

# Local Constitutive Equations, Extended Thermodynamics and Maxwellian Iteration

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**Abstract.** The modern theory of extended thermodynamics, shows that the well known constitutive equations of continuum mechanics of non-local form in space are in reality approximations of balance laws when some relaxation times are neglected. We recall, for example, the Fourier's equation, the Navier-Stokes' equations, the Fick's equation, the Darcy's law and several others. This idea suggests that the "authentic" constitutive equations are local and, therefore, the differential systems of mathematical physics are hyperbolic rather than parabolic. Another consequence is that these equations do not need to satisfy the so called *objectivity principle* that on the contrary still continues to be valid only for the constitutive equations. Under suitable assumptions the conditions dictated by the entropy principle in the hyperbolic case guarantees the entropy principle validity also in the parabolic limit. Considerations are also made with regard to the formal limit between hyperbolic system and parabolic ones and from hyperbolic versus hyperbolic, between a system and a subsystem.

## 1 Constitutive equations and Material Frame Indifference

The physical laws in continuum theories are *balance laws*:

$$\frac{\partial \mathbf{F}^0}{\partial t} + \frac{\partial \mathbf{F}^i}{\partial x^i} = \mathbf{f}. \quad (1)$$

Of course the system is not closed and we need the so called *constitutive equations*. A very roughly mathematical definition of constitutive equations can be considered as the equations that need to close the system i.e., choosing a field  $\mathbf{u} \in R^N$  we have to give the relations between the  $5N$  components of the vectors  $\mathbf{F}^0$ ,  $\mathbf{F}^i$  and  $\mathbf{f}$  and the  $N$  field components of the unknown vector  $\mathbf{u}$ . But of course, as we will see later this definition have no physical meaning because we need that the additive equations must be represents the real constitutive properties of the material.

For a long time the constitutive equation was done in an empiric way and they belong substantially in three big class:

- *Local constitutive equations* - Examples are: stress-strain relations in non-linear elasticity  $\mathbf{t} \equiv \mathbf{t}(\mathbf{E})$  (the Hook law in the linear case), and the caloric and thermal equations of state in Euler fluids that connect internal energy and pressure as function of density and temperature  $\varepsilon \equiv \varepsilon(\rho, T)$ ,  $p \equiv p(\rho, T)$ .

Introducing these constitutive equation in the balance laws we obtain a differential system which, in general, is hyperbolic.

- *Non local type (in space)* - In the case of a single dissipative fluid, examples are: the Fourier law  $\mathbf{q} = L \text{grad}(1/T)$  where  $\mathbf{q}$  is the heat flux, the Navier-Stokes equations  $\boldsymbol{\sigma} = 2\nu \mathbf{D}^D + \lambda \text{div} \mathbf{v} \mathbf{I}$  where  $L, \nu$  and  $\lambda$  are phenomenological coefficients related respectively to the heat conductivity and the viscosity coefficients, while  $\boldsymbol{\sigma}$  is the viscous stress tensor,  $\mathbf{D} = 1/2(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)$  is the deformation velocity and  $\mathbf{D}^D$  indicate the deviatoric part of  $\mathbf{D}$  that is traceless.

In the case of a mixture of dissipative fluids with  $n$  constituents well known examples are the Navier-Stokes, Fourier and Fick laws:

$$\begin{aligned} \boldsymbol{\sigma} &= 2\nu \mathbf{D}^D + \lambda \text{div} \mathbf{v} \mathbf{I}, \\ \mathbf{q} &= L \text{grad} \left( \frac{1}{T} \right) + \sum_{b=1}^{n-1} L_b \text{grad} \left( \frac{\mu_b - \mu_n}{T} \right), \\ \mathbf{J}_a &= \tilde{L}_a \text{grad} \left( \frac{1}{T} \right) - \sum_{b=1}^{n-1} L_{ab} \text{grad} \left( \frac{\mu_b - \mu_n}{T} \right), \end{aligned} \quad (2)$$

where  $\mathbf{J}_a$  are the diffusion flux vectors, the  $\mu$ 's are the chemical potentials and  $\tilde{L}_a, L_b, L_{ab}$ , ( $a, b = 1, 2, \dots, n-1$ ) are phenomenological coefficients related to diffusion.

When we introduce these constitutive equations in the balance laws we obtain a mathematical system of differential equations where the spatial derivatives are of second order and the time derivatives are of first order. These differential systems have a parabolic structure.

- *Non local type (in time)*- Examples are: the visco-elasticity or in general all materials in which the stress depends not only of deformations but also of the history of the deformation (constitutive equations with memory). Except for the case of exponential kernel the mathematical structure of the system is of integro-differential type.

In the modern constitutive theory all the constitutive equations must obey two universal principles:

- *The objectivity principle*: the balance laws are invariant with respect Galilean transformations and the proper constitutive equations are independent of the Observer (*material frame indifference*, Noll, see, e.g [1]);

- *The entropy principle*, that in the Rational Thermodynamics requires that any solutions of the full system satisfies a supplementary entropy balance laws with a non-negative entropy production (Coleman-Noll [2] - Müller [3]):

$$\frac{\partial \rho S}{\partial t} + \frac{\partial}{\partial x^i} (\rho S v^i + \Phi^i) \geq 0 \quad \text{for all processes,}$$

where  $S$  denotes the entropy density and  $\Phi^i$  the entropy flux.

A long debate was present in literature after Ingo Müller published a famous paper [4] in which he proved that the Fourier and Navier-Stokes “constitutive” equations violate the objectivity principle. At that time Müller was convinced that the result indicates that the objectivity principle is not a valid principle and therefore a huge literature start between supporter and not supporter of the objectivity principle. Several authors add also artificial time derivatives to try to recover the objectivity for the heat equation and for the stress. Here we record an independent observation on the subject by Bressan [5] and Ruggeri [6] that may solve in a simple way the problem. Bressan and Ruggeri observe that a possible interpretation of the Müller result is that the objectivity principle is indeed universal, but the Fourier and Navier-Stokes equations are not “true” constitutive equations. The precise and convincing answer was done by the Extended Thermodynamics (ET) [7].

## 2 The Extended Thermodynamics

The idea of Rational Extended Thermodynamics [7] was to view the truncated system of moment equations associated with Boltzmann equation on the same ground of a phenomenological system of continuum mechanics end according with the rational thermodynamic, the restrictions must be imposed only on the basis of *universal principles*, i.e.: *Entropy principle*, *Objectivity Principle* and *Causality and Stability* (convexity of the entropy).

The restrictions are so strong (in particular the entropy principle) that, at least, for processes not too far from the equilibrium the system is completely closed. In the case of 13 moments the results are in perfect agreement with the kinetic closure procedure proposed by Grad [8] (see [9], [7]).

We restrict our attention to the Grad equations only in the one-dimensional

case

$$\left\{ \begin{array}{l} \dot{\rho} + \rho v_x = 0 \\ \rho \dot{v} + (p - \sigma)_x = 0 \\ \rho \dot{\varepsilon} + q_x + (p - \sigma)v_x = 0 \\ \underline{\tau_\sigma \left[ \dot{\sigma} - \frac{8}{15} q_x + \frac{7}{3} \sigma v_x \right] - \frac{4}{3} \mu v_x = -\sigma} \\ \underline{\tau_q \left[ \dot{q} + \frac{16}{5} q v_x - \frac{7}{2} \left( \frac{p}{\rho} \right)_x \sigma - \frac{1}{\rho} (p + \sigma) \sigma_x + \frac{\sigma}{\rho} p_x \right] + \chi T_x = -q,} \end{array} \right. \quad (3)$$

here the dot indicate the material derivative.

We note that together with the conservation of mass, momentum and energy, we have two new balance laws that govern the behaviour of the extended fields  $\sigma$  and  $q$ . When the underlined terms in (3) are negligible the last two equations reduce to the Navier-Stokes, Fourier equations respectively. In particular this limit can be done using the so called *Maxwellian iteration* [10].

## 2.1 Maxwellian Iteration

To reveal the relation between extended and classical model, a formal iterative scheme known as Maxwellian iteration is applied. The first iterates  $q^{(1)}$  and  $\sigma^{(1)}$  are calculated from the right-hand sides of balance laws by putting “zero<sup>th</sup>” iterates — equilibrium values  $q^{(0)} = 0$  and  $\sigma^{(0)} = 0$  on the left-hand sides. In the next step second iterates  $q^{(2)}$  and  $\sigma^{(2)}$  are obtained from the right-hand sides of the same Eqs. by putting first  $q^{(1)}$  and  $\sigma^{(1)}$  on their left-hand sides, and so on. Therefore the Maxwellian iterations is substantially an identification of a relaxation time and a formal power expansion of the solution in terms of it: a sort of Chapman - Enskog procedure at macroscopic level. *Therefore the Fourier and Navier Stokes equations are the first approximation of Maxwellian iteration of the ET balance law system and therefore they are not true constitutive equations and do not need to satisfy the frame indifference principle.*

We observe that this is true not only for rarefied gas but also for real gas as was proved recently in [11].

## 3 The Mixture theory

A similar situation occurs in the case of a mixture of fluids for what concerns the Fick law for the diffusion. Let consider a mixture of  $n$  species and for any

constituents  $\alpha = 1, 2, \dots, n$  we can define the concentration as:

$$c_\alpha = \frac{\rho_\alpha}{\rho}, \quad \rho = \sum_{\alpha=1}^n \rho_\alpha, \quad \left( \sum_{\alpha=1}^n c_\alpha = 1 \right).$$

There are two possible approach to the mixture. A classical approach and an Extended ones.

In the extended framework the description of simple homogeneous mixtures in the context of rational thermodynamics relies on the postulate that each constituent obeys the same balance laws as a single fluid [12]. They express rates of change of mass, momentum and energy with appropriate production terms due to mutual interaction of constituents. In particular the differential system is formed by the conservation laws of mass, momentum and energy of the mixture (as a whole):

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) &= 0; \\ \frac{\partial(\rho \mathbf{v})}{\partial t} + \operatorname{div}(\rho \mathbf{v} \otimes \mathbf{v} - \mathbf{t}) &= \mathbf{0}; \\ \frac{\partial(\frac{1}{2}\rho v^2 + \rho \varepsilon)}{\partial t} + \operatorname{div} \left\{ \left( \frac{1}{2}\rho v^2 + \rho \varepsilon \right) \mathbf{v} - \mathbf{t} \mathbf{v} + \mathbf{q} \right\} &= 0. \end{aligned} \quad (4)$$

and the balance laws for the first  $n - 1$  constituents ( $b = 1, 2, \dots, n - 1$ ) for mass, momentum and energy:

$$\begin{aligned} \frac{\partial \rho_b}{\partial t} + \operatorname{div}(\rho_b \mathbf{v}_b) &= \tau_b; \\ \frac{\partial(\rho_b \mathbf{v}_b)}{\partial t} + \operatorname{div}(\rho_b \mathbf{v}_b \otimes \mathbf{v}_b - \mathbf{t}_b) &= \mathbf{m}_b; \quad (b = 1, \dots, n - 1); \\ \frac{\partial(\frac{1}{2}\rho_b v_b^2 + \rho_b \varepsilon_b)}{\partial t} + \operatorname{div} \left\{ \left( \frac{1}{2}\rho_b v_b^2 + \rho_b \varepsilon_b \right) \mathbf{v}_b - \mathbf{t}_b \mathbf{v}_b + \mathbf{q}_b \right\} &= e_b \end{aligned} \quad (5)$$

The unknown fields of the system (4), (5) are

$$\mathbf{u} \equiv (\rho_\alpha, \mathbf{v}_\alpha, T_\alpha)^T, \quad \text{or} \quad \mathbf{u} \equiv (\rho, c_b, \mathbf{v}, \mathbf{v}_b, T, T_b)^T$$

( $\alpha = 1, 2, \dots, n$ ;  $b = 1, 2, \dots, n - 1$ ), where  $T$  is an appropriate average temperature [14], [13].

### 3.1 Maxwellian Iteration for the Mixture

We observe that in the classical theory of mixture are omitted the last two blocks of equations (5)<sub>2,3</sub> and the field is simple

$$\mathbf{u} \equiv (\rho, c_b, \mathbf{v}, T)^T; \quad (b = 1, 2, \dots, n - 1).$$

The question is which is the classical counterpart of (5)<sub>2,3</sub>?

*It is extremely interesting to observe that applying the Maxwellian iteration scheme to the momentum equation of single constituents (5)<sub>2</sub> after some simple manipulations we obtain the Fick law (2)<sub>3</sub> [7], [13].*

*While we have also as limit of energy balances of each constituents (5)<sub>3</sub> a new non local “constitutive equation” for the temperature differences similar to the Fick laws that is not present in literature [13], [14]:*

$$\Theta_a = T_a - T = - \sum_{b=1}^{n-1} M_{ab} r_b \operatorname{div} \mathbf{v}, \quad (6)$$

where  $M_{ab}$  is a definite positive phenomenological matrix and  $r_b$  for perfect gases

$$r_b = \rho_b c_V^{(b)} (\gamma_b - \gamma_n).$$

The  $\gamma_b$  and  $c_V^{(b)}$  are respectively the ratio of specific heat and the specific heat at constant volume of each constituents. Eq. (6) is not obtained in classical theory and it is interesting to observe that maybe this is due to the fact that if the gas have constituents with the same degree of freedom, i.e. the same  $\gamma$ , then  $r_b \equiv 0$  and all the temperatures are equal in the first Maxwellian iteration. In this last case to reveal difference of the temperature between constituents need to go further to the second order in the Maxwellian iteration and this was done in a recent paper by Ruggeri and Simić [15].

### 3.2 Darcy Law in porous media

Another simple example in the context of mixture theory is that famous Darcy’s equation for porous media in which the relative velocity between the fluid part  $\mathbf{v}_F$  and the solid ones  $\mathbf{v}_S$  is proportional to the pressure gradient of fluid (see, e.g. [16]):

$$\operatorname{grad} p_F = - \frac{k}{\mu} (\mathbf{v}_S - \mathbf{v}_F), \quad (7)$$

where  $k$  and  $\mu$  are respectively the permeability and the viscosity.

*It is well know that Darcy’s law is in reality an approximation to the balance of linear momentum for the fluid that is flowing through the porous solid which is treated as a rigid body, i.e. (7) is a limit case of (see [17]):*

$$\rho_F \dot{\mathbf{v}}_F + \operatorname{grad} p_F = - \frac{k}{\mu} (\mathbf{v}_S - \mathbf{v}_F).$$

## 4 Maxwellian iteration and Entropy Principle

We have seen that using the Maxwellian iteration we can obtain by Extended Thermodynamics- at least formally - the usual non-local constitutive equations of classical theory. Therefore the parabolic systems of classical theories appears, from physical point of view, approximations of hyperbolic systems when some relaxation times are negligible:

- Fourier and Navier Stokes as limit case of moments equations of Extended Thermodynamics;
- Fick law as limit case of momentum equations of each species in mixture with single-temperature;
- The new diffusion equation for difference of temperatures in mixture with multi-temperature as limit case of energy balance of each constituents.
- The Darcy law for porous material is a limit case of momentum equation.

Nevertheless also if the previous non-local equations are not constitutive equations but approximations of balance laws the non-local equations are very useful approximations. In many applications the relaxation times are negligible and they are relevant only in limiting situations: rarefied gas, low temperature, high frequencies, etc. Another advantage of the non-local approximation is that in this limit we are able to measure non-observable quantities like heat flux, viscosity stress and in particular the velocities and the temperature of each species in a mixture of fluids.

Clearly a major open problem in this framework is the rigorous proof of the convergence of the solutions via Maxwellian iterations. To make a little step toward this important result we have first of all to focus our attention to another very subtle point: is the entropy principle preserved in the Maxwellian iteration scheme? In other words: if the “full” hyperbolic theory satisfies the entropy inequality are we sure that the corresponding parabolic limit satisfies automatically a suitable entropy inequality?

We want to prove that the answer is affirmative provided that we have to assume the convexity of entropy also the requirement that the processes are not far from equilibrium.

At it is well know a system of balance laws (1) endowed with a supplementary entropy law:

$$\partial_t h^0 + \partial_{x_i} h^i = \Sigma \leq 0$$

with a convex entropy density  $h^0$  respect the densities field  $\mathbf{u} \equiv \mathbf{F}^0$ , can be put in symmetric form choosing the *main field*  $\mathbf{u}' = \partial h^0 / \partial \mathbf{u}$ . In fact, Boillat in

the context of classical approach [18] and Ruggeri and Strumia in a covariant formulation [19] proved that there exists four potentials

$$h'^{\alpha} = \mathbf{u}' \cdot \mathbf{F}^{\alpha} - h^{\alpha}, \quad \alpha = 0, 1, 2, 3$$

such that

$$\mathbf{F}^{\alpha} = \frac{\partial h'^{\alpha}}{\partial \mathbf{u}'}; \quad \Sigma = \mathbf{u}' \cdot \mathbf{f}.$$

Inserting into (1), the original system becomes symmetric with hessian matrices (note that  $h'^0$  is the Legendre transform of  $h^0$  and therefore convex function of the dual field  $\mathbf{u}'$ ). If we split the system in a block of conservation equations and another of balance laws and in correspondence we split  $\mathbf{u}' \equiv (\mathbf{v}', \mathbf{w}')$  it was proved in [20] that the equilibrium manifold in the main field components is the hyperplane  $\mathbf{w}' = 0$ . Therefore if we assume that the process are not far from equilibrium we can assume without loss of generality that

$$h'^0 = \frac{1}{2} |\mathbf{w}'|^2 + h'_{eq}(\mathbf{v}')$$

and therefore omitting now the prime in the main field, the symmetric system in one-space dimension assume the form:

$$\mathbf{H} \partial_t \mathbf{v} + \mathbf{A} \partial_x \mathbf{v} + \mathbf{B} \partial_x \mathbf{w} = \mathbf{0} \quad (8)$$

$$\partial_t \mathbf{w} + \mathbf{B}^T \partial_x \mathbf{v} + \mathbf{C} \partial_x \mathbf{w} = -\mathbf{L} \mathbf{w} \quad (9)$$

where  $\mathbf{v} \in \mathbf{R}^n$ ,  $\mathbf{w} \in \mathbf{R}^m$ ,  $\mathbf{H} \equiv \mathbf{H}(\mathbf{v})$  ( $m \times m$ )  $\in Sym^+$  (symmetric definite positive matrix),  $\mathbf{A} \equiv \mathbf{A}(\mathbf{v}, \mathbf{w})$  ( $m \times m$ )  $\in Sym$ ,  $\mathbf{C} \equiv \mathbf{C}(\mathbf{v}, \mathbf{w})$  ( $n \times n$ )  $\in Sym$  (symmetric matrices) and  $\mathbf{L} \equiv \mathbf{L}(\mathbf{v})$  ( $n \times n$ )  $\in Sym^+$  for the residual inequality because  $\Sigma = -\mathbf{w}^T \cdot \mathbf{L} \mathbf{w} \leq 0$ . Putting  $\mathbf{w} = 0$  into (9) we have

$$\bar{\mathbf{B}}^T \partial_x \mathbf{v} = -\mathbf{L} \mathbf{w}$$

where  $\bar{\mathbf{B}} \equiv \mathbf{B}(\mathbf{v}, \mathbf{0})$ . Then substituting into (8) we obtain as first Maxwellian iteration:

$$\mathbf{H} \partial_t \mathbf{v} \simeq \mathbf{D} \partial_{xx} \mathbf{v}$$

where the diffusion matrix  $\mathbf{D} = \bar{\mathbf{B}} \mathbf{L}^{-1} \bar{\mathbf{B}}^T \in Sym^+$ . As consequence the entropy principle is preserved in the passage between the hyperbolic system and the parabolic limit.

## 5 The Mathematical Situation

From mathematical point of view seem on the contrary that hyperbolic systems are particular case of parabolic ones. The prototype is Burgers equation



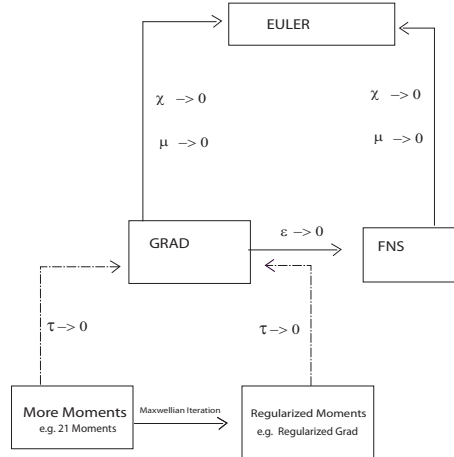


Figure 1. Systems and Sub-Systems and parabolic limit.

with artificial viscosity to restore uniqueness of weak solutions:

$$u_t + uu_x = \mu u_{xx}.$$

Moreover roughly speaking parabolic equations seem from mathematical point more realistic because usual exists regular solutions at the contrary of hyperbolic one for which soon regular solutions become shock or blow up.

I want now to convince that this is not completely true also from mathematical point of view. The first question is in reality in my opinion a misunderstanding due to the confusion between systems and sub-systems. I want to explain this with the simple example of Grad system (3). We have to recall that the relaxation times  $\tau_\sigma, \tau_q$  are proportional to the viscosity and heat conductivity respectively [7]:

$$\tau_\sigma \propto \varepsilon\mu; \quad \tau_q \propto \varepsilon\chi,$$

where  $\varepsilon$  is related to the Knudsen number. If we look the Fig. 1 and (3) we can see that effectively the Euler fluid sub-system is a particular case of the Navier and Fourier system when  $\mu$  and  $\chi$  vanishing. Nevertheless also Euler is a sub-system of Grad system and moreover the Navier-Stokes-Fourier is a particular case of the Grad system when  $\varepsilon$  tends to zero. Therefore the confusing point in literature is that the Euler system is a particular sub-system of both Navier-Stokes-Fourier and Grad system. This situation is also valid if we take an ET with many moments. When we apply the Maxwellian iteration we have as

parabolic counterpart the so called regularized moments [21]. In any case given a  $n$ -moment system all the previous moments are principal sub-systems according the general mathematical *nesting structure* find by Boillat and Ruggeri [22]. Moreover all the parabolic limit are also to be considered as approximations of the hyperbolic system as sketched in Fig.1.

### 5.1 Qualitative Analysis

On the other hand also the question that parabolic systems can have smooth solutions in contrast with hyperbolic systems is also not true because all the ET examples are hyperbolic system with dissipation. It is well known that system of balance law endowed with a convex entropy law, and dissipative, the so called Kawashima-Shizuta K-condition [23] becomes a sufficient condition for the existence of global smooth solutions provided the initial data are sufficiently smooth (Hanouzet and Natalini [24], Wen-An Yong [25], Bianchini, Hanouzet and Natalini [26], see also the Dafermos book [27]):

**Theorem 1** (Global Existence). *Assume that the system of balance laws is strictly dissipative and the K-condition is satisfied. Then there exists  $\delta > 0$ , such that, if  $\|\mathbf{u}(x, 0)\|_2 \leq \delta$ , there is a unique global smooth solution, which verifies*

$$\mathbf{u} \in \mathcal{C}^0([0, \infty); H^2(R)) \cap \mathcal{C}^1([0, \infty); H^1(R)) .$$

Moreover Ruggeri and Serre have proved in the one-dimensional case that the constant states are stable [28]:

**Theorem 2** (Stability of Constant State). *Under natural hypotheses of strongly convex entropy, strict dissipativeness, genuine coupling and “zero mass” initial for the perturbation of the equilibrium variables, the constant solution stabilizes*

$$\|\mathbf{u}(t)\|_2 = O(t^{-1/2}) .$$

Recently Lou and Ruggeri [29] have observed that the weaker K-condition in which we require the K-condition only for the right eigenvectors corresponding to genuine non linear is a necessary (but not sufficient) condition for the global existence of smooth solutions. This is the case of ET in classical [30] and in relativity [31], [32] and in the case of mixture with multi-temperatures [33].

## 6 Conclusions

In conclusion Extended Thermodynamics seems to indicate in clear manner that non local relations are not constitutive equations but approximations of balance laws. The true constitutive equations are in local form and they obey

the material frame difference. The physical systems are hyperbolic in agreement with relativity principle that any disturbance propagate with finite speed. Nevertheless the usual Fourier, Navier-Stokes, Fick, Darcy and others non local equations are useful to measure non-observable quantities and they are good approximation in many practical problems. The Maxwellian iteration preserve the Entropy principle at least for processes not far from equilibrium. Hyperbolic systems with dissipation (balance laws with production terms) can have global smooth solutions provide the initial data are small.

For more details of this talk see [34].

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