Perspectives for ensemble average LES

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1. Motivation and objectives

With the emergence of parallel computing, running several LES’s simultaneously for the same turbulent flow becomes realistic, at least for a rather coarse resolution. We have already investigated this possibility and promising results have been obtained (Carati et al., 1996). In this report, we present several new approaches for subgrid scale modeling that can be developed when an ensemble of LES’s is known.

1.1 Coupling between LES and RANS

First, we remark that the ensemble of LES’s shares some properties with the RANS approach. Indeed, the ensemble average of quantities described by the LES’s is equivalent to the large scale property of the same quantities obtained through the RANS. It is thus natural to investigate the possibility of coupling these methods. One interesting procedure that has been considered in a different context (Cabot, 1996) amounts to decomposing the domain into different regions. In some of these sub-domains, a RANS can be used if LES is too expensive. For example, the RANS can be used in the near wall region while the ensemble of LES’s would be used for the region away from the wall (outer region). Matching conditions for the RANS quantities are easily accessible from averages of the realizations in the outer region. The main theoretical and practical difficulty is then to supply each LES realization with boundary information generated from the single RANS. This task is difficult since these boundary values are an artifact of the domain decomposition and thus do not reflect any physical or mathematical constraints. Boundary conditions for the LES can only be imposed through physically plausible assumptions that must be considered as part of the modeling effort needed in the LES context.

Using RANS models in wall region has a double advantage. First, RANS are much cheaper than LES, which are strongly limited by the problem of resolution close to solid boundaries. Second, RANS represents ensemble average information and thus requires a single simulation independent of the number of realizations in the outer region. The hope in the proposed approach is that (i) the RANS will be improved by the ensemble of LES’s through the information passed at the boundary between the sub-domains, and (ii) the ensemble of LES will be much faster because they will not have to resolve the wall region. This approach has the very reasonable property of letting the LES’s focus on the outer region in which the statistical theories that form the basis of subgrid scale modeling are believed to apply.

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1.2 New models using the ensemble of LES’s

To date, the ensemble of LES’s has been used only in the determination of the model coefficient in the context of the ensemble averaged dynamic model. However, knowledge of an ensemble of realizations for the same flow can be used in a much more general manner. In particular, most of the concepts used in subgrid scale modeling originate from statistical theories of turbulence (Leslie and Quarini, 1979). With the approach we plan to develop, the link between LES and these theories becomes natural. In Section 2 we present some interesting uses of the ensemble of LES’s for subgrid scale modeling purposes.

2. Accomplishments

2.1 The ensemble averaged dynamic model

In a study initiated during the 1996 Center for Turbulence Research Summer Program, we have shown that a collection of LES’s can be used to develop new versions of the dynamic model based on the ensemble average. Indeed, the model coefficient is often seen as a “universal function” that can depend on space when the flow is not homogeneous but that should be independent of a particular realization. In an ensemble of LES’s this is easily achieved. Moreover, the classical dynamic procedure relies on the existence of directions of homogeneity. When the flow is fully inhomogeneous, the dynamic procedure can be applied, but the coefficient evaluation then requires the solution of an integral equation (Ghosal et al., 1995). With the ensemble averaged dynamic model, it has been shown that the model coefficient can be obtained simply even for fully inhomogeneous flows. Some preliminary tests of the ensemble averaged dynamic model have been performed and show good agreement with experimental data. Assuming that the Smagorinsky coefficient is independent of the realization for statistically equivalent flows results in the following model:

\[ \tau_{ij}^r - \frac{1}{3} \tau_{kk}^r \delta_{ij} \approx -2C \Delta^3 |S^r| |S_{ij}^r|, \]  

where \( C \) is independent of the realization index \( r \). Here, \( S_{ij} \) represents the resolved strain tensor. The dynamic procedure can be used to determine \( C \) if the usual average over homogeneous directions is replaced by an average over the ensemble. The error caused by using models for the subgrid scale stresses now depends on the realization. By assuming that for large ensembles, the Smagorinsky coefficient is essentially constant over the scale of the test filter, we have been able to derive an analogous expression for \( C \) as in the spatially averaged version of the dynamic procedure:

\[ C = \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle}, \]  

where the brackets now represent an ensemble average. The Leonard tensor is given by \( L_{ij} = \ddot{u}_i \ddot{u}_j - \ddot{u}_i \ddot{u}_j \) and \( M_{ij} = 2\Delta |S^r| |S_{ij}^r| - 2\Delta |\hat{S}^r| |\hat{S}_{ij}^r| \). Of course, the latter

\[ a \]  

The overline notation \( \overline{\cdot} \) will be used for RANS quantities and not for LES variables. In this report, \( \ddot{u}_i \) represents the resolved field in the LES and \( \ddot{u}_i \) the test field in the dynamic procedure.
assumption has to be verified \textit{a posteriori}. The first conclusion we have reached is quite encouraging. Indeed, it appears that with only 16 simultaneous LES’s, the ensemble averaged dynamic model performs as well as the volume averaged model. Moreover, the spatial variability of $C$ decreases drastically when the number of realizations $R$ increases. The comparison between a $512^3$ decaying isotropic turbulence DNS and a $32^3$ dynamic model LES have shown good agreement both for the total resolved energy and for the spectra (Carati \textit{et al}, 1996).

2.2 Matching conditions for RANS and LES’s

When a RANS is used in some sub-domains and LES’s in others, new boundary conditions are needed. These conditions are not imposed by the physics of the flow but only by the domain decomposition adopted in the numerical integration. There is thus some arbitrariness in their choice. The first and simplest question is how can the LES’s feed the RANS? Clearly, the number of boundary conditions will depend on the RANS model and more specifically on the number of variables predicted by the RANS. The natural assumption is then to impose equality between the RANS quantities and the corresponding ensemble averaged LES quantities. This leads to the following type of equalities:

$$\overline{u}_i = \langle u^r_i \rangle, \quad (3a)$$

$$\overline{u}^{r2}_i = \langle (u^r_i)^2 \rangle - \langle u^r_i \rangle^2. \quad (3b)$$

A much more difficult problem is to determine how one single RANS can be used to derive boundary conditions for an ensemble of LES’s. Indeed, $3R$ boundary conditions are needed for the $u^r_i$, $r = 1 \ldots R$, $i = 1 \ldots 3$. In principle, $3R$ RANS quantities can be matched. In practice, however, only a few RANS quantities are available. Typically, $\overline{u}_i$ plus (maybe) $\overline{k}$, $\overline{v}$, $\overline{w}$, $\overline{w^2}$, $\overline{w'^2}$, $\overline{w''}$, $\overline{w'w''}$. The minimal condition is of course:

$$\langle u^r_i \rangle = \overline{u}_i. \quad (4)$$

However, the simplest choice of imposing $u^r_i = \overline{u}_i \forall r$ appears to be a very poor solution. Indeed, for a stationary channel flow, $\overline{u}_i$ is likely to be zero in the spanwise and wall-normal directions while it should be constant in the streamwise direction. The LES’s for the core flow then reduce to a thinner channel with moving planes which is not realistic. Hence, it can be concluded that the fluctuations should be involved in the boundary conditions for the LES’s. The solution we investigated was obtained by matching both the average velocity and the turbulence intensities. Of course, there is an infinity of solutions for these conditions. They can be written as$^b$:

$$u^r_\alpha = \overline{u}_\alpha + \frac{h^r_\alpha - \langle h^r_\alpha \rangle}{\langle u^r_\alpha (h^r_\alpha - \langle h^r_\alpha \rangle) \rangle} \overline{u}^{r2}_\alpha, \quad (5a)$$

$^b$ We adopt the convention of implicit summation over repeated Latin indices. No summation is implied on Greek indices.
where the quantity $h^r_\alpha$ is arbitrary and has to be determined as part of the modeling effort needed in LES. An equivalent formulation has also been considered:

$$u^r_\alpha = \overline{\pi}_\alpha + \frac{g^r_\alpha - \langle g^r_\alpha \rangle}{\langle (g^r_\alpha - \langle g^r_\alpha \rangle)^2 \rangle^{1/2}} \mu^{1/2}, \tag{5b}$$

where $g^r_\alpha$ is now the arbitrary quantity. Both formulations imply $\langle u^r_\alpha \rangle = \overline{\pi}_\alpha$ and $\langle (\delta u^r_\alpha)^2 \rangle = \mu^2_\alpha$ (here $\delta u^r_\alpha = u^r_\alpha - \langle u^r_\alpha \rangle$). By coupling RANS for the wall region and an ensemble of LES’s for the core flow, the LES model has to deal with both the subgrid scale stress and the boundary conditions. In general, $h^r_\alpha$ is a function of the velocity field and of all its derivatives $h^r_\alpha = h^r_\alpha(u_l, \partial, u_j, \ldots)$. A promising choice for $h^r_\alpha$ has been considered. First, we note that the existence of a continuous boundary provides an unambiguous decomposition of the velocity into a part normal to the boundary $u_\perp$ and a part parallel to the boundary $\overline{u}_\parallel$ (which is a 2D vector). The choice considered so far consists in imposing the following boundary conditions for the parallel part of the velocity:

$$\overline{h}_\parallel = \partial_\perp \overline{u}_\parallel \tag{6}$$

and using continuity:

$$\partial_\perp u^r_\perp = -\nabla_\parallel \overline{u}_\parallel \tag{7}$$

as a boundary condition for $u^r_\perp$. With this choice, the boundary condition for the components of the parallel velocity reduces to:

$$\delta u^r_\| = 2 \frac{\partial_\perp \delta u^r_\|}{\partial_\perp (\langle \delta u^r_\| \rangle^2)} \overline{u}_\parallel^2. \tag{8}$$

The set of boundary conditions (5, 7-8) must now be tested in simple cases.

2.3 Proposals for new subgrid scale models

As already discussed, the additional information provided by the ensemble of LES can be used for constructing new eddy viscosity models. However, it is known that the eddy viscosity gives a very simplified picture of the subgrid scale stress. For that reason, it is also interesting to investigate the possibility of modifying the structure of the subgrid scale model by using some quantities that are directly accessible from the ensemble of LES’s.

2.3.1 Model based on the fluctuating strain tensor

The first model we propose is obtained by subtracting the mean strain:

$$\tau^r_{ij} = -\nu^r_T (S^r_{ij} - \langle S^r_{ij} \rangle) \equiv -\nu^r_T \delta S^r_{ij}. \tag{9}$$

This formulation has some nice properties. The average dissipation is given by

$$\mathcal{E} = \langle \nu_T \delta S^r_{ij} \delta S^r_{ij} \rangle + \nu_0 \langle S^r_{ij} \rangle \langle S^r_{ij} \rangle, \tag{10}$$
and thus the turbulent dissipation only originates from the fluctuating part of the strain tensor. The mean part only contributes to the molecular dissipation. This property ensures that the model will not produce dissipation in a laminar region. In addition, while this model is dissipative on average (provided the eddy viscosity is positive), individual realizations can have negative dissipation thus representing the inverse transfers of energy from the small unresolved scales to the large ones (backscatter). It is generally believed that backscatter originates from fluctuation phenomena on the subgrid scale, and representation of this effect through fluctuations in the strain tensor is thus very reasonable.

2.3.2 Anisotropic model

Although isotropic turbulence has been studied in great detail for many years, the presence of some anisotropy is almost universal in practical instances of turbulent flow. However, anisotropy usually originates from complex interactions between flow direction, solid boundaries, and external constraints like pressure gradient or global rotation. It is thus quite difficult to predict a priori the main direction of anisotropy. In the context of statistical averaged LES, we have access at any instant to mean quantities that will display the anisotropic structure of the turbulence. On the contrary, when only one single LES is accessible, the direction of anisotropy can only be discovered after some averaging in time if there is no direction of homogeneity. A model that would directly take advantage of the ensemble of LES could be:

\[ \tau_{ij}^r \approx -\mu \gamma_{ik} \gamma_{ji} S_{kl}, \]  

where the factor \( \mu \) plays the role of an eddy viscosity but through an anisotropic relation between the subgrid scale stress and the strain tensor. The tensor \( \gamma_{ij} \) should be a measure of the anisotropy. It can be constructed with the velocity fluctuations:

\[ \gamma_{ij} = 3 \frac{\langle \delta u_i^r \delta u_j^r \rangle}{\langle \delta u_k^r \delta u_k^r \rangle}, \]  

This model reduces to the classical eddy viscosity model for isotropic turbulence \( (\gamma_{ij} = \delta_{ij}) \). Moreover, the sign of the dissipation depends only on the sign of \( \mu \) since the product of \( \tau_{ij}^r \) and the strain tensor is given by

\[ -\tau_{ij} S_{ij} = \mu S_{ij} \gamma_{ik} \gamma_{ji} S_{kl} \]  

whose sign only depends on the sign of \( \mu \). Moreover, if there is no turbulence in one direction \( (\delta u_a = 0) \), the model has the property that the component \( \tau_{ia} = \tau_{aj} = 0 \). This is an expected property that is missed by the Smagorinsky model, which dissipates even in the laminar regime.

3. Conclusions and future work

We conclude by stressing that the use of an ensemble of LES's is not per se much more expensive than the use of a single realization. Indeed, let us consider a
stationary LES and denote by $t_t$ the transient period between the beginning of the simulation and the time at which the turbulence becomes fully developed. Let us also denote by $t_s$ the time (beyond $t_t$) required to converge the statistics. Then, the CPU time required for obtaining converged statistics with a single LES is $t_t + t_s$. With an ensemble of realizations, statistics are accumulated over both the ensemble and time. Thus, for equivalent sample, the ensemble only needs to be advanced in time by the amount $t_s/R$. The total CPU cost for the ensemble is thus $R(t_t + t_s/R)$, which amounts in an overhead of $(R - 1)t_t$ over a single realization. If the ratio between the transient phase and the time needed to converge statistics is small, then the additional cost will be acceptable. Moreover, if the LES is not stationary and if there are no homogeneous directions, the ensemble average approach would seem to be the only way to obtain statistics. Finally, a wall model using RANS concepts would greatly reduce the cost of each LES in the ensemble.

Future work must now be devoted to the numerical implementation of the idea developed in this report. A first and very simple test of the matching conditions can be obtained by running an LES in the core flow of a channel with the boundary conditions described in section 2.2 in which the quantities $u_i^{12}$ are obtained from experimental data. In that case, the LES is fed with “exact” RANS quantities, and the test will clearly determine if the boundary conditions performs reasonably well. The channel flow can also be used for testing the new models proposed in section 2.3.

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