Noll's axioms and formulation of the closure relations for the subgrid turbulent tensor in Large Eddy Simulation

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Abstract: - In this paper, the relation between the Noll formulation of the principle of material frame indifference and the principle of turbulent frame indifference in large eddy simulation, is revised. The principle of material frame indifference and the principle of turbulent frame indifference proposed by Hutter and Joenk imposes that both constitutive equations and turbulent closure relations must respect both the requirement of form invariance, and the requirement of frame independence. In this paper, a new rule for the formalization of turbulent closure relations, is proposed. The generalized SGS turbulent stress tensor is related exclusively to the generalized SGS turbulent kinetic energy, which is calculated by means of its balance equation, and the modified Leonard tensor.

Key-Words: - Large eddy simulation, Noll's axioms, frame indifference, form invariance, frame dependence, turbulent closure relations

1 The formulation of the Principle of Material Frame Indifference and the Principle of Turbulent Frame Indifference

In the framework of ordinary fluid dynamics, the turbulence models could be interpreted as constitutive equations, which are necessary to close the equations of motion. The constitutive equations represent, in an idealized form, the behaviour of the materials and, consequently, they must fulfil the principle of material frame indifference [1].

In order to make explicit the relation between the Noll formulation of the principle of material frame indifference and the formulation of the turbulent closure relations, in this section: the Noll formulation of the principle of material frame indifference is shown; the confusion, produced by this formulation, is underlined (it does not emphasize the difference between Euclidean form invariance and frame independence of an equation); the distinction between Euclidean form invariance and frame independence of a constitutive equation or physical law is explained; the Hutter and Joenk [2] formulation of the principle of turbulent frame indifference, that is the equivalent in turbulence of the principle of material frame indifference, is expressed.

Considering an inertial frame, in which a material point has coordinate x_i at time t, and a non-inertial frame, in which the same point has coordinate x_i^* at time t^*, the most general law which governs the transformations of the coordinates and the time expressed in the two frames is that given by the Euclidean transformations

$$x_i = Q_{ij}(t)x_j^* + b_i(t) \qquad t = t^* + a \qquad (1)$$

where $Q_{ij}(t)$ are the components of a time-dependent proper orthogonal tensor, $b_i(t)$ is the time-dependent distance between the origins of the two frames and a is any constant.

It is common knowledge that tensors of rank n ($n = 0,1,2$) are said to be objective, if the components transform according to:

$$
\begin{aligned}
S &= S^* & \text{objective scalar} \\
V_i &= Q_{ij}V_j^* & \text{objective vector} \\
A_{ij} &= Q_{im}Q_{jn}A_{mn}^* & \text{objective tensor}
\end{aligned}
\qquad (2)
$$

A constitutive relation can be expressed in the form

$$T(\vec{\chi},t) = F(\vec{\chi}^t,t) \qquad (3)$$

where $\vec{\chi}^t$ is the history of the motion of the body B up to the time t and $T(\vec{x},t)$ is the stress tensor. The principle of material frame indifference is based on the consideration that the material properties must be independent of the choice of frame. In other words, this basic working principle of continuum mechanics requires the constitutive equations to be the same for observers in inertial systems and in

non-inertial ones. Since constitutive equations are designed to express idealized material properties, the Noll formulation of the principle of material frame indifference requires they shall be frame independent. That is, if the constitutive relation (2) is satisfied by the dynamic process $(\vec{\chi}, T)$, it is satisfied by every equivalent process $(\vec{\chi}^*, T^*)$ that is represented in a non-inertial frame of reference. Formally, the constitutive mapping F in (2) must satisfy the identity

$$T(\vec{\chi}^*, t^*)^* = F\left(\vec{\chi}^{*t}, t^*\right) \qquad (4)$$

For all T^*, $\vec{\chi}^*$ and t^* that may be obtained from T, $\vec{\chi}$ and t by Euclidean transformations of the frame expressed by relations (1) and (2) [1]. The abovementioned Noll formulation of the principle of material frame indifference produces a confusion because it does not emphasize the difference between two distinct requirements on the constitutive equations: form invariance under Euclidean transformations of the frame; frame independence.

1) The requirement of Euclidean form invariance implies the formal expression of the constitutive equations in a non-inertial frame of reference be equal to the formal expression of the constitutive equation in an inertial frame of reference: that is, a constitutive equation is Euclidean form invariant if it does not modify its formal expression under Euclidean transformation of the frame and, consequently, it is constructed only with objective tensors. In other words, each observer uses the constitutive equations in the same functional form, but the quantities appearing in them may have different values due to the used frame, i.e., the values of the quantities appearing in them may be frame dependent.

2) The requirement of frame independence of a constitutive equation implies the values of the quantities, appearing in it, be independent of translational and angular velocity of the frame. It is possible to emphasize the difference between the Euclidean form invariance and the frame independence by underlining the existence of tensors that are objective but dependent on the translational and angular velocity of the frame.

For example, let W_{ij} and W_{ij}^* be, respectively, the representations, in an inertial and non-inertial frame, of the antisymmetric part of the velocity gradient. Let $W_{ij}^{\Omega*}$ be the representation, in a non-inertial frame, of the absolute vorticity tensor, given by the following expression:

$$W_{ij}^{\Omega*} = W_{ij}^* + Q_{ki}Q_{kj} \qquad (5)$$

The law of transformation between the representations of this tensor in the different frames of reference is given by:

$$W_{ij}^{\Omega*} = Q_{im}Q_{jn}W_{mn}^{\Omega*} \qquad (6)$$

The absolute vorticity tensor W_{ij}^{Ω} is an objective tensor, since its representations in the different frames transform according to equation (2), but is frame dependent since its representations depend on the frame by means of the term $Q_{km}\dot{Q}_{kn}$, associated with the angular velocity of the non-inertial frame [2-3].

A constitutive equation, or a physical law, in order to be form invariant under the most general class of transformations of the frame (Euclidean transformations), must be expressed in terms of objective tensors. A constitutive equation, or a physical law, is able to fulfil the principle of material frame indifference if: it is form invariant (under Euclidean transformation of the frame); it is frame independent, i.e. it is expressed exclusively in terms of objective tensors that are independent of the translational and angular velocity of the frame.

The principle of turbulent frame indifference [2] is the equivalent in turbulence of the principle of material frame indifference. The principle of turbulent frame indifference imposes that turbulent closure relation: must be form invariant (or rather, must be expressed in terms of objective tensors); must be frame independent (or rather, must be expressed in terms of objective tensors that are independent of the angular and translational velocity of the frame).

2 Turbulent Balance Equations in Large Eddy Simulation

It must be emphasized that Euclidean form invariance and frame independence are two distinct matters.

The generalised SGS turbulent stress tensor is expressed by the equation

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j \qquad (7)$$

where u_i is the $i - th$ component of the instantaneous velocity and the overbar represents the application of spatial filter.

Following the procedure shown in [4], in order to show the characteristic of the generalised SGS turbulent stress tensor and in order to define the

modalities of formulation of the turbulent closure relations, later on we present:

- the objectivity and the frame independence of the abovementioned tensor;
- the Euclidean form invariance and frame dependence of the generalised SGS turbulent stress tensor transport equation;
- the Euclidean form invariance and frame independence of the generalised SGS turbulent kinetic energy transport equation.

2.1 The generalized SGS turbulent stress tensor

The time derivative of (1) gives

$$u_i = Q_{ij}(t)\, u_j^* + \dot{Q}_{ij}(t)x_j^* + \dot{b}_i(t) \tag{8}$$

Applying a spatial filter to (8) gives

$$\bar{u}_i = Q_{ij}(t)\, \bar{u}_j^* + \dot{Q}_{lJ}(t)x_j^* + \dot{b}_i(t) \tag{9}$$

By introducing (8) and (9) into (7), the relation between the expressions of the generalised SGS turbulent stress tensor in two Euclidean frames is obtained,

$$\tau_{ij} = Q_{il}Q_{jm}\left(\overline{u_l^* u_m^*} - \bar{u}_l^* \bar{u}_m^*\right) = Q_{il}Q_{jm}\tau_{lm}^* \tag{10}$$

Equation (10) shows that the generalised SGS turbulent stress tensor is objective and frame independent. Consequently, all of the turbulent closure relations for the generalised SGS turbulent stress tensor must be: form invariant under Euclidean transformations of the frame; independent of the translational and angular velocity of the frame.

2.2 Transport equation of the generalised SGS turbulent stress tensor

The transport equation of the generalized SGS turbulent stress tensor is:

$$\frac{D\tau(u_k, u_l)}{Dt} = -\frac{\partial \tau(u_k, u_l, u_p)}{\partial x_p} - \tau\left(u_p, u_k\right)\frac{\partial \bar{u}_l}{\partial x_p} - \tau\left(u_p, u_l\right)\frac{\partial \bar{u}_k}{\partial x_p} - \tau\left(u_k, \frac{\partial p}{\partial x_l}\right) - \tau\left(u_l, \frac{\partial p}{\partial x_k}\right) + \nu\tau\left(u_k, \frac{\partial^2 u_l}{\partial x_p \partial x_p}\right) + \nu\tau(u_l, \frac{\partial^2 u_k}{\partial x_p \partial x_p}) \tag{11}$$

The symbols $\tau(f; g)$ and $\tau(f; g; h)$ represent the generalized second and third-order central moments [5] related to the generic quantities f, g and h.

By following the procedure shown in [4], by introducing (1), (8), (9) and (10) in (11), the representation in a non-inertial frame of the

generalized SGS turbulent stress tensor transport equation is:

$$Q_{km}Q_{ln}\left[\frac{D\tau(u_m^*, u_n^*)}{Dt*} + Q_{rn}\dot{Q}_{rp}\tau(u_p^*, u_m^*) + Q_{rm}\dot{Q}_{rp}\tau(u_p^*, u_n^*)\right] =$$
$$Q_{km}Q_{ln}\left[-\frac{\partial \tau(u_p^*, u_m^*, u_n^*)}{\partial x^*_p} - \tau(u_p^*, u_m^*)\frac{\partial \bar{u}^*_n}{\partial x_p^*} - Q_{rn}\dot{Q}_{rp}\tau(u_p^*, u_m^*) - \tau(u_p^*, u_n^*)\frac{\partial \bar{u}^*_m}{\partial x_p^*} - Q_{rm}\dot{Q}_{rp}\tau(u_p^*, u_n^*) - \tau\left(u_m^*, \frac{\partial^* p}{\partial x_n}\right) - \tau\left(u_n^*, \frac{\partial^* p}{\partial x_n}\right) + \nu^*\tau\left(u_m^*, \frac{\partial^2 u_n^*}{\partial x_p^* \partial x_p^*}\right) + \nu^*\tau(u_n^*, \frac{\partial^2 u_m^*}{\partial x_p^* \partial x_p^*})\right] \tag{12}$$

By using the expression $W_{ij}^{\Omega*}$ of the absolute vorticity tensor defined in (6) and the objective time derivative introduced by Weis and Hutter [3], equation (12) reads

$$\frac{\tilde{D}\tau(u_m^*, u_n^*)}{Dt^*} = -\frac{\partial \tau(u_p^*, u_m^*, u_n^*)}{\partial x_p^*} - \tau(u_m^*, u_p^*)(\bar{S}_{pn}^* - \bar{W}_{pn}^{*\Omega}) - \tau(u_p^*, u_n^*)(\bar{S}_{mp}^* - \bar{W}_{mp}^{*\Omega}) - \tau\left(u_m^*, \frac{\partial p^*}{\partial x_n}\right) - \tau\left(u_n^*, \frac{\partial p^*}{\partial x_n}\right) + \nu^*\tau\left(u_m^*, \frac{\partial^2 u_n^*}{\partial x_p^* \partial x_p^*}\right) + \nu^*\tau(u_n^*, \frac{\partial^2 u_m^*}{\partial x_p^* \partial x_p^*}) \tag{13}$$

Since the absolute vorticity tensor $W_{ij}^{\Omega*}$ and the time derivative $\tilde{D}\tau(u_m^*, u_n^*)/Dt^*$ are both objective tensors, equation (13) is expressed exclusively in terms of objective tensors.

From this consideration and for the assumption that an equation is form invariant if it is expressed only in terms of objective tensors, it results that the transport equation of the generalised SGS turbulent stress tensor is form invariant under a Euclidean transformation of the frame but remains frame dependent through the apparition of $W_{ij}^{\Omega*}$.

From the previous considerations, it can be deduced that the principle of turbulent frame indifference proposed by Hutter and Joenk [2] couldn't be applied to the transport equation of the generalized SGS turbulent stress tensor.

2.3 Transport equation of the generalised SGS turbulent kinetic energy

The generalized SGS turbulent kinetic energy E is defined as half the trace of the SGS turbulent stress tensor and is, as can be easily demonstrated, an objective scalar. The generalized SGS turbulent kinetic energy transport equation is [4]:

$$\frac{1}{2}\frac{D\tau(u_k,u_k)}{Dt} = -\frac{1}{2}\frac{\partial\tau(u_k,u_k,u_p)}{\partial x_p} -$$
$$\tau(u_m,u_k)\frac{\partial\bar{u}_k}{\partial x_m} - \tau\left(u_k,\frac{\partial p}{\partial x_k}\right) + \quad (14)$$
$$\nu\tau\left(u_k,\frac{\partial^2 u_k}{\partial x_p \partial x_p}\right)$$

which is equal to

$$\frac{DE}{Dt} = -\frac{1}{2}\frac{\partial\tau(u_k,u_k,u_m)}{\partial x_m} - \tau(u_m,u_k)\frac{\partial\bar{u}_k}{\partial x_m} -$$
$$\frac{\partial\tau(p,u_m)}{\partial x_m} + \nu\frac{\partial^2 E}{\partial x_m \partial x_m} - \nu\tau\left(\frac{\partial u_k}{\partial x_m},\frac{\partial u_k}{\partial x_m}\right) \quad (15)$$

By introducing (1), (8), (9) and (10) in (15), the representation in a non-inertial frame of the generalized SGS turbulent kinetic energy transport equation is:

$$\frac{DE^*}{Dt^*} = -\frac{1}{2}\frac{\partial\tau(u_m^*,u_m^*,u_p^*)}{\partial x_p^*} - \tau\left(u_p^*,u_m^*\right)\frac{\partial\bar{u}^* m}{\partial x_p^*} -$$
$$\frac{\partial\tau(p^*,u_k^*)}{\partial x_k^*} + \nu^*\frac{\partial^2 E^*}{\partial x_p^* \partial x_p^*} - \nu^*\tau\left(\frac{\partial u_p^*}{\partial u_n^*},\frac{\partial u_p^*}{\partial u_n^*}\right) \quad (16)$$

From the comparison between equations (15) and (16), it can be deduced that the transport equation of the generalized SGS turbulent kinetic energy is form invariant and frame independent, in so much that each of the terms that appear in it are representations, in inertial and non-inertial frames, of objective tensors that are independent of the angular and translational velocity of the frame.

3 A New Rule of Turbulent Closure Relations

In the previous section, the Euclidean form invariance and the frame dependence of the generalised SGS turbulent stress tensor transport equation, has been demonstrated. Many authors repute that all of the turbulent closure relations must fulfil the principle of turbulent frame indifference in the formulation proposed by Hutter and Joenk [2]. A contradiction arises from the abovementioned imposition: the generalised SGS turbulent stress tensor transport equation could not be used in the turbulent closure relations, since it doesn't fulfil the principle of turbulent frame indifference. Must all of the turbulent closure relations fulfil the principle of turbulent frame indifference? In other words, if $y = c(x)$ is a turbulent closure relation, does this relation have to be frame independent? No, it does not need to.

It is usually assumed that material laws do not depend on the rotation of the system. This means that in every system the material should show the same behaviour. This is quite a good assumption as

long as the relaxation time of the material is large compared with the typical time scale of the flow.

The turbulent phenomena are not associated to the properties of the materials: consequently, turbulent closure relations do not represent the material behaviour. In such flows the characteristic turbulent time scale can be comparable with the typical time scale of the flow, implying that the rotation of the system can influence the turbulent closure functionals. This means that objective tensors, which depend on the rotation of the reference frame, may enter such functional relations. Constitutive relations of any turbulence theory need not satisfy the principle of turbulent frame indifference.

Turbulent closure relations must always be form invariant but must not necessarily be frame independent. In other words, not all the turbulent closure relations must fulfil the principle of turbulent frame indifference. A new rule of turbulent closure relations can be formulated:

"In a turbulent closure relation, the modelled expressions of an unknown objective tensor must be formulated in terms of objective tensors, allowing the closure relations to fulfil the requirement of Euclidean form invariance, and must retain the same dependence on the angular velocity of the frame of the unknown tensor".

4 Closure Relations

In depth-averaged motion equations models [6-7] and in models based on 3D Navier-Stokes equations [8-10], the turbulent stress tensor is related to the strain rate tensor, which is Reynolds-averaged. In the context of LES models, the generalized SGS turbulent stress tensor, τ_{ij}, is related to the resolved tensors. The generalised SGS turbulent stress tensor, τ_{ij}, can be split into three tensors:

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j = L_{ij}^m + C_{ij}^m + R_{ij}^m \quad (17)$$

where u_i is the i-th component of the instantaneous velocity, the overbar represents the application of the grid filtering operator, L_{ij}^m, C_{ij}^m and R_{ij}^m are the so-called modified Leonard tensor, the modified cross tensor and the modified Reynolds tensor, respectively; u_i' is the i-th component of the fluctuating velocity, $u_i' = u_i - \bar{u}_i$.

Starting from (17), by adopting the scale similarity assumption, by simple mathematical calculations, a closure relation is reached for the generalized SGS turbulent stress tensor, in which there are no coefficients to be calibrated or to be

calculated dynamically, and which is given by the following relation:

$$\tau_{ij} = 2E \frac{L_{ij}^m}{L_{kk}^m} \qquad (18)$$

where $E = \frac{\tau_{kk}}{2}$. See [4] for the details.

The generalised SGS turbulent stress tensor is related exclusively to the generalised SGS turbulent kinetic energy and the modified Leonard tensor that are, respectively, a zero order and a second order objective tensor that are independent of the translational and angular velocity of the frame. Consequently, the closure relation (18) for the generalised SGS turbulent stress tensor: takes into account the anisotropy of the turbulence; removes any balance assumption between the production and dissipation of SGS turbulent kinetic energy; does not use any closure coefficient calculated by means of a dynamic procedure; respects the new rule of turbulent closure relations, proposed in section 3.

The generalised turbulent kinetic energy E is calculated by solving its transport equation (15). The proposed modelled form of Equation (15) is:

$$\frac{DE}{Dt} = \frac{\partial}{\partial x_k}\left(D\sqrt{E}\,\bar{\Delta}\,\frac{\partial E}{\partial x_k}\right) - \left(\frac{2E}{L_{qq}^m}\right)L_{mk}^m\frac{\partial \bar{u}_k}{\partial x_m} + \\ \nu\frac{\partial^2 E}{\partial x_m \partial x_m} - \frac{C_* E^{3/2}}{\bar{\Delta}} \qquad (19)$$

where the 1st and 3rd terms on the right-hand side of the exact balance equation of E (15) are modelled by the 1st term of equation (19); the last term of the right-hand side of equation (15), which represents the viscous dissipation of the turbulent kinetic energy, is modelled by the last term on the right-hand side of equation (19); the values of the coefficients C_* and D are evaluated by means of a dynamic procedure.

5 Results and discussion

Turbulent channel flows (between two flat parallel plates placed at a distance of $2L$) are simulated with the model that uses the presented closure relation, hereinafter called TEM model, at friction-velocity-based Reynolds number Re^* equal to 2340. The numerical results obtained with the TEM model are compared with experimental data [11].

Figure 1a shows the profile of the time-averaged streamwise velocity component for a channel flow at $Re^* = 2340$ obtained with the TEM model, compared with the profile of the analogous velocity component measured experimentally [11]. The agreement between the two velocity profiles is very good.

Figure 1b compares the profile of the component $\{u_1' u_3'\}$ of the Reynolds stress tensor (where the subscripts 1 and 3 denote, respectively, the streamwise and wall-normal directions), calculated with the TEM model, with the profile of the similar component of the Reynolds stress tensor obtained from experimental measurements [11], for a channel flow at $Re^* = 2340$. Figure 1b shows that at the TEM model provides a profile of the component $\{u_1' u_3'\}$ in agreement with the one obtained from the experimental measurements.
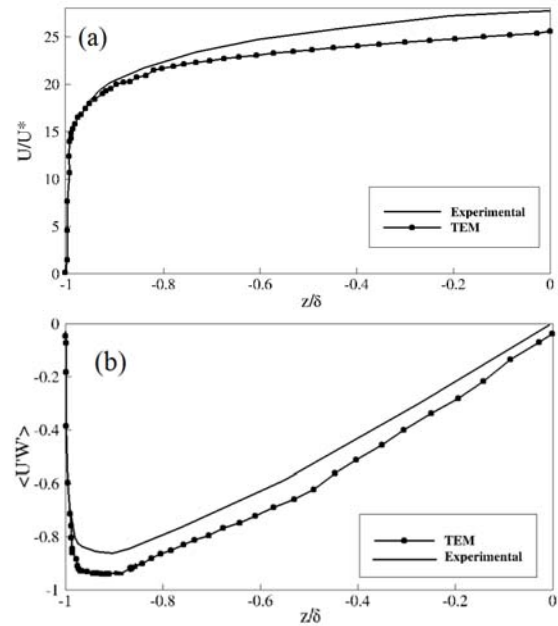

Figure 1. Comparison between experimental measurements and LES results obtained with the TEM model. Channel flow, $Re^* = 2340$. (a): Time-averaged streamwise velocities. (b) Reynolds stress $\{u_1' u_3'\}$.
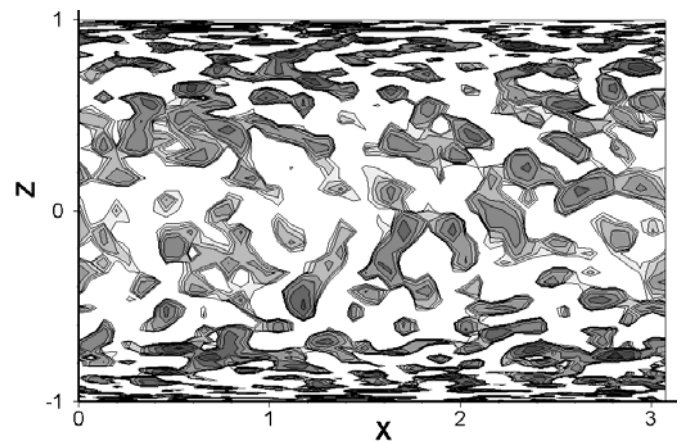

Figure 2. Vortex identification with λ_2 method, x-z plane.

In figure 2 the near-wall vortex structures (inside the turbulent boundary layer) are clearly identified by the λ_2 method of Joeng & Hussain [12]: the

dimensions of the spatial discretization steps allow the optimal simulation of the abovementioned vortex structures that govern the transport, the production and the dissipation of the turbulent kinetic energy. See also [13] and [14].

5 Conclusion

The relation between Noll's formulation of the principle of material frame indifference and the principle of turbulent frame indifference, has been revised. The definition of a new Rule of Turbulent Closure Relations has been proposed. The aforementioned rule of Turbulent Closure Relations has been expressed in the following form: "In a turbulent closure relation, the modelled expressions of an unknown objective tensor must be formulated in terms of objective tensors, allowing the closure relations to fulfil the requirement of Euclidean form invariance, and must retain the same dependence on the angular velocity of the frame of the unknown tensor". The generalized SGS turbulent stress tensor is related exclusively to the generalized SGS turbulent kinetic energy, which has been calculated by means of its balance equation, and the modified Leonard tensor.

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