Analysis of the microscopic-macroscopic structure in real fluid flow

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Abstract: *This paper presents new results concerning the physical coexistence of the molecular chaos and the continuous determinism in real fluid flows. By using the FLUONS mathematical devices [1], the authors investigate the existence of a physical process called MOLECULAR COHERENCE. This particular kind of structure equilibrium needs the fulfilment of the conditions required by the increasing entropy and the minimum of the kinetical as well as the informational energy. Qualitative and quantitative results concerning the fluctuations in real fluid flows support this new point of view in Fluid Mechanics.*

Key Words: *integro-differential formulation, entropy, fluctuations, molecular coherence, fluons.*

1. INTRODUCTION

As it was shown in our previous papers [1], [2], the coordinate transformation and the FLUON expression reveal interesting aspects of the fluctuations associated to a given mean velocity distribution. We continue to exploit the mathematical properties of these FLUONS in a much profound sense, namely the coexistence of the physical molecular chaos and the determinism of the continuous fluid flows.

Essentially, let's consider the $f(\eta)$ normalized distribution ($0 \le f \le 1, 0 \le \eta \le 1$) as an order zero FLUON expression, indicated by the notation $F^{(0)}(\eta)$.

For the various order of FLUONS expressions, namely $F^{(k)}(\eta)$, where $k = 0,1,2,\dots,N$, we get the algorithm:

$$F^{(k)}(\eta) = \frac{\int_0^\eta \eta \cdot F^{(k-1)}(\eta)\, d\eta - \eta \left[\int_0^1 F^{(k-1)}(\eta)\, d\eta - \int_0^\eta F^{(k-1)}(\eta)\, d\eta \right]}{\int_0^1 \eta \cdot F^{(k-1)}(\eta)\, d\eta} \tag{1}$$

In the figure 1 (a, b, c) we show some examples of various $F^{(0)}(\eta)$ discrete and continuous distributions leading to about the same $F^{(1)}(\eta), F^{(2)}(\eta)$, $F^{(3)}(\eta)$ distributions.

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This very interesting feature of the expressions $F^{(0)}, F^{(1)}, F^{(2)}, \ldots$ concerning the tendency towards typical $F^{(k>2)} \sim \eta(2-\eta)$ distribution in spite of the great variety of the continuous or discrete $f = F^{(0)}$ distributions needs a complete and correct mathematical treatment. This remains, however, beyond the aims of the present paper.

Physically, the linear combination of the integrals $\int_0^{\eta} \eta^m f \, d\eta$ and of the constants $\int_0^{1} \eta^m f \, d\eta$ involved in the $F^{(k)}$ distributions leading to about the same distribution $\left(F^{(k+1)} - F^{(k)} \cong 0\right)$ raises a lot of questions.

Firstly, the very ordered or very disordered macroscopic boundary conditions imposed to real flows with undisturbed pressure, temperature, density and viscosity, but with eventually various degrees of wall roughness or impurities require the fulfillment of the entropy principle (i.e. the Boltzmann law) for a given system. This condition – a given system – is very important, because it needs a definite amount of macroscopic energy which ensures the normalization of $0 \le F^{(k)}(\eta) \le 1$ and of $0 \le \eta \le 1$. Let's mention, in this respect, the turbulent spot and the biological cell.

Secondly, the equilibrium structure of this given system requires a permanent connection from $F^{(0)}$ towards $F^{(k>1)}$ as well as, inversely, from $F^{(k>1)}$ towards $F^{(0)}$. In both cases the entropy principle is not violated and we can assume that the molecular organization is perturbed as structure involving a molecular coherence.

Thirdly, this molecular coherence needs some energy for the interconnections at the microscopic scale. We call this kind of energy information energy and, naturally, this kind of energy tends towards a minimum. The paper presents some considerations about $F^{(k)}(\eta)$ leading to such minimum. The structure stability around this minimum explains the existence of macroscopic fluctuations. We mention also the algorithmic character of the $F^{(k)}(\eta)$ succession which facilitates the implementation in some microscopic structures, like in biological neuron activity.

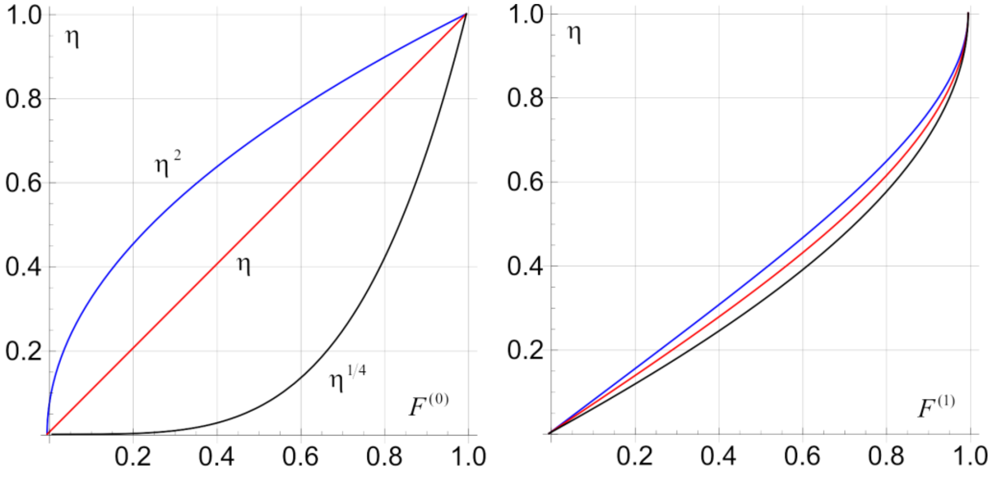


Figure 1a. $F^{(0)} \rightarrow F^{(1)}$ transformation for different η^m distributions.

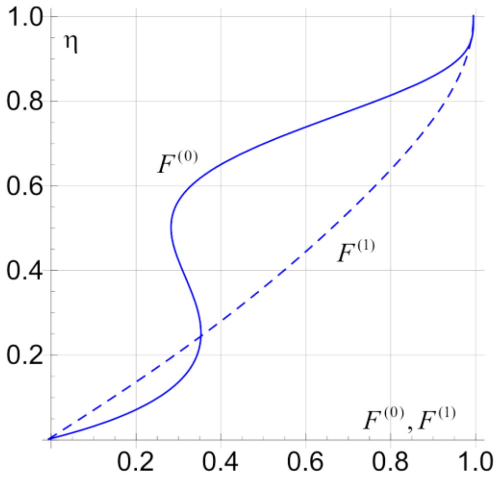


Figure 1b. $F^{(0)} = 1 - (1-\eta)^4 (1+2\eta^2)^6$

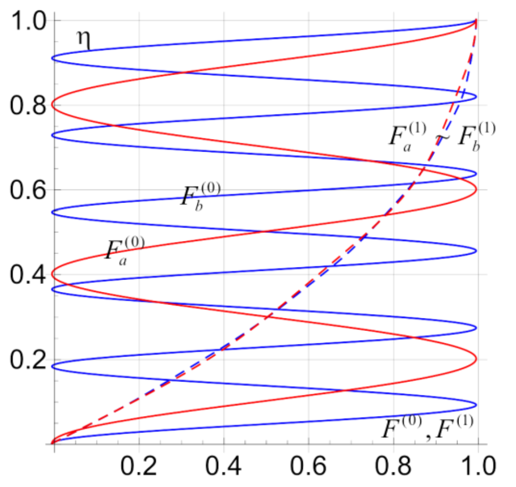


Figure 1c. $F^{(0)} = \sin^2\left(k \frac{\pi}{2}\eta\right)$, $k_a = 5$, $k_b = 11$

2. THE ANALYSIS OF THE COHERENCE PROCESS

In the introduction we point out the idea of the existence of a special kind of molecular organization at the micro-scale that we've called a coherence process. The physical motivation lies on the fulfillment of the Gibbs-Boltzmann entropy principle [3][4][5], usually conceived as a transition (order towards disorder) in a well-defined space-time domain. The classical example presents a usual object destroyed and transformed in a disordered mass of its fragments. However, let's consider a disorder ensemble of such objects which can be destroyed to form a macroscopic "ordered" mass of fragments. In order to respect the entropy principle, we have to consider this ensemble at a some microscopic scale, which really presents a very disordered mass of very small fragments. Therefore, the finite space-domain stands for an essential requirement of the entropy principle. In this respect, the molecular organization at a some microscopic scale becomes a physical condition for the existence of a permanent connection between the molecular chaos and the macroscopic deterministic degree of disorder.

Accordingly, the coordinate transformation and the integro-differential formulation (IDF) of the macroscopic conservation law [6][7] play a fundamental role when we analyze the fluctuations associated to a macroscopic deterministic distribution. Mathematically, when we have a normalized mean distribution $f(\eta)$ ($0 \le f \le 1, 0 \le \eta \le 1$), we have to associate the following expressions:

$$F^{(0)}(\eta) = f(\eta)$$

$$\eta_2(\eta) = \left(\int_0^\eta f^2\, d\eta\right) \Big/ \left(\int_0^1 f^2\, d\eta\right) \tag{2}$$

$$e(\eta) = f^*(\eta) - f(\eta),\ h(\eta) = \eta - \eta_2(\eta)$$

and the finite global quantity:

$$\varphi_{U,BL} = (1-Q_{1a})\frac{(Q_{2a}-Q_{4a})}{(Q_{2a}-Q_{3a})} - (1-Q_{2a}) \tag{3}$$

with:

$$Q_{ra} = \int_0^1 f^r \, d\eta \tag{4}$$

for the boundary-layer flow, as well as corresponding expressions $\varphi_{U,CN}$, $\varphi_{U,PIPE}$ for the channel and pipe flows.

The above expressions are involved in the calculation of the intensity and distribution of the fluctuations arising in the mentioned turbulent flows. The FLUON expression:

$$f^{\oplus}(\eta) \equiv F^{(1)}(\eta) = \frac{\int_0^{\eta} \eta \cdot f \, d\eta - \eta \cdot \left(\int_0^1 f \, d\eta - \int_0^{\eta} f \, d\eta \right)}{\int_0^1 \eta \cdot f \, d\eta} \tag{5}$$

as well as the $F^{(k)}(\eta)$, is now analyzed in order to explain the coupling between the microscopic molecular chaos and the macroscopic fluctuations irregularities (disorder). We will examine some macroscopic aspects of the turbulent and transitional flows, pointed out in experiments, but without any theoretical explanation.

First of all, let's examine the chaotic character of the turbulent fluctuations associated to a well-established mean velocity profile in boundary-layer, channel and pipe flows. We have to observe that the molecular chaos objectively exist, contrary to the so called fluctuations which are, more or less, subjectively defined quantities, depending on a lot of microscopic and macroscopic (Reynolds number etc.) conditions. The existence of a coherent molecular process is related, particularly, to the equilibrium turbulent flow. In this respect, let's examine the first order FLUON given as a difference between two FLUON expressions:

$$\Delta = F^{(1)}(f^*) - F^{(1)}(f) = \eta(1-\eta) \cdot K(f, f^*) \tag{6}$$

where f^* is the transferred distribution of f by means of the integral:

$$\eta_r = \frac{\int_0^{\eta} f^r d\eta}{\int_0^1 f^r d\eta} \tag{7}$$

For instance, for $f = \eta^n$ we get $f = \eta_r^{\frac{n}{1+nr}}$ and $f^* = \eta^{n^*}$, where $n^* = \dfrac{n}{1+nr}$, leading to:

$$\Delta(n, r, \eta) = \eta(1-\eta) \cdot K(n, n^*, \eta) \tag{8}$$

where:

$$K(n,n^*,\eta) = \frac{n-n^*}{(1+n)(1+n^*)}\left[\frac{1-\eta^{1+n^*}}{1-\eta} - \frac{1+n^*}{n-n^*}\eta^{1+n^*}\frac{1-\eta^{n-n^*}}{1-\eta}\right] \tag{9}$$

We can observe that $\Delta(n,r,\eta)$ presents the invariant distribution $\eta(1-\eta)$.

Now we suppose that the macroscopic fluctuations are related to this Δ. In the figure 2 we show a possibility to achieve the micro-scale coherence by discrete change of η belonging always to Δ. It is a kind of coupling between the molecular chaos and the macroscopic fluctuations. We can write:

$$\eta_{k+1} = K_C \eta_k (1-\eta_k) \tag{10}$$

where

$$K_C = K\frac{U_e L}{v_m \lambda} \tag{11}$$

with U_e a typical macroscopic velocity, L a typical macroscopic length, v_m the mean molecular velocity, λ the mean molecular path.

The chaotic behavior of the η_k sequence depends on the conditions $K_C \geq 3.9$, what means $K\frac{U_e L}{v_m \lambda} \geq 3.9$ or $\mathrm{Re} \sim \frac{3.9}{K}$. However, $K(n,n^*,\eta)$ decreases drastically when $n-n^*$ is small or when the FLUON order increases. The discretization of the invariant expression $\eta(1-\eta)$ depends essentially on the coupling between the very small scale of the difference $\Delta(n,n^*,\eta) = \eta(1-\eta)\cdot K(n,n^*,\eta)$ and the discrete molecular motion (λ_m, v_m).

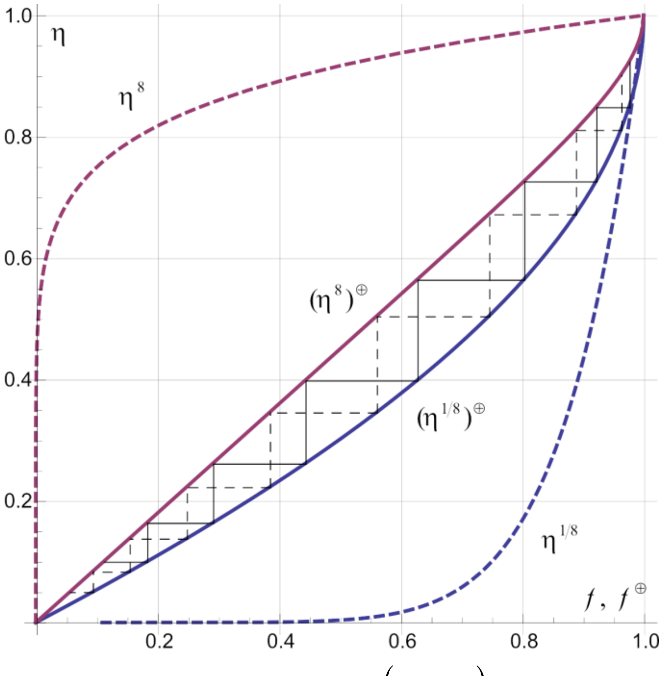
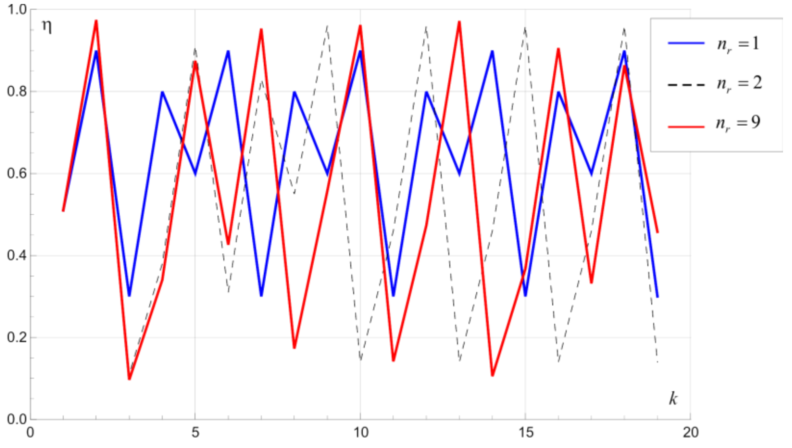


Figure 2. The covering of the $\Delta(n,n^*,\eta)$ difference

On the figure 2 we present (at an exaggerated step scale) the covering of Δ by various distances. These distances, limited by the f and its transform function f^* as macroscopic boundaries, are finally achieved by the molecular motions. At some microscopic scale, the covering of Δ becomes a discrete motion, realized by bonds from η_k to η_{k+1}. This coupling involves some kinetic energy, naturally supplied by the macroscopic flow characteristics (high Reynolds number, perturbations etc.).

Another kind of discretization lies on the following observation concerning the simple numerical expression $\eta_{k+1} = K \cdot \eta_k (1 - \eta_k)$, where $3.5 < K < 4$, in order to fulfill the $0 \le \eta \le 1$ condition. The chaotic character of the sequence $k = 0, 1, 2, \ldots$ can be pointed out only as a very small variation of the numerical values of η_k, what means that a great amount of information energy has to be stored in order to see the differences. When we restrict the value of η_k to the first or second order figures, we get a more regular sequence, which shows a fixed periodical variation. The table on the figure 3 stands for an example.



k	η_k		
	$n_r = 1$	$n_r = 2$	$n_r = 9$
1	0.51	0.51	0.51
2	0.9	0.97	0.97461
3	0.3	0.11	0.096507
4	0.8	0.38	0.340054
5	0.6	0.91	0.875227
6	0.9	0.31	0.425898
7	0.3	0.83	0.953585
8	0.8	0.55	0.172618
9	0.6	0.96	0.557001
10	0.9	0.14	0.962328
11	0.3	0.46	0.141385
12	0.8	0.96	0.473442
13	0.6	0.14	0.972249
14	0.9	0.46	0.105225
15	0.3	0.96	0.367195
16	0.8	0.14	0.906215
17	0.6	0.46	0.331459
18	0.9	0.96	0.864216
19	0.3	0.14	0.457653

Figure 3. Variation of $\eta_{k+1} = K \cdot \eta_k (1 - \eta_k)$, for $K = 0.9$, $\eta_{k=1} = 0.51$

At the molecular micro-scale the coherence process can be related to the tendency towards a periodic variation which needs a smaller quantity of energy by comparison to the chaotic variations. However, at the macro-scale level, the fluctuations seem to be chaotic and consequently the entropy principle is not violated.

In the normalized space-time ensemble $(0 \le \eta \le 1, 0 \le t_a \le 1)$ the general form concerning the microscopic-macroscopic coherence process could be:

$$\Delta(\eta, t_a) = O\left(\frac{\partial^p \Delta}{\partial t^p}, \frac{\partial^q \Delta}{\partial \eta^q}\right) \tag{12}$$

where $p, q \in N$ and Δ is given by (6). Previously we examined the most simple case, where the operator $O\left(\frac{\partial^p \Delta}{\partial t^p}, \frac{\partial^q \Delta}{\partial \eta^q}\right) \sim \eta_{k+1}$. The physical justification lies on the supposition that at the microscopic scale the discrete variation of Δ for a given η_k could be assumed to provide the next η_{k+1} in a sequence of bonds which ensures the covering of $\Delta(\eta)$. This kind of motion points out the importance of the $v^{/}$ fluctuations (normal to the main flow direction), because the $u^{/}$ fluctuations involve the influence of the macroscopic convection (along the main flow direction).

Another interesting application of this coherence process concerns the evaluation of the quantity $\int_0^1 \overline{u^{/}v^{/}} / U_e^2 \, d\eta$ for the same normalized space-time ensemble (boundary layer, channel or pipe flows). By reference to figure 4 we can write the relation:

$$\int_0^1 \frac{\left|\overline{u^{/}v^{/}}\right|}{U_e^2} d\eta_0 \sim \frac{1}{2^3} \int_0^1 \frac{\overline{\left(u^{/}\right)^2} + \overline{\left(v^{/}\right)^2}}{U_e^2} d\eta_0 \qquad (13)$$

which is confirmed by the above mentioned flows experimental results.

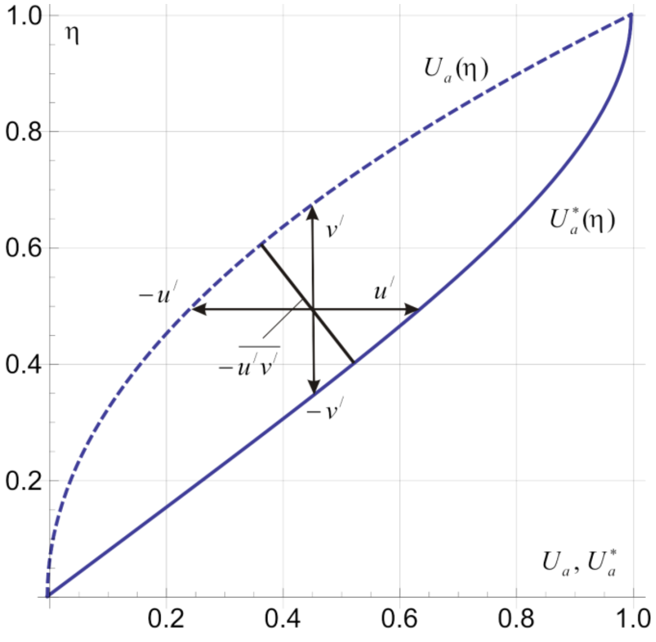


Figure 4. Turbulent fluctuations between U_a and U_a^*

3. CONCLUSIONS

The main conclusion of this paper concerns the existence of a physical coherence process in the domain of molecular chaos-deterministic macro-scale real flows.

This coherence process explains various qualitative and quantitative aspects of the fluctuations field associated to a mean velocity distribution normal to the flow direction. The mathematical expression of this coherence process is based on the FLUON essential properties to drastically reduce the great values of the various differences between $U_a(\eta_0)$ and its associated distribution $U_a^*(\eta_0)$, when we use the relation:

$$\Delta\left(U_a, U_a^*\right) = \eta_0\left[\frac{\int_0^1 U_a^* d\eta_0}{\int_0^1 \eta_0 U_a^* d\eta_0} - \frac{\int_0^1 U_a d\eta_0}{\int_0^1 \eta_0 U_a d\eta_0}\right] + \frac{\int_0^{\eta_0} \eta_0 U_a^* d\eta_0}{\int_0^1 \eta_0 U_a^* d\eta_0} - \frac{\int_0^{\eta_0} \eta_0 U_a d\eta_0}{\int_0^1 \eta_0 U_a d\eta_0} - \eta_0\left[\frac{\int_0^{\eta_0} U_a^* d\eta_0}{\int_0^1 U_a^* d\eta_0} - \frac{\int_0^{\eta_0} U_a d\eta_0}{\int_0^1 U_a d\eta_0}\right] \tag{14}$$

which involves the invariant $\eta_0\left(1-\eta_0\right)$, a source of chaos at a very small scale of molecular discrete bonds.

REFERENCES

[1] Şt. N. Săvulescu, Fl. Băltăreţu, H. Dumitrescu, The analysis of the process tending towards equilibrium in transitional and turbulent wall flows, *INCAS Bulletin*, Vol. **2**, No. 2, 2010.
[2] Şt. N. Săvulescu, Eine Beziehung zwischen der Energieverteilung der Grundströmung und entsprechenden Schwankungsgrößen in Grenzschichten, *Z.A.M.M.*, **52**, T418-423, 1972.
[3] F. Reif, *Statistical Physics*, McGraw-Hill, New York, 1967.
[4] K. Huang, *Statistical Mechanics*, 2nd Edition, John Wiley & Sons, New York, 1987.
[5] R. S. Ellis, The theory of large deviations: from Boltzmann's 1877 calculation to equilibrium macrostates in 2D turbulence, *Physica D: Nonlinear Phenomena*, Volume **133**, Issues 1–4, 10 September 1999, 106-136.
[6] Fl. Băltăreţu, Şt. N. Săvulescu, O formulare integro-diferenţială a ecuaţiilor Navier-Stokes cu proprietăţi remarcabile, *Conferinţa a IX-a "Eficienţă, confort, conservarea energiei şi protecţia mediului"*, Bucureşti, 2002.
[7] H. Dumitrescu, Comparative study of turbulence models for prediction of transitional boundary layer, *Rev. Roum. Sci. Tech. - Méc. Appl.*, Tome **43**, No. 3, 1998.