion equation with source term is investigated in this study. Terms involving anomalous diffusion and the fractional derivative is defined using Grünwald Letnikov formula. The Keller box finite difference scheme to solve the spatiotemporal governing equation is developed implicitly with second order accuracy. Here, the stability of the scheme is carried out using well-known Von Neumann stability method. It is proven that the Keller box scheme for the governing equation is unconditionally stable with order of the time fractional derivative is taken between 0 and 1.
Keywords: Time fractional differential equation; Keller box method; Grünwald Letnikov formula; Von Neumann method.

1 Introduction

Over the last few decades, fractional differential equation (FDE) has grabbed the eye of numerous researchers as its both principle and applications are strong and developing [1]. Not only in pure and applied mathematics, but the significance of fractional derivatives development is also remarkable in physics, chemistry and engineering. For various materials and processes, their definition of memory and hereditary properties can be brilliantly provided by using fractional differential equation. Ever since the question of the meaning of $\frac{\delta^{\eta} f}{\delta x^{\eta}}$ if $\eta = \frac{1}{2}$ has been raised by L'Hopital in 1695 [2], many definitions of a fractional derivative, new derivatives and fractional integrals have arisen. Each of them has different fundamentals that makes the definitions varies [1]. Two of the popular fractional derivatives are Riemann-Liouville and Caputo definitions.

This study is focused on fractional differential equations problems with time fractional diffusion equation. The finite difference scheme to solve these problems is developed implicitly based on Keller box method and the stability of the scheme is analysed. Central difference scheme is used that yields a second order accuracy in both time and space. Definition of fractional derivative like Grünwald-Letnikov formula is used to discretise the time fraction. Stability of the scheme is analysed by using Vonn-Neumann method.

2 Literature Review

Derivation of time fractional diffusional equation is from considering continuous time random walk problems, and they are in general non-Markovian process [3]. Some analytical solutions for time fractional differential equations problem have been constructed in [4] and [5] where time-fractional diffusion wave equation is considered. In both studies, the Green function and their properties are taken in terms of Fox function. In terms of wright function, Gorenflo et al. [6] and Gorenflo et al. [7] obtained the scale-invariant solution by using the similarity method and the method of Laplace transform.

First devised by Keller and Cebeci [8], Keller box method is based on a developed new accurate finite difference method for parabolic partial differential equation. One of the fundamental concepts for this method is to write the first order system of the governing partial differential equations [8]. A study analysed a steady boundary layer flow and heat transfer over a stretching sheet with Newtonian heating in which the heat transfer from the surface is proportional to the local surface temperature [9]. Equations with nonlinear boundaries are converted into ordinary differential equations, which are then numerically solved by Keller box method.

Osman and Langlands [10] in their study, discretised the fractional diffusion equation by using Keller box method and a modified L1 scheme (ML1) based on Oldham and Spanier [11] to approximate the Riemann-Liouville fractional derivative. The closed form analytic solutions are either do not exist or involve special functions that are hard to evaluate causes developing numerical techniques to find approximate solutions of fractional partial differential equation is important. They developed a method that can be used for a more general equations such as fractional cable equation [12]. The numerical method developed could be modified to include a source term $f(x,t)$ which then be solved on the finite spatial domain $0 \leq x \leq L$ and for times $0 \leq t \leq T$. The accuracy was found to be in order $1+\gamma$ in time and second order in space.

A study used Keller box to obtain a numerical scheme for one-dimensional time fractional diffusion equation with functions as boundary values [13]. In this scheme, Grünwald-Letnikov is used to replace the fractional derivatives term. Two first-order equations are obtained from the second order diffusion equation. By using central difference in space and time, a system of equations is acquired and represented in a tridiagonal matrix form. Then, this is solved by using Thomas algorithm.

3 Mathematical Formulation

3.1 One Dimensional Time Fractional Diffusion Equation

The one dimensional time fractional diffusion equation is given by,

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \qquad 0 < x < L, \qquad 0 < t < T, \tag{1}$$

where $f(x,t)$ is a source term, L is maximum length of space x and T is the maximum time, t. The equation (1) has broad applications in real world applications like chemotaxis and relaxation problems. Given the initial condition,

$$u(x,0) = 0; \qquad\qquad 0 \leq x \leq L \tag{2}$$

and the boundary conditions:

$$\begin{aligned} u(0,t) &= g_0(t), \\ u(1,t) &= g_1(t); \qquad\qquad 0 < t < T. \end{aligned} \tag{3}$$

The functions g_0 and g_1 are known while the function u is the unknown function to be determined.

3.2 Finite Difference Scheme

3.2.1 Discretization for the First Case

For the first case, $\alpha = 1$ is substituted into equation (1). Therefore, equation (1) becomes,

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t). \tag{4}$$

Let,

$$\frac{\partial u(x,t)}{\partial x} = v(x,t), \tag{5}$$

then equation (4) becomes,

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial v(x,t)}{\partial x} + f(x,t). \tag{6}$$

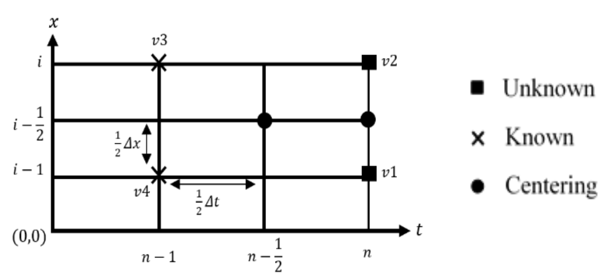

Figure 1 Grid points for finite difference of Keller box scheme.

Based on Figure 1, central difference for space is applied in equation (5) using $\left(n, i-\frac{1}{2}\right)$ of the segment $v_1 v_2$ and central difference in space and time is employed in equation (6) for $\left(n-\frac{1}{2}, i-\frac{1}{2}\right)$ of rectangle $v_1 v_2 v_3 v_4$. Therefore,

$$\frac{u_i^n - u_{i-1}^n}{\Delta x_i} + O(\Delta x^2) = v_{i-\frac{1}{2}}^n, \tag{7}$$

$$\frac{u_{i-\frac{1}{2}}^n - u_{i-\frac{1}{2}}^{n-1}}{\Delta t_n} + O(\Delta t^2) = \frac{v_i^{n-\frac{1}{2}} - v_{i-1}^{n-\frac{1}{2}}}{\Delta x_i} + O(\Delta x^2) + f_{i-\frac{1}{2}}^{n-\frac{1}{2}}. \tag{8}$$

Assume

$$t_{n-\frac{1}{2}} = \frac{1}{2}(t_n + t_{n-1}) \qquad \text{and} \qquad x_{i-\frac{1}{2}} = \frac{1}{2}(x_i - x_{i-1}) \tag{9}$$

and neglecting the truncation errors, equations (7) and (8) yield

$$u_i^n - u_{i-1}^n - \frac{\Delta x_i}{2}(v_i^n + v_{i-1}^n) = 0, \tag{10}$$

$$u_i^n + u_{i-1}^n + \frac{\Delta t_n}{\Delta x_i}(v_{i-1}^n - v_i^n) = u_i^{n-1} + u_{i-1}^{n-1} + \frac{\Delta t_n}{\Delta x_i}\left(v_i^{n-1} - v_{i-1}^{n-1}\right) + 2\Delta t_n f_{i-\frac{1}{2}}^{n-\frac{1}{2}}, \tag{11}$$

respectively. Equations (10) and (11) are represented in the form of tridiagonal matrix and is solved using Thomas algorithm.

3.2.2 Discretization for the Second Case

Now, the second-order diffusion equation (4) is recalled and the order of α is taken between 0 and 1.

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t).$$

This equation is reduced to a system of two-first order partial differential equations. Let,

$$\frac{\partial u(x,t)}{\partial x} = v(x,t). \tag{12}$$

Then the second-order diffusion equation (4) becomes

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial v(x,t)}{\partial x} + f(x,t). \tag{13}$$

By using central differences of $(n, i - \frac{1}{2})$ in equation (12) and $(n - \frac{1}{2}, i - \frac{1}{2})$ in equation (13), and discretize the time fraction in equation (13) using standard Grünwald-Letnikov formula which is defined as,

$${}_0D_t^\alpha f(t) = \frac{1}{b^\alpha}\sum_{s=0}^{\left[\frac{t}{b}\right]} \omega_s^{(\alpha)} f(t - sb) + O(b); \quad t \geq 0,$$

then, the equations (12) and (13) become

$$\frac{u_i^n - u_{i-1}^n}{\Delta x_i} + O(\Delta x^2) = v_{i-1/2}^n, \tag{14}$$

$$\begin{aligned} \frac{\partial^\alpha u(x_i, t_n)}{\partial t^\alpha} &= \frac{1}{2\Delta t_n^\alpha} \sum_{s=0}^{n} \omega_s^{(\alpha)} u_{i-1/2}^{n-s} + O(\Delta t) \\ &= \frac{v_i^{n-1/2} - v_{i-1}^{n-1/2}}{\Delta x_i} + O(\Delta x^2) + f_{i-1/2}^{n-1/2}, \end{aligned} \tag{15}$$

respectively. By using the central difference expressions in (9) and neglecting the truncation error terms, equations (14) and (15) become,

$$u_i^n - u_{i-1}^n - \frac{\Delta x_i}{2}(v_i^n + v_{i-1}^n) = 0, \tag{16}$$

$$\begin{aligned} &\frac{1}{2\Delta t_n^\alpha}\left(\sum_{s=0}^{n} \omega_s^{(\alpha)} u_i^{n-s} + \sum_{s=0}^{n} \omega_s^{(\alpha)} u_{i-1}^{n-s}\right) \\ &\qquad = \frac{1}{2\Delta x_i}\left(v_i^n + v_i^{n-1} - v_{i-1}^n - v_{i-1}^{n-1}\right) + f_{i-1/2}^{n-1/2}. \end{aligned} \tag{17}$$

The coefficients $\omega_s^{(\alpha)}$ are the first coefficients of Taylor series expansions of the function $(1-z)^\alpha$, where

$$\omega_0^{(\alpha)} = 1 \qquad \text{and} \qquad \omega_s^{(\alpha)} = \left(1 - \tfrac{a+1}{s}\right)\omega_{s-1}^{(\alpha)}.$$

The series in (17) is expanded and simplified as

$$\begin{aligned} &u_i^n + u_{i-1}^n + \frac{\Delta t_n^\alpha}{\Delta x_i}(v_{i-1}^n - v_i^n) \\ &\qquad = \alpha\left(u_i^{n-1} + u_{i-1}^{n-1}\right) + \frac{\Delta t_n^\alpha}{\Delta x_i}\left(v_i^{n-1} - v_{i-1}^{n-1}\right) - \sum_{s=2}^{n} \omega_s^{(\alpha)} u_i^{n-s} \\ &\qquad - \sum_{s=2}^{n} \omega_s^{(\alpha)} u_{i-1}^{n-s} + 2\Delta t_n^\alpha f_{i-\frac{1}{2}}^{n-\frac{1}{2}}. \end{aligned} \tag{18}$$

The system of equations (16) and (18) is represented in the form of tridiagonal matrix and is solved using Thomas algorithm. For simplification, let $h = \Delta x$ and $m = \Delta t$.

Newton's method is used to linearize the nonlinear system of equations (16) and (18). Linearizing these equations yield,

$$\delta u_i - \delta u_{i-1} - \tfrac{h}{2}(\delta v_i + \delta v_{i-1}) = -u_i + u_{i-1} + \tfrac{h}{2}(v_i + v_{i-1}), \tag{19}$$

$$\delta u_i + \delta u_{i-1} + \frac{m}{h}\left(\delta v_{i-1} - \delta v_i\right) = G^{n-1} - u_i - u_{i-1} - \frac{m^\alpha}{h}(v_{i-1} - v_i), \tag{20}$$

where

$$G^{n-1} = \alpha\left(u_i^{n-1} + u_{i-1}^{n-1}\right) + \frac{m^\alpha}{h}\left(v_i^{n-1} - v_{i-1}^{n-1}\right)$$
$$-\sum_{s=2}^{n} \omega_s^{(\alpha)} u_i^{n-s} - \sum_{s=2}^{n} \omega_s^{(\alpha)} u_{i-1}^{n-s} + 2m^\alpha f_{i-\frac{1}{2}}^{n-\frac{1}{2}}.$$

The linear system (19) and (20) is solved by using the block-elimination method that involves forward and backward sweeps.

4 Results and Discussion

4.1 Stability of Fractional Implicit Keller Box Method

The stability of fractional implicit Keller box method developed is analysed using Von Neumann method following the work from Chen *et al*. [14]. The system of equations (16) and (18) is rewritten with no source term for simplicity. By letting U_i^n and V_i^n as the approximate solutions of difference equations and the errors, then

$$u_i^n = U_i^n + \varepsilon_i^n,$$
$$v_i^n = V_i^n + z_i^n. \tag{21}$$

Hence, substituting (21) into equations (16) and (18) yields,

$$U_i^n + \varepsilon_i^n - U_{i-1}^n - \varepsilon_{i-1}^n - \frac{h}{2}(V_i^n + z_i^n + V_{i-1}^n + z_{i-1}^n) = 0, \tag{22}$$

$$\begin{aligned} U_i^n + \varepsilon_i^n + U_{i-1}^n + \varepsilon_{i-1}^n + \frac{m^\alpha}{h}(V_{i-1}^n + z_{i-1}^n - V_i^n - z_i^n) \\ = \alpha\left(U_i^{n-1} + \varepsilon_i^{n-1} + U_{i-1}^{n-1} + \varepsilon_{i-1}^{n-1}\right) \\ + \frac{m^\alpha}{h}\left(V_i^{n-1} + z_i^{n-1} - V_{i-1}^{n-1} - z_{i-1}^{n-1}\right) \\ -\sum_{s=2}^{n} \omega_s^{(\alpha)} (U_i^{n-s} + \varepsilon_i^{n-s}) - \sum_{s=2}^{n} \omega_s^{(\alpha)} (U_{i-1}^{n-s} + \varepsilon_{i-1}^{n-s}). \end{aligned} \tag{23}$$

Since U_i^n and V_i^n are the approximate solutions, therefore it satisfies the difference equations. Then,

$$U_i^n - U_{i-1}^n - \frac{h}{2}(V_i^n + V_{i-1}^n) = 0, \tag{24}$$

$$\begin{aligned} U_i^n - U_{i-1}^n + \frac{m^\alpha}{h}(V_{i-1}^n - V_i^n) = \alpha\left(U_i^{n-1} + U_{i-1}^{n-1}\right) + \frac{m^\alpha}{h}\left(V_i^{n-1} - V_{i-1}^{n-1}\right) \\ -\sum_{s=2}^{n} \omega_s^{(\alpha)} U_i^{n-s} - \sum_{s=2}^{n} \omega_s^{(\alpha)} U_{i-1}^{n-s}. \end{aligned} \tag{25}$$

Subtracting equations (24) and (25) from equations (22) and (23) respectively give,

$$\varepsilon_i^n - \varepsilon_{i-1}^n - \frac{h}{2}(z_i^n + z_{i-1}^n) = 0. \tag{26}$$

$$\begin{aligned}\varepsilon_i^n + \varepsilon_{i-1}^n + \frac{m^\alpha}{h}(z_{i-1}^n - z_i^n) &= \alpha\left(\varepsilon_i^{n-1} + \varepsilon_{i-1}^{n-1}\right) + \frac{m^\alpha}{h}\left(z_i^{n-1} - z_{i-1}^{n-1}\right) \\ &\quad - \sum_{s=2}^{n} \omega_s^{(\alpha)} \varepsilon_i^{n-s} - \sum_{s=2}^{n} \omega_s^{(\alpha)}\, \varepsilon_{i-1}^{n-s} \quad ,\end{aligned} \tag{27}$$

where,

$$\varepsilon_0^n = \varepsilon_n^n = 0 \quad \text{and} \quad z_0^n = z_J = 0, \quad \text{for } n = 1, 2, \ldots, N. \tag{28}$$

Proposition 1 [13] The coefficient $\omega_s^{(\alpha)}$ $(s = 0,1, \ldots)$ satisfies

(1) $\omega_0^{(\alpha)}$=1; $\omega_1^{(\alpha)} = -\alpha$; $\omega_s^{(\alpha)} < 0$, $s = 1, 2, \ldots;$

(2) $\sum_{s=0}^{\infty} \omega_s^{(a)} = 1$; $-\sum_{s=1}^{n} \omega_s^{(\alpha)} < 1$, $\forall n \in N^+$.

The error functions $\varepsilon(ih) = \varepsilon_i$ and $z(ih) = z_i$ where, $i = 0,1, \ldots, J$ are represented as Fourier series respectively,

$$\varepsilon_i = \sum_{j=0}^{J} A_j e^{\sqrt{-1}qih},$$

$$z_i = \sum_{j=0}^{J} B_j e^{\sqrt{-1}qih},$$

where q is a real number. For the purpose of studying the propagation of errors, the summation and constant A_j and B_j are omitted. Now, supposed that the solution of equations (26), (27) and (28) are in the form,

$$\begin{aligned}\varepsilon_i^n &= e^{\sqrt{-1}qx} e^{\beta t} \\ &= e^{\sqrt{-1}qih} e^{\beta nm} \\ &= \xi_n e^{\sqrt{-1}qih},\end{aligned} \tag{29}$$

$$z_i^n = \zeta_n e^{\sqrt{-1}qih}, \tag{30}$$

where β is a complex number. When $n = 0$, the solutions are reduced to $e^{\sqrt{-1}qih}$, where $\xi_0 = 1$ and $\zeta_0 = 1$. By substituting (29) and (30) into equations (26) and (27) respectively,

$$\xi_n e^{\sqrt{-1}qih} - \xi_n e^{\sqrt{-1}q(i-1)h} - \frac{h}{2}(\zeta_n e^{\sqrt{-1}qih} + \zeta_n e^{\sqrt{-1}q(i-1)h}) = 0, \tag{31}$$

$$\begin{aligned}\xi_n e^{\sqrt{-1}qih} + \xi_n e^{\sqrt{-1}q(i-1)h} + \frac{m^\alpha}{h}\left(\zeta_n e^{\sqrt{-1}q(i-1)h} - \zeta_n e^{\sqrt{-1}qih}\right) \\ = \alpha\left(\xi_{n-1} e^{\sqrt{-1}qih} + \xi_{n-1} e^{\sqrt{-1}q(i-1)h}\right)\end{aligned} \tag{32}$$

$$+\frac{m^{\alpha}}{h}\left(\zeta_{n-1}e^{\sqrt{-1}qih}-\zeta_{n-1}e^{\sqrt{-1}q(i-1)h}\right)$$
$$-\sum\nolimits_{s=2}^{n}\omega_s^{(\alpha)}\xi_{n-s}e^{\sqrt{-1}qih}-\sum\nolimits_{s=2}^{n}\omega_s^{(\alpha)}\,\xi_{n-s}e^{\sqrt{-1}q(i-1)h}.$$

Simplifying equations (31) and (32),

$$\xi_n=\frac{h}{2}\frac{(1+e^{-\sqrt{-1}qh})}{\left(1-e^{-\sqrt{-1}qh}\right)}\zeta_n. \tag{33}$$

$$\xi_n-\frac{m^{\alpha}}{h}\zeta_n\frac{\left(1-e^{-\sqrt{-1}qh}\right)}{\left(1+e^{-\sqrt{-1}qh}\right)}=\alpha\xi_{n-1}+\frac{m^{\alpha}}{h}\frac{\left(1-e^{-\sqrt{-1}qh}\right)}{\left(1+e^{-\sqrt{-1}qh}\right)}\zeta_{n-1}$$
$$-\sum_{s=2}^{n}\omega_s^{(\alpha)}\xi_{n-s}\,. \tag{34}$$

Rearranging (33) becomes,

$$\zeta_n=\frac{2}{h}\left(\frac{1-e^{-\sqrt{-1}qh}}{1+e^{-\sqrt{-1}qh}}\right)\xi_{n.} \tag{35}$$

Substituting (35) into equation (34), then

$$\xi_n-2S^{\alpha}\left(\frac{1-e^{-\sqrt{-1}qh}}{1+e^{-\sqrt{-1}qh}}\right)^2\xi_n=\alpha\xi_{n-1}+2S^{\alpha}\left(\frac{1-e^{-\sqrt{-1}qh}}{1+e^{-\sqrt{-1}qh}}\right)^2\xi_{n-1}$$
$$-\sum\nolimits_{s=2}^{n}\omega_s^{(\alpha)}\xi_{n-s}, \tag{36}$$

where

$$S^{\alpha}=\frac{m^{\alpha}}{h^2}\,.$$

Using the Euler identities,

$$e^{\sqrt{-1}qh}=\cos(qh)+\sqrt{-1}\sin(qh),$$

$$e^{-\sqrt{-1}qh}=\cos(qh)-\sqrt{-1}\sin(qh),$$

therefore equation (36) becomes,

$$\xi_n=\frac{(\alpha-\mu)\xi_{n-1}-\sum\nolimits_{s=2}^{n}\omega_s^{(\alpha)}\xi_{n-s}}{(1+\mu)}\,, \tag{37}$$

where

$$\mu = \frac{2S\sin^2(qh)}{(1+\cos(qh))^2} \geq 0. \tag{38}$$

Proposition 2 [13] The solution of equation (37) is assumed to be ξ_n for $n = 1, 2, \dots, N$.

$$|\xi_n| \leq |\xi_0| \qquad \text{for} \qquad n = 1, 2, \dots, N.$$

Proof Mathematical induction is used to prove Proposition 2 according to several studies [1,2]. Starting with $n = 1$ from equation (37),

$$\xi_1 = \frac{(\alpha - \mu)\xi_0}{(1+\mu)}. \tag{39}$$

Since $\mu \geq 0$ and $0 < \alpha < 1$, then

$$|\xi_1| \leq \frac{(\alpha-\mu)}{(1+\mu)}|\xi_0| \leq |\xi_0|.$$

Assume that,

$$|\xi_m| \leq |\xi_0|, \text{ for } m = 1, 2, \dots, n-1,$$

then from equation (37) and by applying Proposition 1, it is obtained

$$\begin{aligned}
|\xi_n| &\leq \frac{(\alpha-\mu)}{(1+\mu)}|\xi_{n-1}| + \frac{1}{1+\mu}\sum_{s=2}^{n}|\omega_s^{(\alpha)}|\,|\xi_{n-s}| \\
&\leq \left[\frac{(\alpha-\mu)}{(1+\mu)} + \frac{1}{1+\mu}\sum_{s=2}^{n}|\omega_s^{(\alpha)}|\right]|\xi_0| \\
&\leq \left[\frac{(\alpha-\mu)}{(1+\mu)} + \frac{1}{1+\mu}\sum_{s=2}^{n}\left(|\omega_s^{(\alpha)}| - |\omega_1^{(\alpha)}|\right)\right]|\xi_0| \\
&= \left[\frac{(\alpha-\mu)}{(1+\mu)} + \frac{1}{1+\mu}\left(-\sum_{s=2}^{n}\omega_s^{(\alpha)} - \alpha\right)\right]|\xi_0| \\
&\leq \left[\frac{(\alpha-\mu)}{(1+\mu)} + \frac{1}{1+\mu}(1-\alpha)\right]|\xi_0| \\
&= \frac{1-\mu}{1+\mu}|\xi_0| \\
&\leq |\xi_0|.
\end{aligned} \tag{40}$$

Hence, it is proven that $|\xi_n| \leq \frac{1-\mu}{1+\mu}|\xi_0| \leq |\xi_0|$. According to Von Neumann's method, this gives the stability requirement for the solution of the difference equation (16) and (18) to be unconditionally stable.

5 Conclusion

The finite difference scheme to solve one dimensional time fractional diffusion equation is developed in this study. The scheme is based on Keller box method. The system of equations then can be linearized using Newton's method and then solved using block elimination. The stability of the scheme is investigated. It is proven that the scheme build is unconditionally stable.

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