Ensemble averaged dynamic modeling

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The possibility of using the information from simultaneous equivalent large eddy simulations for improving the subgrid scale modeling is investigated. An ensemble average dynamic model is proposed as an alternative to the usual spatial average versions. It is shown to be suitable independently of the existence of any homogeneity directions, and its formulation is thus universal. The ensemble average dynamic model is shown to give very encouraging results for as few as 16 simultaneous LES's.

1. Introduction

The equation for large eddy simulation (LES) is obtained by applying a spatial filter to the Navier-Stokes equation. The LES equation thus describes the evolution of a filtered velocity field $\overline{u}_i$ which explicitly depends on the small scales through the subgrid scale stress $\tau_{ij} = \overline{u_i u_j} - \overline{u}_i\ \overline{u}_j$:

$$\partial_t \overline{u}_i + \partial_j \overline{u}_j \overline{u}_i = -\partial_i \overline{p} + \nu_0 \nabla^2 \overline{u}_i - \partial_j \tau_{ij}. \tag{1.1}$$

For simplicity, we only consider incompressible flows. The pressure p is then chosen to satisfy the incompressibility condition. Clearly, τ_{ij} is a large scale quantity depending mainly on the small scale velocity field. However, it is usually modeled as a function of the resolved velocity field as in the Smagorinsky eddy viscosity model (Smagorinsky, 1963):

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} \approx -2C\overline{\Delta}^2 |\overline{S}| \overline{S}_{ij}, \tag{1.2}$$

where $\overline{S}_{ij} = \frac{1}{2}\ (\partial_i \overline{u}_j + \partial_j \overline{u}_i)$ and $|\overline{S}| = (2\overline{S}_{ij}\overline{S}_{ij})^{1/2}$. In the original formulation of the Smagorinsky model, the parameter C must be obtained from some fitting procedure. Recently, this model has been improved by the introduction of the dynamic procedure, which allows a self calibration of the parameter C and gives an explicit expression as a function of the resolved field $C = C(\overline{u}_k)$. However, any procedure that determines the subgrid scale stress in terms of the resolved field can only be an approximation. Indeed, the same resolved field may be compatible with many different small scale velocity fields. This is reflected in the *a priori* tests which show very poor correlations between the models $\tau_{ij} \approx \tau_{ij}^M(\overline{u}_k)$ and the actual τ_{ij} obtained from direct numerical simulations (see Winckelmans *et al*, in this volume).

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Clearly more information is needed to properly reconstruct the subgrid-scale stress. The introduction of stochastic model for τ_{ij} is a first attempt to introduce models that are not fully determined by the resolved field (Carati *et al*, 1995; Chasnov, 1991; Leith, 1990; Mason & Thomson, 1992). Here, we explore another approach which consists in running simultaneously several statistically equivalent LES's and constructing the model by using information from the set of resolved velocity fields:

$$\partial_t \overline{u}_i^r + \partial_j \overline{u}_j^r \overline{u}_i^r = -\partial_i \overline{p}^r + \nu_0 \nabla^2 \overline{u}_i^r - \partial_j \tau_{ij}^r \qquad r = 1, \ldots, R. \tag{1.3}A$$

Here, r is a new index corresponding to the realization and R is the total number of realizations. The concept of *statistically equivalent* LES's will be defined in Section 3. The model we propose to test should generalize the classical subgrid scale model ($\tau_{ij}^r = \tau_{ij}^r(\overline{u}_k^r)$) by allowing an explicit dependence on the velocity field from other members in the set:

$$\tau_{ij}^r = \tau_{ij}^r(\{\overline{u}_k^s\}) \tag{1.4}$$

Clearly, in that case the subgrid scale model in the LES labeled r will not be a function of the resolved velocity field $\overline{u}_k^r$ only.

In the following section, we will present the dynamic procedure and its generalization to several LES's. We also present an alternative formalism to the classical dynamic model. Some results for decaying and forced isotropic turbulence and for channel flow are discussed.

2. The dynamic procedure

The dynamic procedure is based on an exact relation between subgrid scale stresses for different filter widths (Germano, 1992; Ghosal *et al* 1995; Lilly, 1992). This relation is obtained by introducing a second filter G_t, usually referred to as the *test filter*, denoted by $\widehat{\ }$; we will call the original filter G_1. The application of this new filter to Eq. (1.1) yields:

$$\partial_t \widehat{\overline{u}}_i + \partial_j \widehat{\overline{u}}_j \widehat{\overline{u}}_i = -\partial_i \widehat{\overline{p}} + \nu_0 \nabla^2 \widehat{\overline{u}}_i - \partial_j \widehat{\tau}_{ij} - \partial_j L_{ij}, \tag{2.1}$$

where $L_{ij} = \widehat{\overline{u}_i \overline{u}_j} - \widehat{\overline{u}}_i \, \widehat{\overline{u}}_j$ is the Leonard tensor. This equation governs the evolution of the field $\widehat{\overline{u}}$ obtained by the application of the filter $G_2 \equiv G_t \star G_1$ to the fully resolved velocity. Thus, an equivalent equation should be obtained by applying G_2 directly to the Navier-Stokes equation:

$$\partial_t \widehat{\overline{u}}_i + \partial_j \widehat{\overline{u}}_j \widehat{\overline{u}}_i = -\partial_i \widehat{\overline{p}} + \nu_0 \nabla^2 \widehat{\overline{u}}_i - \partial_j T_{ij}. \tag{2.2}$$

Here, the subgrid stress tensor is defined by $T_{ij} = \widehat{\overline{u_i}\,\overline{u_j}} - \widehat{\overline{u}}_i \, \widehat{\overline{u}}_j$. The comparison between equations (2.1) and (2.2) readily leads to the Germano identity:

$$L_{ij} + \widehat{\tau}_{ij} - T_{ij} = 0. \tag{2.3}$$

When approximate models $\tau_{ij} \approx \tau_{ij}^M$ and $T_{ij} \approx T_{ij}^M$ are used, this identity is violated. However, the error $E_{ij} \equiv L_{ij} + \hat{\tau}_{ij}^M - T_{ij}^M \neq 0$ may be used to calibrate the models. When the Smagorinsky model is used at both grid and test levels, the error is a linear function of the Smagorinsky parameter:

$$E_{ij} = L_{ij} + \widehat{C\beta_{ij}} - C\alpha_{ij} \tag{2.4}$$

where

$$\alpha_{ij} = -2\widehat{\overline{\Delta}}^2 |\widehat{\overline{S}}|\widehat{\overline{S}}_{ij}$$
$$\beta_{ij} = -2\overline{\Delta}^2 |\overline{S}|\overline{S}_{ij}$$

The calibration of C is usually achieved by using a least square method for minimizing E_{ij}. The integral

$$I[C] = \int_V d\mathbf{y} \sum_{ij} E_{ij}^2(\mathbf{y}) \tag{2.5}$$

is thus minimized with respect to C.

A first difficulty encountered when using the dynamic procedure for determining C has been pointed out by Ghosal *et al* (1993,1995), who showed that this procedure requires the solution of an integral equation for C unless both of the following conditions are satisfied:

1. There are one or more directions of homogeneity in the flow.
2. The flow is fully resolved in the other direction(s).

In that case, C is assumed to be constant along the direction of homogeneity and can be taken out of the test filter operation $\widehat{\ }$. Moreover, the flow being fully resolved in the other direction(s), the test filter must only act in the homogeneous direction. The error (2.4) then reduces to:

$$E_{ij} = L_{ij} + CM_{ij} \tag{2.6}$$

where $M_{ij} = \alpha_{ij} - \widehat{\beta_{ij}}$ and the dynamic prediction for C reads:

$$C = \frac{\langle L_{ij} M_{ij} \rangle_h}{\langle M_{ij} M_{ij} \rangle_h}$$

where the brackets $\langle\ \rangle_h$ represent a spatial average in the homogeneous direction(s). If the two aforementioned conditions for replacing expression (2.4) by (2.6) are not fulfilled, one could argue that C is slowly varying in space and that (2.6) should be a valid approximation independently of the existence of a direction of homogeneity. The minimization of the global quantity $I[C]$ then leads to a local expression for C:

$$C = \frac{L_{ij} M_{ij}}{M_{ij} M_{ij}},$$

Unfortunately, this approximation has proved to be very poor, and the resulting C depends strongly on space. Since in almost all LES's at least one of the aforementioned conditions is violated, a mathematically clean implementation of the dynamic model always requires the solution of an integral equation (Ghosal *et al.* 1995).

A second difficulty with the dynamic model is that C takes negative as well as positive values. Positive values correspond to the classical eddy dissipation picture for the subgrid scales. The negative values were first interpreted as the capability of the dynamic model to predict reverse energy transfer (backscatter). Unfortunately, the modeling of backscatter by a negative Smagorinsky coefficient leads to numerical instabilities. This problem is easily solved by constraining *a priori* the minimization of $I[C]$ so that only positive values of C are accepted. The resulting C (obtained either by solving an integral equation or by using a spatial average) is the same as before but clipped to positive value. Thus, C must then be replaced by $(C + |C|)/2$. Although this clipping procedure can be derived properly from a constrained minimization procedure, it is usually considered an undesirable extension of the dynamic model. In particular, the clipping corresponds to turning off the model where the dynamic procedure "tries to build a model for backscatter." In some sense, the resulting model does not use all the information available from the dynamic procedure. Hence, it is desirable to have a dynamic model with as few clipped values as possible for C.

We will discuss in the following sections how the simultaneous use of several statistically equivalent LES's may solve these two difficulties.

3 Statistical LES & dynamic model

3.1 Definition of the ensemble

We first discuss the problem of defining the ensemble of runs needed for the statistical tests without considering the modeling problem. The equations (1.3) correspond to R different LES's. In order to have a "good" ensemble, these LES's should correspond to *statistically equivalent* and *statistically independent* realizations of the same problem. Although these requirements are intuitively clear, it is worthwhile to define them as properly as possible. The first step consists in defining precisely what is an "acceptable" simulation for a given problem. From the strict mathematical point of view, a flow described by the Navier-Stokes equation or by an LES equation is completely defined by the knowledge of

1. The domain $\mathcal{D}$ in which the flow is considered.
2. The conditions on the boundary $\partial\mathcal{D}$ of this domain $v(\partial\mathcal{D}, t) = f(t)$.
3. The initial conditions $v(\mathbf{x}, 0) = v_0(\mathbf{x}) \quad \forall x \in \mathcal{D}$.

However, in a simulation of a turbulent flow only the domain and the boundary conditions are rigorously fixed. Indeed, because of the lack of sensitivity to initial conditions in a turbulent flow, different simulations with different initial conditions sharing some properties are considered to characterize the same flow. Thus, the

requirement that the initial conditions are known is usually replaced by some weaker constraints, and point (3) is replaced by

3'. The initial conditions $v(\mathbf{x},0) = v_0(\mathbf{x};w_l)$ are generated using random numbers w_l and satisfy some constraints: $P_s[v_0] = p_s, \quad s = 1,\dots S.$

For example, in homogeneous turbulence, the first constraint $s = 1$ will be on the spectrum of v_0. For the channel flow, one could impose the profile of the velocity and of the fluctuation in each direction. We will not discuss in detail the minimal constraints that must be imposed on the initial conditions in order to have a reasonable simulation. We only suppose that these constraints do exist. Now, it is possible to give some precise definition of the ensemble of LES's:

Definition 1: *Two LES's are* **statistically equivalent** *if the domain of the flow and the boundary conditions are exactly the same and if the initial conditions satisfy the same set of constraints.*

Definition 2: *Two LES's are* **statistically independent** *if the initial conditions are generated with uncorrelated random numbers* w_l.

For a stationary flow, such equivalent and independent initial conditions can be obtained by running a single LES and recording several velocity fields separated by at least one large eddy turnover time when turbulence is fully developed.

3.2 Ensemble average dynamic model

In what follows, we will focus on a simple generalization of the Smagorinsky model which reads:

$$\tau_{ij}^r - \frac{1}{3}\tau_{kk}^r\delta_{ij} \approx -2C\overline{\Delta}^2|\overline{S^r}|\overline{S}_{ij}^r. \tag{3.2.1}$$

Thus, we basically use the Smagorinsky model in every realization with the following additional assumption :

Hypothesis 1: *The Smagorinsky coefficient is independent of the realization for statistically equivalent flows.*

This assumption defines the model in such a way that the unknown parameter in the LES is "universal". The formulation thus mixes some aspects of both LES and Reynolds average simulations.

The dynamic procedure can also be used to determine C when several LES's are run in parallel. In that case, the model depends on the resolved flow from other realizations (1.3). Indeed, the quantity that needs to be minimized is a straightforward generalization of $I[C]$:

$$\mathcal{I}[C] = \sum_r \int_V d\mathbf{y} \sum_{ij} \left(E_{ij}^r(\mathbf{y})\right)^2 \tag{3.2.2}$$

where now E_{ij} as well as L_{ij}, β_{ij}, and α_{ij} depend on the realization ($E_{ij}^r = L_{ij}^r + \widehat{C\beta_{ij}^r} - C\alpha_{ij}^r$). We now make another assumption:

Hypothesis 2: *For large ensembles, the Smagorinsky coefficient is slowly dependent on space and can be taken out of the test filter.*

The quantity $\mathcal{I}[C]$ then reduces to

$$\mathcal{I}[C] = \sum_{r=1}^{R} \sum_{ij} \left(L_{ij}^r - C\, M_{ij}^r\right)^2,$$

which leads to the same expression for C as in the spatial average version of the dynamic procedure:

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

where now the brackets represent an ensemble average. We will see in the next section that hypothesis 2 is very well justified by the numerical results.

3.3 Alternative formalism for the dynamic model

The usual formulation of LES Eq. (1.1) is not fully satisfactory because the evolution of the filtered velocity is given in terms of quantities that are not filtered, whereas all numerically computed quantities are filtered in some way. This is well known, but, to our knowledge, its effect on the dynamic model formulation has never been carefully considered. In this section, we propose an alternative dynamic model formulation which should be fully self-consistent with the filtered equation for the resolved field. First, we assume that all the quantities in the LES equation are filtered and Eq. (1.1) must then be replaced by

$$\partial_t \overline{u}_i = \nu_0 \nabla^2 \overline{u}_i - \partial_j \overline{\overline{u}_j \overline{u}_i} - \partial_j \overline{\tau}_{ij} - \partial_i \overline{p}. \tag{3.3.1}$$

This redefines the subgrid scale stress as

$$\overline{\tau}_{ij} = \overline{u_i u_j} - \overline{\overline{u}_i\, \overline{u}_j}$$

The application of the test filter to the LES equation (3.3.1) yields:

$$\partial_t \widehat{\overline{u}}_i + \partial_j \widehat{(\overline{\overline{u}_j \overline{u}_i})} = \nu_0 \nabla^2 \widehat{\overline{u}}_i - \partial_i \widehat{\overline{p}} - \partial_j \widehat{\overline{\tau}}_{ij} - \partial_j \widehat{\overline{L}}_{ij},$$

and the comparison with the "one-step" application of G_2 to u_i leads to the following equality:

$$\widehat{\overline{L}}_{ij} + \widehat{\overline{\tau}}_{ij} - \widehat{\overline{T}}_{ij} = 0. \tag{3.3.2}$$

where now

$$\widehat{\overline{L}}_{ij} = \widehat{\overline{\overline{u}_i \overline{u}_j}} - \widehat{\overline{\overline{u}}_i \overline{\overline{u}}_j},$$

$$\widehat{\overline{T}_{ij}} = \widehat{\overline{u_i\, u_j}} - \widehat{\overline{\overline{u}}_i\, \overline{\overline{u}}_j}.$$

At this point it is important to ensure that the model for the subgrid scale is also expressed in terms of a filtered quantity. The simplest generalization of the Smagorinsky model would then be $\overline{\tau_{ij}} = \overline{C\beta_{ij}}$ and $\widehat{\overline{T_{ij}}} = \widehat{\overline{C\alpha_{ij}}}$. The dynamic procedure is then easily implemented and yields

$$C = \frac{\langle \widehat{\overline{L}}_{ij} \widehat{\overline{N}}_{ij} \rangle}{\langle \widehat{\overline{N}}_{ij} \widehat{\overline{N}}_{ij} \rangle} \tag{3.3.3}$$

where $N_{ij} = \beta_{ij} - \alpha_{ij}$. Of course, the expression (3.3.3) also relies on the assumption that C can be taken out from the filtering operators. This assumption is very important here because, in the equality (3.3.2), the Smagorinsky coefficient only appears in filtered quantities. This means that the integral equation formulation of this alternative dynamic model would be much more complicated than the classical formalism. However, if hypothesis 2 is valid, the present formalism appears to be more consistent with the LES equation.

4. Test on isotropic turbulence

4.1 Decaying turbulence

The statistical average dynamic model described in section 3.1 has been tested in decaying turbulence for 32^3 LES. A first series of numerical experiments have determined how large the ensemble of simultaneous LES's must be (*i.e.* how large R should be). The criteria used to determine the minimal size of the ensemble were focused on

1. The spatial variability of C.
2. The percentage of negative C.
3. Comparison with the volume average dynamic model.
4. Comparison with direct numerical simulations.

The first conclusion we have reached is quite encouraging. Indeed, it appears that with only 16 simultaneous LES's, the ensemble average dynamic model performs as well as the volume average model. The spatial variability of C decreases drastically when R increases (see Fig. 1). This is also reflected on the probability distribution function (PDF) of C (see Fig. 2).

The comparison between a 512^3 DNS and dynamic model shows good agreement both for the total resolved energy (see Fig. 3) and for the spectra. The results for $R = 16$ are indistinguishable for the volume average and for the ensemble average. Here the comparison with the dynamic model has been made by running an ensemble of unrelated volume average LES's. This allows comparison of the both the means and the standard deviations. The standard deviations are computed for the 3-d energy spectra at each k, and quantities such as total resolved energy and compensated spectra are then computed from the mean and mean$\pm\sigma$ spectra.

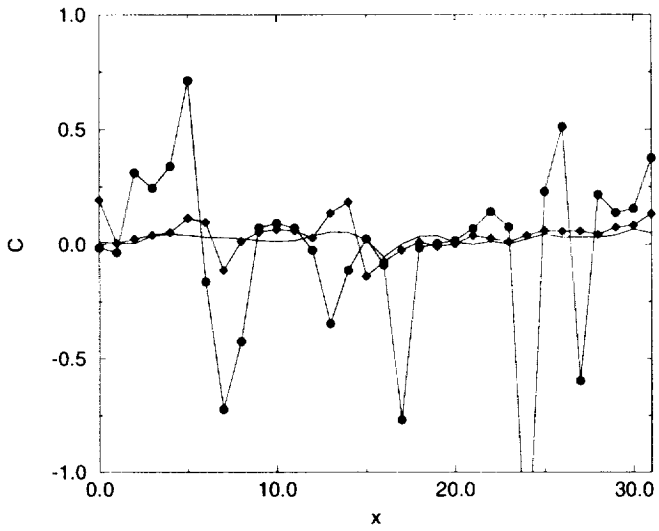

FIGURE 1. Typical profile of C in decaying isotropic turbulence. R=1:—● — ; R=4:— ◆ — ; R=16:——— .

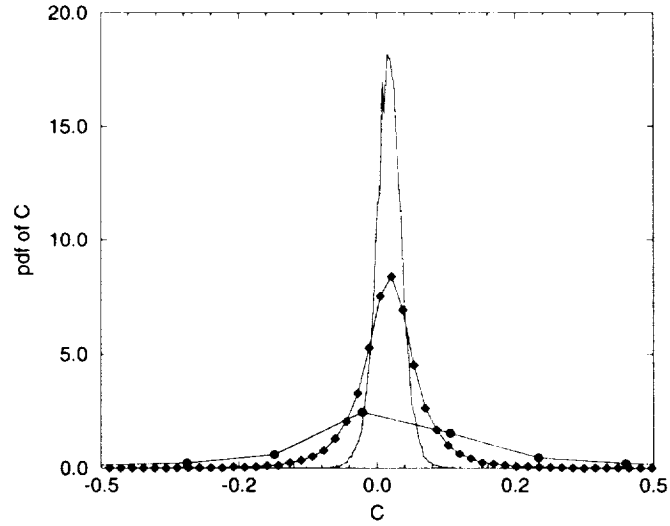

FIGURE 2. PDF of C in decaying isotropic turbulence. Symbols as in Fig. 1.

4.2 Forced turbulence

We have run an ensemble of 32^3 forced turbulence LES's with zero molecular viscosity. Fig. 4 shows that the mean resolved energy and the standard deviation evolve in a very similar way for both the volume and the ensemble average models.

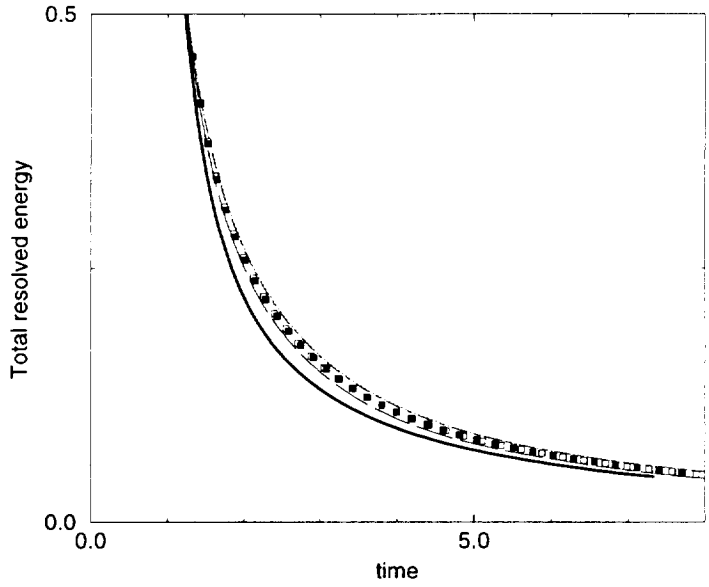

FIGURE 3. Energy decay: comparison with DNS and volume average. DNS:——— ; ensemble-averaged (mean):□ ; ensemble-averaged (mean+sigma):— - — ; ensemble-averaged (mean-sigma):— — — ; volume-averaged (mean):■ ; volume-averaged (mean+sigma):····· ; volume-averaged (mean-sigma):- - - -

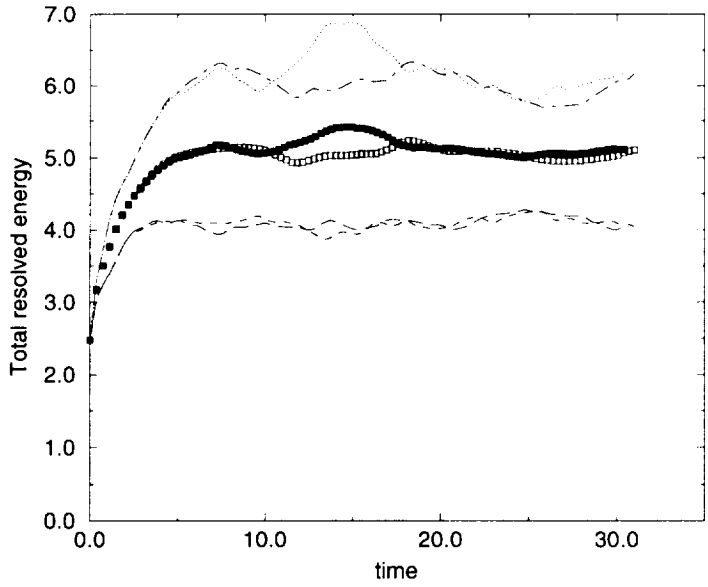

FIGURE 4. Resolved energy in forced isotropic turbulence: average vs volume. Symbols as in Fig. 3, without DNS.

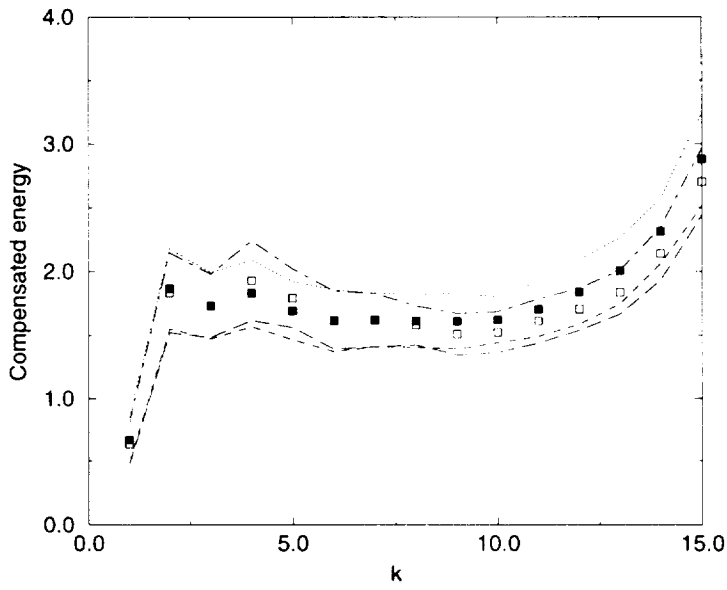

FIGURE 5. Compensated energy spectrum in forced isotropic turbulence: average vs volume. Symbols as in Fig. 3.

It is also very important to notice that the standard deviation saturates so that the LES's in the ensemble do not evolve towards very different states.

It is also interesting to compare the compensated energy spectrum to check if an inertial range is observed. Of course, with 32^3 LES, we do not expect to obtain a very good estimate of the Kolmogorov constant. However, the results in Fig. 5 show that the observed "Kolmogorov constant" is in a reasonable range of values. These spectra are at time ≈ 27 in the units of Fig. 4.

5. Tests in channel flow

We did not reach the stage of "production runs" for the channel flow, so the tests presented here are very preliminary and have been focused on the behavior of C as a function of the ensemble size (R). The data collected from the runs concern the PDF of C and the fraction of negative C. Because of the channel flow inhomogeneity, the PDF of C depends on the wall normal coordinate. However, the trends for increasing numbers of runs (R) is similar across the channel, and we only present in Fig. 6 the results for $y = 0.1$ near midchannel.

We also show the fraction of negative C (Fig. 7). Since the channel flow simulations used in these tests have a non-zero molecular viscosity, the relevant stability condition is the percentage of C leading to a total (molecular + eddy) negative viscosity. Here again, the results are encouraging for $R \approx 16$ (less than 15% of the points need to be clipped) while the local version of the dynamic model for only one LES requires about 40% clipping.

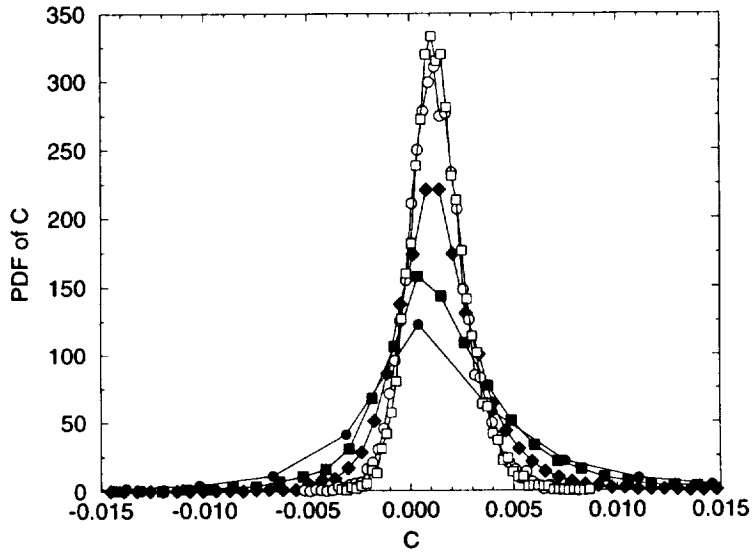

FIGURE 6. Probability distribution function of C for different ensemble sizes at $y = 0.1$. R=1:● ; R=2:■ ; R=4: ◆ ; R=8;o ; R=16:□ .

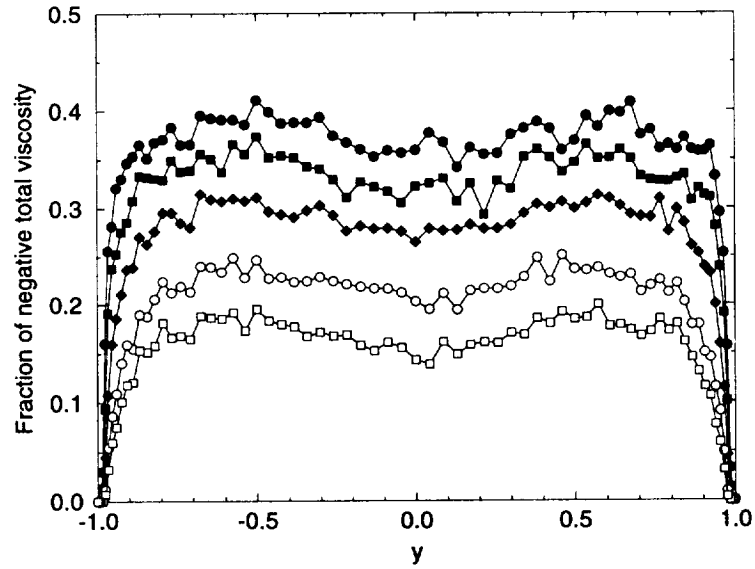

FIGURE 7. Fraction of negative total viscosity as a function of y for different ensemble sizes. Symbols as in Fig. 6.

6. Conclusion

The statistical tests presented in this report have shown that the knowledge of statistically equivalent resolved velocity fields may be useful in deriving new subgrid scale models. We have used the additional information available from the different LES's to create an ensemble average version of the dynamic model. This dynamic model has the following advantages:

1. A local version of the ensemble average dynamic model may be derived in the limit of large ensemble sets.
2. The local formulation does not rely on any homogeneity assumption. It can thus be adapted to any geometry, unlike to the classical volume (or surface or line) average dynamic model.
3. The theoretical limit of large ensemble sets is closely approached for $R \approx 16$. This is indicated by the PDF of C, which is very peaked for $R = 16$. Also, the spatial variations of C decrease drastically for increasing ensemble sizes and seem to be quite mild for $R = 16$.

For the examples treated in this work (decaying and forced isotropic turbulence), the volume average version of the dynamic model is justified. Remarkably, in those cases, the results from the ensemble average and the volume average versions are almost indistinguishable.

The next interesting step in the investigation of statistical LES is to apply this model to fully inhomogeneous problems (for which the mathematically consistent classical dynamic model requires the solution of an integral equation). The additional cost of multiple simultaneous LES's may be ameliorated by a reduction in the time of simulation since the statistics should converge more rapidly.

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