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Abstract. In the paper the different current approaches to the Large Eddy Simulations of turbulent flows are examined and critically discussed. A LES is usually defined as a numerical computation in which some scales are captured and others are modelled, but different procedures are used for such decomposition. As regards the modeling of the unresolved scales they are in the paper tentatively classified as *exact modeling* and *statistical modeling*. A third procedure, the *dynamic modeling* is examined as a technique based on the use of general relations that connect the subgrid scale turbulent stresses at different levels. Their implementation to standard models, like the Smagorinsky eddy viscosity one, can improve the results and can efficiently extend the range of their application. The connections between LES and RANS, the simulations based on the Reynolds Averaged Navier-Stokes equations, are finally examined and some critical issues related to the extraction of the statistical averages from LES databases are discussed.

### 1. Introduction

An overview of the many approaches that can be classified as Large Eddy Simulations, (LES), of turbulent flows, cannot be done without considering the limiting procedures of the Direct Numerical Simulation, (DNS), and the Reynolds Averaged Navier-Stokes Simulation, (RANS). If compared with the complex scenario of different definitions, filtering operators, truncations and models adopted by the current different LES techniques, these two asymptotic approaches to the simulation of turbulent flows should appear well defined, consolidated basic points, but that is far from true. As regards the Reynolds averages the only thing that we can say, following Frisch (1995), is that for the moment the partial understanding of chaos in deterministic systems gives us the confidence that a probabilistic descrip-

tion of turbulence is justified, and as regards the DNS it is important to remark with Lee (1995) that an instantaneous flowfield of direct numerical simulation must be viewed not as the true solution of the Navier Stokes equations, but only as a snapshot of the evolving flowfield at some fictitious time. Uncomfortable as it can be, anyway we can only conclude with Lee (1995) that, due to the chaotic nature of the turbulent field, the only viable outcome of both approaches, DNS and RANS, is prediction of the averaged flow quantities, and that is only the beginning of a lot of problems. A statistical description needs the definition of a statistical ensemble of flow realizations, and following with the citations let us notice now with Aubry (1991) that this definition in the applications has been quite flexible. As a matter of fact the *statistical* ensemble usually consists of a temporal domain under the ergodicity assumption, or of a symmetry group under which the equations for that particular flow are invariant, or of an ensemble of discrete times conditionally determined. The basic ensemble, a set of initial conditions, is usually never considered, for obvious practical considerations.

Let us now examine the LES. From the basic point of view a Large Eddy Simulation should produce a filtered representation  $\langle a \rangle_f$ 

$$\langle a \rangle_f \equiv \mathcal{F}(a) \tag{1}$$

of the original quantity a, where  $\mathcal{F}$  is a general filtering operator provided with some particular smoothing properties. One particular aim of this approach is to derive, given the evolutionary equation of a, the evolutionary equation for the filtered quantity  $\langle a \rangle_f$ . That is not so easy, and different approaches can be imagined. Let us define as usual, Leonard (1974), the filtered quantity  $\langle a \rangle_f$  as given by

$$\langle a \rangle_f = \int a(t')F(t-t')dt'$$
 (2)

where F(z) is a frequency function, see Hirschman & Widder (1955). If

$$\frac{da}{dt} = A(a) \tag{3}$$

is the evolutionary equation for a, the evolutionary equation for  $\langle a \rangle_f$ 

$$\frac{d\langle a\rangle_f}{dt} = \cdots \tag{4}$$

will usually contain, if non linear, unresolved moments. Three basic approaches can be conceived, one strictly deterministic and the others statistical in order to *close* this filtered equation. The first one, that we will call *exact modeling*, is based on the analytic properties of the convolution

kernel, the frequency function F(z), and it is clear that for very high resolutions a LES is similar to a DNS, so that statistical ingredients seem unadapted. We remark that the statistical approaches are based on a probabilistic interpretation of the definition (2), and that seems a little difficult to understand. It is however easy to see that we can read this physical deterministic average in terms of a filtered density function  $p_f(a, t)$ . We can write

$$\langle a \rangle_f = \int p_f(a, t) a da$$
 (5)

where

$$p_f(a,t) = \int \delta[a-a(t)]F(t-t')dt'$$
(6)

and two statistical procedures can be conceived, the first one based on the derivation of the evolutionary equations for the different moments that appear in the evolutionary equation of  $\langle a \rangle_f$  and the second one based on the evolutionary equation for the filtered density function  $p_f(a, t)$ . That is similar to RANS. Also in this case the usual definition of the mean, easy to compare with the experiments, is based on an infinite time average, but from the fundamental point of view it is more correct to think in terms of an ensemble operator  $\mathcal{E}$  based on a set of initial conditions

$$\langle a \rangle_e = \int P_e(\alpha) a(\alpha, t) d\alpha$$
 (7)

where  $P_e(\alpha)$  is a probability density function on the initial states at the time t = 0

$$\alpha = a(0) \tag{8}$$

If

$$\frac{da}{dt} = A(a) \tag{9}$$

is the evolutionary equation for a, also in this case the basic problem is to derive the evolutionary equation for  $\langle a \rangle_e$ 

$$\frac{d\langle a\rangle_e}{dt} = \cdots \tag{10}$$

and we remark that if we write

$$\langle a \rangle_e = \int p_e(a,t) a da$$
 (11)

where now  $p_e(a, t)$  is a probability density function on a, given by

$$p_e(a,t) = \int \delta[a - a(\alpha,t)] P_e(\alpha) d\alpha$$
(12)

another challenging problem is to derive the evolutionary equation for  $p_e(a,t)$ 

$$\frac{\partial p_e}{\partial t} = \cdots \tag{13}$$

In the following we will examine these two approaches, the *exact modeling* and the *statistical modeling*, in some detail and we will finally make some comments on a third modeling technique that is of some usefulness in improving dynamically the previous procedures. We will call it *dynamic modeling* and we remark that it is based on general operational relations that any modeling procedure, deterministic or not, must verify, like the tensorial or the Galilean invariance.

# 2. Exact modeling

We tentatively classify as exact modeling the procedures based on the analytical properties of an explicit convolutional filtering operator  $\mathcal{F}$ 

$$\mathcal{F}(a) \equiv \langle a \rangle_f = \int_{-\infty}^{\infty} a(t') F(t-t') dt'$$
(14)

where, as remarked in the introduction, the kernel F(z) is a frequency function. It is interesting to notice, Hirschman & Widder (1955), that if L(s) is the inverse of the bilateral Laplace transform of F(z)

$$\frac{1}{L(s)} = \int_{-\infty}^{\infty} F(z)e^{-zs}dz \tag{15}$$

a useful inversion formula is the following

$$L(\mathcal{D})\langle a \rangle_f = a \tag{16}$$

where  $\mathcal{D}$  stands for the derivative operator

$$\mathcal{D} \equiv \frac{d}{dt} \tag{17}$$

From the operational point of view the differential operator  $L(\mathcal{D})$  is the inverse of the integral operator  $\mathcal{F}$ 

$$L(\mathcal{D}) \equiv \mathcal{F}^{-1} \tag{18}$$

and an interesting class of filters is the following

$$\mathcal{F}^{-1} = (1 - \alpha_1 \mathcal{D})((1 - \alpha_2 \mathcal{D}) \cdots (1 - \alpha_n \mathcal{D})$$
(19)

It can be shown that these filters are variation diminishing in the sense that the number of changes of sign of the filtered function  $\langle a \rangle_f$  never exceeds the

number of changes of sign of the original function a, and other interesting properties are related to the mean  $m_f$  and the variance  $v_f$  of the kernel of the inverse convolutional filter, the frequency function F(z), given by

$$m_f = -\sum_{1}^{n} \frac{1}{\alpha_k}$$
  $v_f = \sum_{1}^{n} \frac{1}{\alpha_k^2}$  (20)

We remark that the smoothing properties of the variation diminishing transform are particularly interesting for LES, and till now unexplored. Historically they were first introduced by Schoenberg, and are connected to the *zero crossing* rate of a turbulent fluctuation that, as remarked in the past by Liepmann, is directly related to the dissipation.

Many other different filters have been proposed for LES, and a complete review of all them should require many pages. We refer for that to the recent book of Sagaut (2001) where definitions and properties of classical filters for LES are discussed both for the homogeneous and the inhomogeneous case. This last issue is very important for the applications, and we remark that a general class of *differential filters*, Germano (1986), is particularly interesting in order to explore what happens when nonhomogeneous filtering operators do not commute with differentiation, Germano (2000). As an example let us consider a linear differential form of the second order

$$\mathcal{D} = \mathcal{I} + \vartheta \mathcal{D}_t + \Delta_k \mathcal{D}_k + \Delta_{kl} \mathcal{D}_k \mathcal{D}_l \tag{21}$$

where

$$\mathcal{D}_t \equiv \frac{\partial}{\partial t} \qquad \qquad \mathcal{D}_k \equiv \frac{\partial}{\partial x_k}$$
 (22)

and let us associate to this differential operator a filtering operator  $\mathcal F$  defined as

$$\mathcal{I} = \mathcal{DF} \tag{23}$$

where  $\mathcal{I}$  is the identity. It is interesting to remark that the differential operator  $\mathcal{D}$  is by definition the inverse of the filtering operator  $\mathcal{F}$ 

$$\mathcal{D} = \mathcal{F}^{-1} \tag{24}$$

and formally  $\mathcal{F}$  can be expressed by an integral convolution with a kernel given by the Green's function associated to  $\mathcal{D}$ . We notice that if the parameters  $\vartheta, \Delta_k, \Delta_{kl}$  are not constant the operator  $\mathcal{F}$  does not commute with the derivatives  $\mathcal{D}_t$  and  $\mathcal{D}_k$ , and what is interesting with these filters is that provided with the exact inverse of  $\mathcal{F}$  we can easily write the exact expressions for the commutative terms

$$\mathcal{F}\mathcal{D}_t - \mathcal{D}_t\mathcal{F} \qquad \qquad \mathcal{F}\mathcal{D}_k - \mathcal{D}_k\mathcal{F}$$
(25)

In fact if  $\mathcal{G}$  is a generic operator we obtain by applying the relation (23)

$$\mathcal{GDF} = \mathcal{DFG} \tag{26}$$

and we can write

$$(\mathcal{GD} - \mathcal{DG})\mathcal{F} = \mathcal{D}(\mathcal{FG} - \mathcal{GF})$$
<sup>(27)</sup>

If we now compare this relation with the relation (23) we obtain

$$\mathcal{FG} - \mathcal{GF} = \mathcal{F}(\mathcal{GD} - \mathcal{DG})\mathcal{F}$$
(28)

that provides the exact form for the commutative *errors* in terms of the filtered quantities.

#### 3. Statistical modeling

As remarked before statistical modeling reads the filtering length as an interval of indeterminacy that separates what can be calculated analytically from what has to be guessed statistically. This point of view can be similarly applied to a projection. If we express the generic turbulent velocity field  $u_i$  in terms of a generalized Fourier expansion

$$u_i = \sum_{1}^{\infty} u_{ik} \varphi_k \tag{29}$$

where  $\varphi_k$  is a particular set of basis functions and  $u_{ik}$  are random Fourier coefficients, following Yoshizawa (1982) we can define a *partial* statistical operator  $\mathcal{E}_f$  that applied to  $u_i$  gives the  $\mathcal{F}$ -level statistical representation

$$\mathcal{E}_f(u_i) = \sum_{1}^{f} u_{ik} \varphi_k + \sum_{f+1}^{\infty} \langle u_{ik} \rangle_e \varphi_k \tag{30}$$

The partial statistical theory of turbulence is at the beginning, and in the opinion of the author the Large Eddy Simulation has stimulated the research in the field. We recall that the probability density function approach has been pioneered in turbulence by Lundgren (1967). His method derives directly the evolutionary equation for the ensemble pdf from the differential equations which define the conservation laws, and the principal fields of application are the reacting turbulent flows, but recently this approach has been extended to LES, see Pope (1990) and Gao & O'Brien (1993). This concept of a pdf within the subgrid, Madnia & Givi (1993), is very promising for LES and some first simulations based on a velocity filtered density function computed by a Lagrangian Monte Carlo procedure have been recently performed by Gicquel et al. (2001).

As remarked in the introduction the *exact* and the *partial statistical* modeling based on filtered pdf could seem incompatible. If the filtering operation is defined as a convolution in the physical space

$$\langle a \rangle_f = \int_X a(x')F(x-x')dx'$$
 (31)

we have

$$\tau_f(a,b) = \tau_f(-a,-b) \tag{32}$$

where by definition the generalized central moment associated to the quantities a and b is given by

$$\tau_f(a,b) = \langle ab \rangle_f - \langle a \rangle_f \langle b \rangle_f \tag{33}$$

and this condition of *reversibility* should be respected by modeling. It is however important to recall that the Smagorinsky model, based on statistical considerations and applied to the anisotropic part of the subgrid turbulent stress,

$$\tau_f^a(u_i, u_j) \sim M_f(u_i, u_j) = -2\nu_f \langle s_{ij} \rangle_f \tag{34}$$

is such that

$$M_f(u_i, u_j) = -M_f(-u_i, -u_j)$$
(35)

and this condition is violated. This situation is reminiscent of the *reversibility paradox* related to the connections between the statistical kinetic theory and the microscopic laws of mechanics that are invariant under time reversal. We remark, Germano (2001), that if we rewrite the integral (31) in its Lebesgue version

$$\langle a \rangle_f = \int_X a(x')F(x-x')dx' = \int_A ap(x,a)da \tag{36}$$

where

$$p(x,a) = \int_X F(x-x')\delta[a-a(x')]dx'$$
(37)

the Smagorinsky model could be recovered by an assumed probability distribution  $p(x, C_i)$  given by

$$p(x, C_i) = (2\pi U^2)^{-3/2} \exp[-C^2/2U^2] \cdot \left\{ 1 - \frac{\nu_f}{U^2} \left[ \left( \frac{C^2}{2U^2} - \frac{5}{2} \right) \frac{C_i}{U^2} \frac{\partial U^2}{\partial x_i} + \frac{C_i \langle s_{ij} \rangle_f C_j}{U^2} \right] \right\}$$
(38)

where  $C_i = u_i - \langle u_i \rangle_f$ ,  $C^2 = C_i C_i$  and

$$3U^2 = \tau_f(u_i, u_i) \tag{39}$$

It seems in conclusion that the eddy viscosity model could only be justified on the basis of probabilistic arguments, and that the irreversible LES could only find its formulation in the large eddy probabilistic density function.

## 4. Dynamic modeling

The dynamic modeling procedures are based on identities that relate the subgrid scale stresses at different resolution levels. The simplest one is the following

$$\tau_{fg}(u_i, u_j) = \langle \tau_f(u_i, u_j) \rangle_g + \tau_g(\langle u_i \rangle_f, \langle u_j \rangle_f)$$
(40)

where the various terms are given by definition by the expressions

$$\tau_{f}(u_{i}, u_{j}) = \mathcal{F}(u_{i}u_{j}) - \mathcal{F}(u_{i})\mathcal{F}(u_{j})$$
  

$$\tau_{fg}(u_{i}, u_{j}) = \mathcal{GF}(u_{i}u_{j}) - \mathcal{GF}(u_{i})\mathcal{GF}(u_{j})$$
  

$$\langle \tau_{f}(u_{i}, u_{j}) \rangle_{g} = \mathcal{GF}(u_{i}u_{j}) - \mathcal{G}(\mathcal{F}(u_{i})\mathcal{F}(u_{j}))$$
  

$$\tau_{g}(\langle u_{i} \rangle_{f}, \langle u_{j} \rangle_{f}) = \mathcal{G}(\mathcal{F}(u_{i})\mathcal{F}(u_{j})) - \mathcal{GF}(u_{i})\mathcal{GF}(u_{j})$$
  
(41)

and where  $\mathcal{F}$  and  $\mathcal{G}$  are respectively the LES filter and the test filter. Also in this case to discuss the many applications and variants adopted since the first dynamic model, Germano et al. (1991), should require a lot of space, and we refer to a recent paper of Piomelli (1999) for a critical analysis. It is perhaps more interesting for this brief review to remark that this procedure is based on purely formal properties and can only improve an existing model, like the Smagorinsky eddy viscosity model, or the structure function model. That is good from one side, because as such its range of application is very large, and we recall a recent interesting extension, Im et al. (1997), of the dynamic procedure applied to the so called G-equation that predicts the evolution of the propagating front of laminar flamelets corrugated by turbulent eddies. From the other side however that is a limit, because in some sense there is nothing new that is added *physically* by this procedure, and the improvement is due to a better consistency with the formal properties of the real subgrid stresses. This point seems to the author very important and has been the matter of an interesting criticism by Pruett (1997). With reference to the relation (40) he states that this identity is mathematically tautological, and unnecessary as a basis for dynamic SGS models, and in our opinion this criticism is applicable or not according to the situation. Let us examine the identity (40) from the point of view of the exact modeling. In this case we assume that both the test filter  $\mathcal{G}$  and the LES filter  $\mathcal{F}$  are explicitly known, and as in Brun & Friedrich (2000) we can expand them in one dimension as follows

$$\mathcal{F} = \mathcal{I} + a_f \mathcal{D} + b_f \mathcal{D}^2 + c_f \mathcal{D}^3 \cdots$$

$$\mathcal{G} = \mathcal{I} + a_g \mathcal{D} + b_g \mathcal{D}^2 + c_g \mathcal{D}^3 \cdots$$
(42)

where  $\mathcal{D}$  stands for the derivative. If the problem is to find an expression for the turbulent stress at the  $\mathcal{FG}$ 

$$\tau_{fg}(u_i, u_j) = \mathcal{GF}(u_i u_j) - \mathcal{GF}(u_i)\mathcal{GF}(u_j)$$
(43)

we can in this case derive an explicit expression for  $\mathcal{FG}$ 

$$\mathcal{GF} = \mathcal{I} + a_{fg}\mathcal{D} + b_{fg}\mathcal{D}^2 + c_{fg}\mathcal{D}^3 \cdots$$
(44)

where

$$a_f + a_g = a_{fg}$$
  

$$b_f + a_f a_g + b_g = b_{fg}$$
  

$$c_f + b_f a_g + a_f b_g + c_g = c_{fg}$$
  
... (45)

and it is clear that in this case Pruett is right. In fact we can easily derive directly that

$$\tau_{fg}(u_i, u_j) = (2b_{fg} - a_{fg}^2)\mathcal{D}(u_i)\mathcal{D}(u_j) + \cdots$$
(46)

and the identity (40) is unessential. On the contrary if we are provided only with an explicit LES *model*, and we do not exactly know the explicit originating LES *filter*, we can only write that

$$\langle \tau_f(u_i, u_j) \rangle_g = \tau_f(u_i, u_j) + a_g \frac{\partial \tau_f(u_i, u_j)}{\partial x} + b_g \frac{\partial^2 \tau_f(u_i, u_j)}{\partial x^2} + \cdots$$
  
$$\tau_g(\langle u_i \rangle_f, \langle u_j \rangle_f) = (2b_g - a_g^2) \mathcal{D}(\langle u_i \rangle_f) \mathcal{D}(\langle u_j \rangle_f) + \cdots$$
(47)

and the only way to derive the turbulent stress at the  $\mathcal{FG}$  level remains to apply the identity (40).

## 5. Connections between LES and RANS

The comparisons among DNS, LES and RANS databases pose a lot of problems that in some cases can be neglected, but that conceptually remain. The first concerns the recovery of the statistical data from a LES database. We remark that what we produce by LES are filtered quantities, for example the filtered values of the velocity field,  $\langle u_i \rangle_f$ . When we apply an explicit model we have no idea of its explicit generating filter, if ever exist. If we define the LES fluctuations  $u'_i$  to the statistical mean as

$$u_i' = \langle u_i \rangle_e - \langle u_i \rangle_f \tag{48}$$

we notice that only in the case  $\langle u'_i \rangle_e = 0$  the simple usual relations

$$\tau_e(u_i, u_j) = \langle u'_i u'_j \rangle_e + \langle \tau_f(u_i, u_j) \rangle_e$$
  
$$\tau_e(u_i, u_j, u_k) = \langle u'_i u'_j u'_k \rangle_e + \langle \tau_f(u_i, u_j, u_k) \rangle_e + \langle u'_i \tau_f(u_j, u_k) \rangle_e + \langle u'_j \tau_f(u_k, u_i) \rangle_e + \langle u'_k \tau_f(u_i, u_j) \rangle_e$$
(49)

are valid, and that is not so good. As remarked in Hussaini *et al.* (1989) if higher order turbulence statistics are needed beyond the mean velocity, the problem of defiltering arises, and this problem becomes most critical when more than 10 - 20% of the turbulent kinetic energy is in the subgrid scale motions. The literature on the estimation of the second and the third order statistical moments based on LES databases is relatively poor, and in some cases we are obliged to think that probably the subgrid models are considered very important dynamically, in order to compute the mean values, but not so reliable in order to be implemented in the relations (49). We remark, Germano (2001), that only in the case that the following chain of relations is satisfied

$$\langle u'_i \rangle_e = 0 \langle \tau_f(u_i, u_j) \rangle_e = 0 \langle u'_i \tau_f(u_j, u_k) \rangle_e = 0 \langle \tau_f(u_i, u_j, u_k) \rangle_e = 0 \cdots = \cdots$$
 (50)

the filtering procedure produces statistical moments simply given by

$$\tau_e(u_i, u_j) = \langle u'_i u'_j \rangle_e$$
  

$$\tau_e(u_i, u_j, u_k) = \langle u'_i u'_j u'_k \rangle_e$$
  

$$\tau_e(u_i, u_j, u_k, u_l) = \langle u'_i u'_j u'_k u'_l \rangle_e$$
  

$$\cdots = \cdots$$
(51)

and the study of explicit filters or explicit models that implement these statistical constraints are currently under way.

# 6. Conclusions

The various modeling approaches and numerical procedures that since the first applications in meteorology have been applied to simulate the large scales of turbulence, have stimulated during the time a lot of different interests and have raised a lot of different questions. A general overview of all

that is nearly impossible, and inevitably is a little biased by the particular attitudes or tendencies of the reviewer. If we look at the agenda of this meeting we can see that the applications of LES are very promising and wide-spread on a lot of different fields of application, from the aeronautical engineering to the estimate of the pollution dispersion, in reactive flows as in heat transfer. Industrial needs and interests motivate obviously the future of LES, that will probably still remain for a long time the only viable way for accurate calculations of turbulent flows. Hybrid RANS-LES strategies like the Detached Eddy Simulation or time dependent RANS are presently developed in order to simulate complex turbulent flows and to combine LES with standard and well developed computational and modeling procedures. In this particular case, as in many others, practical and theoretical issues are strongly intermixed. From one side the motivation of these hybrid procedures is mainly practical : LES remains after all very expensive, and simplest computational strategies remain very attractive. From another side however the final goal is very ambitious and aims to construct a unified turbulence model useful for all purposes, from wall modeling to the wake. This point, as many others, is a real challenge and imposes a big effort in a lot of different fields, from the exploration of higher order computational schemes to the basic research on turbulence, from the study of unstructured grids to the speculations about statistical and deterministic issues in chaotic systems. The fundamentals of turbulence remain one of the most fascinating unresolved problem and the hopes placed in a more rational design of aircraft, automobiles, turbines and many others industrial processes based on an improved computational ability of fluid flows are more and more increasing. In order to cope with all these problems we need the effort of everybody and a strong cooperation among different partners.

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