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On the modelling of the subgrid-scale and filtered-scale stress tensors in large-eddy simulation

By DANIELE CARATI[1], GRÉGOIRE S. WINCKELMANS[2] AND HERVÉ JEANMART[2]

[1]Université Libre de Bruxelles, Bruxelles, Belgium

[2]Université catholique de Louvain, Louvain-la-Neuve, Belgium

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The large-eddy simulation (LES) equations are obtained from the application of two operators to the Navier–Stokes equations: a smooth filter and a discretization operator. The introduction *ab initio* of the discretization influences the structure of the unknown stress in the LES equations, which now contain a subgrid-scale stress tensor mainly due to discretization, and a filtered-scale stress tensor mainly due to filtering. Theoretical arguments are proposed supporting eddy viscosity models for the subgrid-scale stress tensor. However, no exact result can be derived for this term because the discretization is responsible for a loss of information and because its exact nature is usually unknown. The situation is different for the filtered-scale stress tensor for which an exact expansion in terms of the large-scale velocity and its derivatives is derived for a wide class of filters including the Gaussian, the tophat and all discrete filters. As a consequence of this generalized result, the filtered-scale stress tensor is shown to be invariant under the change of sign of the large-scale velocity. This implies that the filtered-scale stress tensor should lead to reversible dynamics in the limit of zero molecular viscosity when the discretization effects are neglected. Numerical results that illustrate this effect are presented together with a discussion on other approaches leading to reversible dynamics like the scale similarity based models and, surprisingly, the dynamic procedure.

1. Introduction

The large-scale velocity field $\bar{u}_i$ described by a large-eddy simulation (LES) is usually regarded as the convolution between the velocity u_i and a filter that smooths the high wavenumber (i.e. short wavelength) structures (Leonard 1974):

$$\bar{u}_i(x) = \int G_r(x-y)\, u_i(y)\, \mathrm{d}y, \tag{1.1}$$

where G_r represents the filter kernel in real space (G will be used for the filter kernel in wave space). For an incompressible flow, the LES equations based on the filter G_r read:

$$\partial_t \bar{u}_i + \partial_j(\bar{u}_j \bar{u}_i) = -\partial_j \tau_{ij} - \partial_i \bar{p} + \nu \nabla^2 \bar{u}_i, \tag{1.2}$$

where ν is the molecular viscosity, p is the pressure and $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$ is an additional stress that is not expressed in terms of the filtered velocity. It will be represented here as the commutator between the operators ‘product’ and ‘filtering’, acting on the complete velocity u_i. We do not consider here possible commutation errors between the filtering and the derivation operators. Although these effects might be important in some cases, their inclusion in the present work would obfuscate some of the results we want to stress. The description given by (1.2) is, however, only an ideal picture of the LES since the filtered velocity field defined by (1.1) cannot, for most filters, be represented on a numerical grid without further approximation (representing discretization errors). The necessary discretization procedure required for solving the LES equations can thus be seen as an additional operator $\mathscr{D}$ applied to the filtered equation (1.2). The quantity predicted by the discrete LES equations is thus:

$$\tilde{\bar{u}}_i = \mathscr{D}[\bar{u}_i]. \tag{1.3}$$

The exact nature of the operator $\mathscr{D}$ is usually unknown. For numerical schemes using a basis of orthogonal functions, such as the Fourier waves or the Chebyshev polynomials, $\mathscr{D}$ is simply a projector into a finite subset of these functions. However, for finite-difference schemes, the operator $\mathscr{D}$ is not clearly defined. In the following, we will systematically assume that the filtering and the discretization operations are commutative ($\tilde{\bar{u}}_i = \bar{\tilde{u}}_i$). The LES equations that are actually computed thus correspond to:

$$\partial_t \bar{\tilde{u}}_i + \partial_j \widetilde{\bar{\tilde{u}}_j \bar{\tilde{u}}_i} = -\partial_j \widetilde{\mathscr{T}_{ij}} - \partial_i \bar{\tilde{p}} + \nu \nabla^2 \bar{\tilde{u}}_i, \tag{1.4}$$

where the stress to be modelled is given by the discretized version of $\mathscr{T}_{ij} = \overline{u_i u_j} - \bar{\tilde{u}}_i \bar{\tilde{u}}_j$. We have deliberately written the nonlinear term as the application of the operator $\mathscr{D}$ on the product $\bar{\tilde{u}}_j \bar{\tilde{u}}_i$ since we assume that all the terms in the LES equations are discretized in the same way. For a pseudospectral code, this amounts to assuming that the code is de-aliased.

Clearly, the total LES stress $\mathscr{T}_{ij}$ takes its origin from two different ranges of velocity scales. First, $\mathscr{T}_{ij}$ depends on the scales that are outside the resolution domain of the LES. It thus has an explicit subgrid-scale dependence. Secondly, $\mathscr{T}_{ij}$ also depends on the difference between the exact velocity field and the filtered velocity field inside the resolution domain of the LES. Hence, it also has a resolved filtered-scale dependence. In § 2, the total LES stress $\mathscr{T}_{ij}$ is decomposed into two terms closely related to these two different dependences. An exact expansion is derived for the filtered-scale stress tensor in § 3. Phenomenological and numerical arguments are proposed in § 4 that support the modelling of the subgrid-scale stress by an eddy viscosity term. Examples of filtered-scale stress tensors obtained for classical filters are presented in § 5 and the convergence of the expansion is discussed in § 6. As a consequence of the expansion for the filtered-scale stress tensor, it is shown that this tensor cannot be responsible for any irreversible effect in the LES dynamics. This important property is discussed in detail in § 7 and existing models with this property are discussed in § 8. In particular, the dynamic procedure, a recently developed method for calibrating filtered-scale models, is proved to systematically produce reversible models. To our knowledge, this fundamental property of the dynamic procedure has not been widely recognized so far.

2. Filtered-versus subgrid-scale stress tensors

The stress $\mathscr{T}_{ij}$ can be decomposed into two terms:

$$\mathscr{T}_{ij} \equiv \overline{u_i u_j} - \bar{\tilde{u}}_i \bar{\tilde{u}}_j = \underbrace{(\overline{u_i u_j} - \overline{\tilde{u}_i \tilde{u}_j})}_{\overline{\mathscr{A}_{ij}}} + \underbrace{(\overline{\tilde{u}_i \tilde{u}_j} - \bar{\tilde{u}}_i \bar{\tilde{u}}_j)}_{\mathscr{B}_{ij}}. \tag{2.1}$$

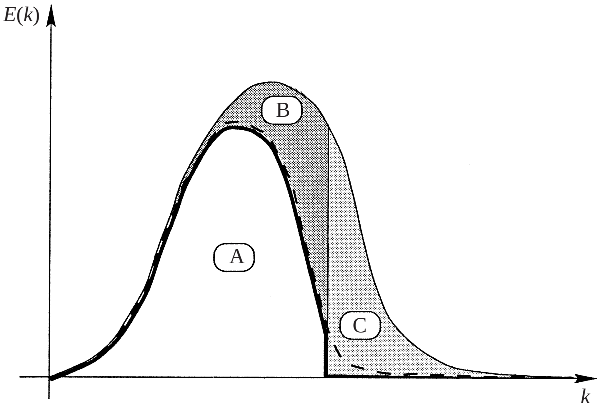

FIGURE 1. Effect of the discretization and of the filtering on a typical turbulent energy spectrum. For simplicity, the discretization is here represented as a sharp Fourier cutoff.

The decomposition (2.1) shows that the total stress contains two terms of very different nature. The first term is obtained by applying the filtering operation to the tensor $\mathscr{A}_{ij} = u_i u_j - \tilde{u}_i \tilde{u}_j$, which represents the difference between the total nonlinear term and the nonlinear term that can be captured on the grid. The second term is closer to the classical stress appearing in the LES equation. It is the commutator between the operators 'product' and 'filtering', acting on the discretized velocity $\tilde{u}_i$: $\mathscr{B}_{ij} = \overline{\tilde{u}_i \tilde{u}_j} - \bar{\tilde{u}}_i \bar{\tilde{u}}_j$. These two terms can be rewritten as follows

$$\mathscr{A}_{ij} = u_i^C u_j^C + (u_i^C u_j^A + u_i^A u_j^C) + (u_i^C u_j^B + u_i^B u_j^C), \tag{2.2}$$

$$\mathscr{B}_{ij} = \overline{(u_i^A + u_i^B)(u_j^A + u_j^B)} - u_i^A u_j^A, \tag{2.3}$$

where the total velocity $u_i = u_i^A + u_i^B + u_i^C$ has been decomposed into three parts. The first term $u_i^A = \bar{\tilde{u}}_i$ is the LES field that is resolved in an actual simulation, whereas $u_i^B = \tilde{u}_i - \bar{\tilde{u}}_i$ is the difference between the total and the LES velocity fields within the numerical domain of the LES. Finally, the remainder $u_i^C = u_i - \tilde{u}_i$ corresponds to scales that are beyond the resolution limit of the scheme used for solving the LES equations numerically. The respective spectral domains of these three contributions to the total velocity are shown in figure 1.

We investigate the important limits obtained when one of the operators G or $\mathscr{D}$ reduces to the unity operator U. The first case, $G \to U$ can be interpreted as the DNS limit since no filter is applied to the Navier–Stokes equations. The following properties are derived straightforwardly from the decomposition of u_i:

$$\lim_{G \to U} u_i^B = 0 \quad \forall \mathscr{D}, \tag{2.4}$$

$$\lim_{G \to U} \mathscr{B}_{ij} = 0 \quad \forall \mathscr{D}. \tag{2.5}$$

Hence, $\mathscr{B}_{ij}$ vanishes for a DNS (when no filtering is applied), independently of the discretization scheme $\mathscr{D}$ used for solving the equations. This tensor is thus mainly generated by the filtering operator and, accordingly, it will be called *filtered-scale stress* tensor. The second limit, $\mathscr{D} \to U$, corresponds to a simulation with an infinite resolution. Again, the following properties are derived straightforwardly from the decomposition of u_i:

$$\lim_{\mathscr{D} \to U} u_i^C = 0 \quad \forall G, \tag{2.6}$$

$$\lim_{\mathscr{D}\to U} \mathscr{A}_{ij} = 0 \quad \forall G. \tag{2.7}$$

Clearly, $\mathscr{A}_{ij}$ vanishes for an infinite resolution, independently of the filter G. Its origin is thus mainly in the discretization procedure. Hence, $\mathscr{A}_{ij}$ corresponds to a *subgrid-scale stress* tensor.

The terminology adopted here is purposely not the classical one. In the LES literature, the tensor $\mathscr{B}_{ij}$ is usually called the subgrid-scale stress tensor. This has caused some confusion since the filtering and the discretization are rarely distinguished. In this work, mathematical and physical motivations will be given for a different modelling of the two contributions to $\mathscr{T}_{ij}$. In particular, in § 3 it is shown that, for a wide class of filters, an exact expansion of the second term $\mathscr{B}_{ij}$ in terms of spatial derivatives of $u_i^A = \tilde{\bar{u}}_i$ can be obtained. As a consequence, there is no closure problem related to this term which can be expressed as $\mathscr{B}_{ij} = \mathscr{B}_{ij}[\tilde{\bar{u}}]$. Moreover, the resulting expression for $\mathscr{B}_{ij}$ has the following property:

$$\mathscr{B}_{ij}(\tilde{\bar{u}}_l) = \mathscr{B}_{ij}(-\tilde{\bar{u}}_l). \tag{2.8}$$

Hence, $\mathscr{B}_{ij}$ is invariant under the change of sign of the resolved LES velocity $\tilde{\bar{u}}_i$.

3. Exact expansion for the filtered-scale stress tensor

In the LES literature, the unknown stress tensor is usually supposed to represent the effects of the filter G only, while the discretization effects are not taken into account explicitly. Such a viewpoint amounts to considering the limit (2.7). However, adopting this limit is not a prerequisite to the derivation of exact results for the filtered-scale stress tensor. The main purpose of this section is to show that $\mathscr{B}_{ij}$ can be expressed, in many cases, in terms of $\tilde{\bar{u}}_i$ without the need for any models and independently of the nature of the discretization operator $\mathscr{D}$.

Before proving that there is no closure problem related to the filtered-scale stress tensor, this property can be easily understood from the expression (2.3). Indeed, $\mathscr{B}_{ij}$ is independent of the unresolved velocity u_i^C. Moreover, if the filtering operator is invertible inside the resolution domain of the LES, then u_i^B can be expressed in terms of u_i^A only. As a consequence, under some constraints on the filter G, $\mathscr{B}_{ij}$ should be a function of the LES velocity $\tilde{\bar{u}}_i = u_i^A$ only, and no closure problem should arise from this term.

3.1. *Known results: the Gaussian filter*

Yeo (1987) – see also Yeo & Bedford (1988) – and Leonard (1997) have both recently and independently derived an expression for the filtered-scale stress in the case of Gaussian filters. Consider first the one-dimensional Gaussian filter given by $\Delta G_r(x) = \exp(-x^2/2\Delta^2)/\sqrt{2\pi}$ and $G(k) = \exp(-k^2\Delta^2/2)$. They have shown that, for any function a and b, the filtered-scale stress can be expressed only in terms of the spatial derivatives of the filtered functions $\bar{a}$ and $\bar{b}$:

$$\overline{ab} - \bar{a}\,\bar{b} = \sum_{n=1}^{\infty} \frac{\Delta^{2n}}{n!} \partial_x^n \bar{a}\, \partial_x^n \bar{b}. \tag{3.1}$$

The extension to the three-dimensional Gaussian filter is easily obtained and can be used for determining $\mathscr{B}_{ij}$:

$$\mathscr{B}_{ij} = \Delta^2\, \partial_k \tilde{\bar{u}}_i\, \partial_k \tilde{\bar{u}}_j + \frac{\Delta^4}{2!}\, \partial_{kl}^2 \tilde{\bar{u}}_i\, \partial_{kl}^2 \tilde{\bar{u}}_j + \frac{\Delta^6}{3!}\, \partial_{klm}^3 \tilde{\bar{u}}_i\, \partial_{klm}^3 \tilde{\bar{u}}_j + \cdots, \tag{3.2}$$

where we assume summation over the repeated indices. This result can also be extended to an anisotropic three-dimensional Gaussian filter with $\Delta_1 \neq \Delta_2 \neq \Delta_3$:

$$\mathscr{B}_{ij} = \sum_k \Delta_k^2\, \partial_k \tilde{\bar{u}}_i\, \partial_k \tilde{\bar{u}}_j + \sum_{kl} \frac{\Delta_k^2 \Delta_l^2}{2!}\, \partial_{kl}^2 \tilde{\bar{u}}_i\, \partial_{kl}^2 \tilde{\bar{u}}_j + \sum_{klm} \frac{\Delta_k^2 \Delta_l^2 \Delta_m^2}{3!}\, \partial_{klm}^3 \tilde{\bar{u}}_i\, \partial_{klm}^3 \tilde{\bar{u}}_j + \cdots . \quad (3.3)$$

In some sense, the expansion (3.1) gives the exact model LES practitioners have always been looking for. Obviously, this model is not directly implementable since it requires the evaluation of an infinite number of terms. Moreover, in the realistic case where the LES is performed with a limited resolution, only a few spatial derivatives can be computed with confidence starting from an actual LES field. Nevertheless, this result is very important since it shows that, for LES based on the Gaussian filter, a mathematical expression can be derived for the filtered-scale stress tensor $\mathscr{B}_{ij}$. In the following section, we extend this result to a wide class of filters.

3.2. *General expansion for the filtered-scale stress tensor*

We now show that the expansion (3.1) can be generalized for a wide class of filters. In order to simplify the developments, only one-dimensional filters are considered in the first step. Let us consider that the kernel of the filter defined by equation (1.1) has a Fourier transform, $G(k)$, which is C^∞. This is true for most filters that are defined in real space such as the Gaussian, the tophat and all the discrete filters $[G_r(x) = \sum_i \delta(x - x_i)]$. In addition, we introduce two fields $a(x)$ and $b(x)$ for which the Fourier transform is assumed to exist. The first part of this section proves that there always exists a generalized expansion of the form:

$$\overline{ab} = \sum_{r,s=0}^{\infty} c_{rs}\, \partial_x^r \bar{a}\, \partial_x^s \bar{b}. \quad (3.4)$$

It is then shown how to derive the coefficients c_{rs} from a generating function. The proof consists of writing the assumed expansion in Fourier space:

$$G(k) \int \mathrm{d}q\, a(q)\, b(k-q) = \sum_{r,s=0}^{\infty} c_{rs} \int \mathrm{d}q\, (\mathrm{i}q)^r\, G(q)\, a(q)\, (\mathrm{i}(k-q))^s\, G(k-q)\, b(k-q). \quad (3.5)$$

Assuming that integration and summation commute, we have, on both sides of (3.5), an expression of the type $\int \mathrm{d}q\, a(q)\, b(k-q)\, Z(q,k)$ where Z is a function of the wavevectors k and q and of the Fourier transform of the filter. Since the expansion should be true for any fields a and b, we have to prove the equality between the Z terms. This leads to

$$G(k) = \sum_{r,s=0}^{\infty} c_{rs}\, (\mathrm{i}q)^r\, (\mathrm{i}(k-q))^s\, G(q)\, G(k-q). \quad (3.6)$$

We now introduce the function $F[\phi,\psi]$ defined by its double Taylor expansion $F[\phi,\psi] = \sum_{r,s} c_{rs} \phi^r \psi^s$. Using the change of variable $q = -\mathrm{i}\phi$, $(k-q) = -\mathrm{i}\psi$ and $k = -\mathrm{i}(\phi + \psi)$, it is easy to verify that expansion (3.4) is valid if and only if it is possible to define the real function F as

$$F[\phi,\psi] = \frac{G(-\mathrm{i}(\phi+\psi))}{G(-\mathrm{i}\phi)\, G(-\mathrm{i}\psi)}. \quad (3.7)$$

This will always be true for symmetric filters (i.e. that are such that $G(k) = G(-k)$) since, in this case, F will be invariant under the change $\mathrm{i} \to -\mathrm{i}$ and thus F will be real. Hence, we conclude that, for all the symmetric filters, it is possible to derive a generalized expansion (3.4). At this point, it is convenient to adopt the scaling convention that the width of the filter is given by the following formula:

$$\Delta^2 = \int_{-\infty}^{+\infty} x^2\, G_r(x)\,\mathrm{d}x = -\left.\frac{\mathrm{d}^2 G}{\mathrm{d}k^2}\right|_{k=0}. \tag{3.8}$$

This expression assumes filters that have a well-defined and non-zero second moment in real space. The leading terms in the multiple Taylor expansion of $F[\phi,\psi]$ are easily obtained from (3.7) using the normalization property of the filter ($G(0)=1$) and the symmetry ($G(-k)=G(k)$):

$$F[\phi,\psi] = 1 - \left.\frac{\mathrm{d}^2 G}{\mathrm{d}k^2}\right|_{k=0} \phi\psi + \cdots\ . \tag{3.9}$$

The generalized expansion (3.4) thus always starts with:

$$\overline{ab} - \bar{a}\,\bar{b} = \Delta^2\, \partial_x \bar{a}\, \partial_x \bar{b} + \cdots\ . \tag{3.10}$$

We stress that this result is valid for any symmetric filter with a well-defined second moment in real space. Let us mention that filters with a vanishing second moment have been recently considered (Vasilyev, Lund & Moin 1998) in the study of the commutation error between the filtering and the differentiation. However, the most commonly used filters do have a non-vanishing second moment. It is also interesting to note that this proof of the existence of the generalized expansion gives a very simple way to explicitly construct the series in (3.4). The Taylor coefficients of the function $F[\phi,\psi]$ are simply the coefficients that appear in the expansion. Hence, $F[\phi,\psi]$ is the generating function of the generalized expansion (3.4).

The case of three-dimensional filters is a direct generalization of the one-dimensional filters. The generalized expansion for the filtered-scale stress tensor reads:

$$\mathscr{B}_{ij} = \sum_{r_1,s_1=0}^{\infty} \sum_{r_2,s_2=0}^{\infty} \sum_{r_3,s_3=0}^{\infty} c_{r_1r_2r_3s_1s_2s_3}\, (\partial_1^{r_1}\, \partial_2^{r_2}\, \partial_3^{r_3}\, \tilde{\bar{u}}_i)\, (\partial_1^{s_1}\, \partial_2^{s_2}\, \partial_3^{s_3}\, \tilde{\bar{u}}_j), \tag{3.11}$$

where ∂_j represents the derivative with respect to x_j. The coefficients $c_{r_1r_2r_3s_1s_2s_3}$ are obtained from the Taylor expansion of the function:

$$F[\phi_1,\phi_2,\phi_3,\psi_1,\psi_2,\psi_3] = \frac{G(-\mathrm{i}(\boldsymbol{\phi}+\boldsymbol{\psi}))}{G(-\mathrm{i}\boldsymbol{\phi})\, G(-\mathrm{i}\boldsymbol{\psi})}, \tag{3.12}$$

where G is a function of a vector variable. Very often, three-dimensional filters are taken as the product of three one-dimensional filters. In this case, the coefficients factorize $c_{r_1r_2r_3s_1s_2s_3} = c^1_{r_1s_1} c^2_{r_2s_2} c^3_{r_3s_3}$ and the parameters $c^j_{r_js_j}$ ($j = 1,\ldots,3$) are obtained from the Taylor expansion of the function

$$F^j[\phi,\psi] = \frac{G^j(\mathrm{i}(\phi+\psi))}{G^j(\mathrm{i}\phi)\, G^j(\mathrm{i}\psi)}, \tag{3.13}$$

where $G^j(k)$ is the one-dimensional filter in the jth dimension. The particular case of the three-dimensional Gaussian filter has already been given in (3.2).

We conclude this section by stressing that the result (3.11) is independent of the discretization operator. Its validity clearly depends on the type of filter used in the LES (which is here assumed to be symmetric and C^∞). However, the combination of the discretization and the filtering operator makes this condition not very restrictive.

Examples and further discussion on the consequences of the expansion (3.11) will be presented in §§4–6.

4. Modelling of the subgrid-scale stress tensor

So far, we have focused on the description of the filter-scale stress tensor. However, in a practical LES, the subgrid-scale stress tensor cannot be neglected. Indeed, an LES in which the subgrid-scale stress tensor is negligible contains as much information as a DNS. Hence, we must conclude that any practical LES approach will require some information loss. Since $\tilde{\mathscr{B}}_{ij}$ can be expressed exactly as a function of the resolved LES field independently of the discretization scheme $\mathscr{D}$, the expected information losses in an LES must have their origin in the subgrid-scale stress tensor $\tilde{\tilde{\mathscr{A}}}_{ij}$. This property is quite obvious when considering the expressions (2.2) and (2.3). Indeed, the information losses are represented by the unresolved velocity u_i^C which only appears in $\tilde{\tilde{\mathscr{A}}}_{ij}$. Since the information contained in u^C is not accessible in an LES, there is no chance of reconstructing the term $\tilde{\tilde{\mathscr{A}}}_{ij}$ from a purely mathematical analysis. Modelling is thus required for taking into account the subgrid-scale stress.

The subgrid-scale tensor appears in the equation for u^A and, following the expression (2.2), it will correspond to triad interaction with modes from $\{u^A, u^C, u^C\}$ for the term $\mathscr{A}_{ij}^{ACC} \equiv u_i^C u_j^C$, with modes from $\{u^A, u^A, u^C\}$ for the term $\mathscr{A}_{ij}^{AAC} \equiv u_i^C u_j^A + u_i^A u_j^C$ and with modes from $\{u^A, u^B, u^C\}$ for the term $\mathscr{A}_{ij}^{ABC} \equiv u_i^C u_j^B + u_i^B u_j^C$. Although strictly speaking u^A and u^B have the same spectral support, the effect of the filtering is such that we can, as a first approximation, consider u^A as the large-scale field and u^B as the intermediate-scale field (see figure 1). Therefore, $\mathscr{A}_{ij}^{ABC}$ could be regarded as a local triad interaction, while $\mathscr{A}_{ij}^{ACC}$ and $\mathscr{A}_{ij}^{AAC}$ correspond to non-local triad interactions. If, for any reason, $\mathscr{A}_{ij}^{ABC}$ could be neglected, then the effective subgrid-scale stress tensor $\tilde{\tilde{\mathscr{A}}}_{ij}$ would mainly correspond to interactions between u^A and u^C. In that case, figure 2 indicates that, owing to the combined effects of the smooth filtering G and of the discretization $\mathscr{D}$, a scale separation might be created between the spectra of u_i^A and u_i^C. This scale separation and the unavoidable information loss due to the discretization would make plausible the modelling of the first two terms in $\tilde{\tilde{\mathscr{A}}}_{ij}$ by an eddy viscosity term:

$$\tilde{\tilde{\mathscr{A}}}_{ij} \approx -2\nu_e \tilde{\tilde{S}}_{ij}, \tag{4.1}$$

where $\tilde{\tilde{S}}_{ij} = \frac{1}{2}(\partial_i u_j^A + \partial_j u_i^A)$ is the filtered and discretized strain rate tensor. We have performed some tests on DNS fields that show that $\mathscr{A}_{ij}^{ABC}$ is indeed small under certain conditions. This does not mean that the dynamics of u^A is entirely dominated by the non-local interactions. Indeed, the filtered-scale stress tensor that also enters the equation for u^A uniquely corresponds to local triad interactions from modes $\{u^A, u^A, u^B\}$ and is supposed to be taken into account thanks to the expansion discussed in the previous section.

Our numerical tests have been carried out on a 256^3 DNS of forced isotropic turbulence. Two quantities have been used to determine whether the term $\mathscr{A}_{ij}^{ABC}$ is negligible or not: the amplitude $\mathscr{Q}$ of $\mathscr{A}_{ij}^{ABC}$ normalized by the total amplitude of the subgrid-scale stress and the fraction $\mathscr{H}$ of the subgrid-scale dissipation generated by

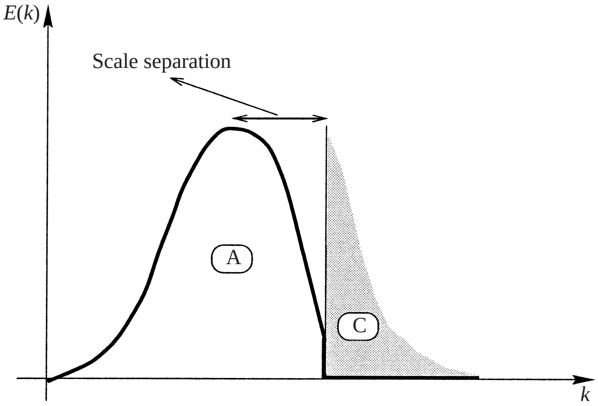

FIGURE 2. The spectra corresponding to domains A and C show that some scale separation does exist between the velocities $u - \tilde{u}$ and $\tilde{\tilde{u}}$.

DNS	LES	Δ	$\mathscr{Q}$	$\mathscr{H}$
256^3	24^3	0.00	0.00	0.00
256^3	24^3	0.05	0.01	0.08
256^3	24^3	0.10	0.10	0.23
256^3	32^3	0.00	0.00	0.00
256^3	32^3	0.05	0.02	0.14
256^3	32^3	0.10	0.19	0.35
256^3	48^3	0.00	0.00	0.00
256^3	48^3	0.05	0.07	0.27
256^3	48^3	0.10	0.36	0.48

TABLE 1. Comparison of the relative amplitude $\mathscr{Q}$ and dissipation $\mathscr{H}$ associated to the term $\mathscr{A}_{ij}^{ABC}$ for various discretizations and various widths of the Gaussian filter.

this term. These quantities are defined by

$$\mathscr{Q} \equiv \frac{\int_V \mathrm{d}^3 r\, \tilde{\tilde{\mathscr{A}}}_{ij}^{ABC}\, \tilde{\tilde{\mathscr{A}}}_{ij}^{ABC}}{\int_V \mathrm{d}^3 r\, \tilde{\tilde{\mathscr{A}}}_{ij}\, \tilde{\tilde{\mathscr{A}}}_{ij}}, \tag{4.2}$$

$$\mathscr{H} \equiv \frac{\int_V \mathrm{d}^3 r\, \tilde{\tilde{\mathscr{A}}}_{ij}^{ABC} \tilde{\tilde{S}}_{ij}}{\int_V \mathrm{d}^3 r\, \tilde{\tilde{\mathscr{A}}}_{ij} \tilde{\tilde{S}}_{ij}}, \tag{4.3}$$

and are reported in table 1. In the DNS, the forcing is acting in a fairly wide range of wavevectors ($2 < k < 10$) in order to produce a field which is not decaying too fast (otherwise u^C is too small for reasonable *a priori* tests). Since our DNSs are obtained with a fully de-aliased pseudospectral code, the natural choice for the discretization operator is the sharp Fourier cutoff. Several levels of discretization have been considered (from 24^3 to 48^3). The type of filter (Gaussian, tophat, ...) appears to have a very weak influence and we report results only for the Gaussian filter. On the

DNS	LES	Δ	$E[u^C]/E$	$E[u^A]/E$	Correlation
256^3	24^3	0.00	0.30	0.70	0.224
256^3	24^3	0.05	0.30	0.58	0.234
256^3	24^3	0.10	0.30	0.37	0.256
256^3	32^3	0.00	0.19	0.81	0.173
256^3	32^3	0.05	0.19	0.64	0.181
256^3	32^3	0.10	0.19	0.38	0.203
256^3	48^3	0.00	0.08	0.92	0.128
256^3	48^3	0.05	0.08	0.51	0.096
256^3	48^3	0.10	0.08	0.38	0.094

TABLE 2. Correlation between the subgrid-scale stress tensor and the discretized and filtered strain rate tensor. The filter is Gaussian. The discretization operator is systematically a sharp Fourier cutoff. The ratio $E[u^C]/E$ and $E[u^A]/E$ refer to the fraction of energy captured by u^C and u^A, respectively.

contrary, the value of the filter width is shown to play a very important role. The value of the filter width has been chosen so that the fraction of the energy captured by u^A, i.e. the actual LES field, is always larger than 35% of the DNS energy (this fraction of captured energy by u^A is reported in table 2). It appears clearly that, in most of the cases, the term $\mathscr{A}_{ij}^{ABC}$ does not contribute to a large fraction of the amplitude of the total subgrid-scale stress. The contribution of this term to the subgrid-scale dissipation is, however, not always negligible. These results support, or at least do not contradict, the theoretical arguments leading to the eddy viscosity model for $\tilde{\tilde{\mathscr{A}}}_{ij}$. The measure (reported in table 2) of the correlation between $\tilde{\tilde{\mathscr{A}}}_{ij}$ and $\tilde{\tilde{S}}_{ij}$ using *a priori* tests gives a more direct evaluation of the possible performance of the model (4.1).

According to the results of *a priori* tests of table 2, the modelling of the discretization error (represented by $\tilde{\tilde{\mathscr{A}}}_{ij}$) in terms of an eddy viscosity model might be a rather crude approximation. The maximal correlation of $\tilde{\tilde{\mathscr{A}}}_{ij}$ with the strain rate tensor in our DNS is indeed of the order of 0.25. Increasing the filter width should correspond to a wider spectral gap between u^A and u^C. When u^C contains a significant part of the total energy, it appears that the correlation between $\tilde{\tilde{\mathscr{A}}}_{ij}$ and $\tilde{\tilde{S}}_{ij}$ is increasing with the spectral gap, supporting the idea that the eddy viscosity picture is somewhat better justified in that case. However, for well-resolved LES (48^3), the correlation is small and even decreases with the filter width.

As a conclusion of this section, the model for $\tilde{\tilde{\mathscr{A}}}_{ij}$ might be seen as the necessary additional ingredient in the equation for $\tilde{\tilde{u}}_i$, the role of which is to ensure that the numerical solution of this equation remains correctly captured on the grid. In this case, adding a subgrid-scale viscosity probably corresponds to the simplest approach without any pretension on modelling correctly the interaction between resolved and unresolved scales. On the other hand, models based on the exact expansion for $\mathscr{B}_{ij}$ will provide an excellent approximation of the interactions between filtered and unfiltered scales in the resolution domain of the LES. This discussion strongly motivates the use of mixed models for the total effective stress $\tilde{\mathscr{T}}_{ij}$ (see e.g. Vreman, Geurts & Kuerten 1996, 1997; Winckelmans *et al.* 1998, 2001; Leonard & Winckelmans 1999),

$$\tilde{\mathscr{T}}_{ij} \approx \Delta^2(\widetilde{\partial_k\tilde{\tilde{u}}_i\,\partial_k\tilde{\tilde{u}}_j}) - 2\nu_e\tilde{\tilde{S}}_{ij}, \tag{4.4}$$

which have already proved to be good candidates for modelling the effective stress appearing in the LES equations.

5. Examples of exact expansions for the filtered-scale stress tensor

The explicit expression for the expansion (3.4) in the case of the Gaussian filter has already been presented. We show here how this expansion is trivially derived from the generating function $F[\phi, \psi]$ and extend this result to the tophat filter and to discrete filters.

5.1. *One-dimensional Gaussian filter*

The one-dimensional Gaussian filter considered before satisfies the normalization (3.8). It is an easy matter to show that the function $F[\phi, \psi]$ defined by (3.7) is $F[\phi, \psi] = \exp(\phi\psi\Delta^2)$. The proof of (3.1) is then straightforward. Since F is a function of the product $\phi\psi$ only, its multiple Taylor series only has diagonal terms:

$$F[\phi, \psi] = \sum_{r=0}^{\infty} \frac{\Delta^{2r}}{r!} \phi^r \psi^r, \tag{5.1}$$

and the expansion (3.4) reads:

$$\overline{ab} = \sum_{r=0}^{\infty} \frac{\Delta^{2r}}{r!} \partial_x^r \bar{a}\, \partial_x^r \bar{b}. \tag{5.2}$$

5.2. *One-dimensional tophat filter*

The one-dimensional tophat filter that follows normalization (3.8) is given in Fourier space by $G(k) = \sin(\sqrt{3}k\Delta)/(\sqrt{3}k\Delta)$. Using the property $\sin(\mathrm{i}\phi) = \mathrm{i}\sinh(\phi)$, and expanding $\sinh(\phi + \psi)$ the function F simplifies to:

$$F[\phi, \psi] = (\coth(\sqrt{3}\phi\Delta) + \coth(\sqrt{3}\psi\Delta)) \frac{\sqrt{3}\Delta\phi\psi}{\phi + \psi}. \tag{5.3}$$

In this case, the general expression for the coefficient c_{rs} is not as simple as in the case of the Gaussian. The leading terms in the expansion of F are obtained as:

$$F[\phi, \psi] = 1 + \Delta^2\phi\psi - \frac{\Delta^4}{5}\phi\psi(\phi^2 - \psi\phi + \psi^2) + \cdots, \tag{5.4}$$

and thus

$$\overline{ab} - \bar{a}\,\bar{b} = \Delta^2\, \partial_x\bar{a}\, \partial_x\bar{b} - \frac{\Delta^4}{5}(\partial_x^3\bar{a}\, \partial_x\bar{b} - \partial_x^2\bar{a}\, \partial_x^2\bar{b} + \partial_x\bar{a}\, \partial_x^3\bar{b}) + \cdots. \tag{5.5}$$

5.3. *One-dimensional first-neighbour discrete filters*

We call ‘first-neighbour discrete filters’ filters that correspond to a local averaging of the field using the first (grid) neighbours only. These can be defined in real space by a sum of δ functions: $G_r(x) = \beta\delta(x) + (1-\beta)/2(\delta(x+d) + \delta(x-d))$ where d is the grid spacing. In Fourier space, these filters are given by $G(k) = \beta + (1-\beta)\cos(kd)$. The width is thus obtained from the normalization (3.8) as $\Delta^2 = (1-\beta)d^2$. The generating function F is here obtained as

$$F[\phi, \psi] = \frac{\beta + (1-\beta)\cosh((\phi + \psi)d)}{(\beta + (1-\beta)\cosh(\phi d))(\beta + (1-\beta)\cosh(\psi d))}. \tag{5.6}$$

An interesting case arises for the choice $\beta = 0$. This is the case of the 'arithmetical mean' filter: $\bar{a}(x) = \frac{1}{2}(a(x+d) + a(x-d))$ and $G(k) = \cos(kd)$. The function F then simplifies into a product of functions of ϕ and ψ only:

$$F[\phi, \psi] = 1 + \tanh(\phi d) \tanh(\psi d), \tag{5.7}$$

and the expansion (3.4) reads:

$$\overline{ab} - \bar{a}\,\bar{b} = \left(\sum_{r=1}^{\infty} \tilde{c}_r\, \partial_x^r \bar{a} \right) \left(\sum_{r=1}^{\infty} \tilde{c}_r\, \partial_x^r \bar{b} \right), \tag{5.8}$$

where the coefficients $\tilde{c}_r$ are obtained from the Taylor series expansion of the function: $\tanh(x) = x - \frac{x^3}{3} + \frac{2x^5}{15} - \cdots$.

Another interesting case is the choice $\beta = \frac{2}{3}$. This case corresponds to what LES practitioners usually use as an 'approximate way of applying the tophat filter using grid values'. It has $\Delta^2 = 4d^2$, and thus $\Delta = 2d$. It is easily obtained as the Simpson quadrature for the integral:

$$\bar{a}(x) = \frac{1}{2d} \int_{x-d}^{x+d} a(y)\,\mathrm{d}y \approx \tfrac{2}{3} a(x) + \tfrac{1}{6}(a(x+d) + a(x-d)). \tag{5.9}$$

6. Convergence of the expansion for the filtered-scale stress tensor

For simplicity of notation, we again focus the discussion on one-dimensional filters. Before considering the convergence itself of the series (3.4), it is legitimate to first investigate the possibility that this series degenerates into a finite summation. It would be most interesting to find special filters that would lead to an expansion with only a finite number of terms. Indeed, if such filters do exist, the exact $\mathscr{B}_{ij}$ would be accessible without the need to evaluate an infinite number of velocity derivatives. Unfortunately, it is quite easy to show that such filters do not exist. Indeed, replacing ψ by $-\phi$ in expression (3.7) leads to $G(\mathrm{i}\phi) = (F[\phi, -\phi])^{-1/2}$ (here, we explicitly use the fact that G is a symmetric filter). Replacing this expression in the relation defining F, we obtain, after some simple algebraic manipulations,

$$F[\phi, \psi]^2\, F[\phi + \psi, -\phi - \psi] = F[\phi, -\phi]\, F[\psi, -\psi], \tag{6.1}$$

which can never be satisfied if F is a polynomial of order $n < \infty$. Indeed, the order of the polynomial on the right-hand side will be $2n$ while that on the left-hand side will be $3n$. We thus conclude that the generalized expansion (3.4) will always contain an infinite number of terms.

The convergence of the series (3.4) is closely related to the convergence of the series defining $F[\phi, \psi]$. Since F is defined by the expression (3.7), the series $\sum_{rs} c_{rs} \phi^r \psi^s$ clearly converges to $F[\phi, \psi]$. A very simple condition for the convergence of expansion (3.4) can then be derived. Indeed, if it is possible to find two real positive numbers such that

$$\left| \frac{\partial^n \bar{a}}{\partial x^n} \right|, \left| \frac{\partial^n \bar{b}}{\partial x^n} \right| < \alpha\, \rho^n \quad \forall n, \tag{6.2}$$

then, the following inequality is satisfied

$$\sum_{rs} c_{rs}\, \partial_x^r \bar{a}\, \partial_x^s \bar{b} < \alpha^2 \sum_{rs} c_{rs} \rho^{r+s} = \alpha^2 F[\rho, \rho]. \tag{6.3}$$

$K\Delta$	Filtered *vs.* DNS energy	1 term	2 terms	3 terms
8	0.53	0.61	0.80	0.89
6	0.66	0.73	0.88	0.94
4	0.81	0.84	0.94	0.98
3	0.88	0.90	0.97	0.99
2	0.94	0.95	0.99	1.00

TABLE 3. Correlation between the exact filtered-scale stress tensor and the truncated series (3.4) with 1, 2 and 3 terms. The 128^3 DNS corresponds to forced isotropic turbulence, $K = 64$ is the maximal DNS wavenumber and Δ is the filter width. The filter is Gaussian.

Clearly, the inequalities (6.2) give minimal conditions for having a convergent expansion. In the context of filtered-scale modelling, the parameter α is a velocity scale and ρ is the inverse of a lengthscale. Here, it must be stressed that the evaluation of the magnitude of $|\partial^n \bar{u}_i/\partial x^n|$ is far from being obvious. At first sight, we could assume that $|\partial^n \bar{u}_i/\partial x^n| \sim u^*/\Delta^n$ where u^* is some characteristic velocity scale. Indeed, such an evaluation could be justified by that fact that $\bar{u}_i$ is a quantity that should only vary on scale of the order of the filter width Δ. However, this analysis does not hold in general for the derivatives of $\bar{u}_i$. For example, considering the tophat filter, it is easily proved that:

$$\frac{\partial^n \overline{a(x)}}{\partial x^n} = \frac{1}{\Delta}\left(\frac{\partial^{n-1}\, a(x+\frac{1}{2}\Delta)}{\partial x^{n-1}} - \frac{\partial^{n-1}\, a(x-\frac{1}{2}\Delta)}{\partial x^{n-1}}\right), \tag{6.4}$$

and, consequently, there is little chance that $|\partial^n \bar{u}_i/\partial x^n|$ behaves like u^*/Δ^n.

In the absence of a proof of the convergence for expansion (3.4) we have checked numerically that the series converges for an actual turbulent velocity field. Using the *a priori* testing technique, we have compared the correlation between the exact filtered-scale stress tensor that can be derived from a DNS field and the model consisting of only the first terms in the series (3.4). The DNS field is a 128^3 simulation of isotropic forced turbulence in a cubic box of length 2π. The largest wave vector is thus $K = 64$. Results are summarized in table 3. Not surprisingly, the correlations increase with the ratio between the filtered and the DNS energy. When the filtered (not truncated) field captures about 50% of the DNS energy, the correlation between the exact filtered-scale stress tensor and the first term only already reaches 0.61. This correlation is larger than 0.90 when the filtered field captures more than 90% of the DNS energy and the first three terms reproduce almost exactly the exact filtered-scale stress tensor. Although such a numerical check cannot be considered as a proof of the convergence of the generalized expansion, it certainly supports it.

7. Reversibility of the filtered-scale stress tensor

It has long been recognized that filtering cannot be strictly interpreted as an average (see, e.g. Germano 1992). However, filtering has often been considered as a spatial 'averaging' procedure and most of the concepts developed for the closure of the Reynolds-averaged Navier–Stokes (RANS) equations have been applied in the context of LES modelling. For example, the very popular Smagorinsky (1963) model draws its inspiration from the turbulent viscosity concept developed in RANS equations and models the traceless part of the LES stress tensor in terms of an effective viscosity. Many constraints (realizability, tensorial invariance, Galilean invariance) imposed on RANS models have naturally been used for LES models. However, the decomposition of the total LES stress into two terms (2.1) allows us to introduce an additional constraint for the filtered-scale stress tensor that is drastically different from the Reynolds stress tensor: the *reversibility*. Indeed, the exact expansion derived in § 3 shows that the filtered-scale stress tensor is invariant under the change of sign of the LES velocity (2.8). Since the convective nonlinearity term has obviously the same property, the LES equations can be written as

$$\partial_t \tilde{\bar{u}}_i = -\partial_j \tilde{R}_{ij} - \partial_j \tilde{\bar{\mathscr{A}}}_{ij} - \partial_i \tilde{\bar{p}} + \nu \nabla^2 \tilde{\bar{u}}_i, \tag{7.1}$$

with $R_{ij}[-\tilde{\bar{u}}_l] = R_{ij}[\tilde{\bar{u}}_l] = \tilde{\bar{u}}_i \tilde{\bar{u}}_j + \mathscr{B}_{ij}[\tilde{\bar{u}}_l]$. Hence, in the limit of zero molecular viscosity and if the discretization operator is neglected ($\mathscr{D} \to U$), the LES equations can be rewritten $\partial_t \tilde{\bar{u}}_i = f_i[\tilde{\bar{u}}_l]$ where $f_i[\tilde{\bar{u}}_l] = f_i[-\tilde{\bar{u}}_l]$. This property implies that, in the limit of zero molecular viscosity and when the subgrid-scale stress tensor $\tilde{\bar{\mathscr{A}}}_{ij}$ is neglected, the evolution of the large-scale velocity field, $\tilde{\bar{u}}_i$, will be purely reversed if its sign is flipped. Indeed, the LES equations are then invariant for the simultaneous changes $t \to -t$ and $\tilde{\bar{u}}_i \to -\tilde{\bar{u}}_i$.

We have checked this property numerically by computing the free decay of a randomly generated isotropic field with $\nu = 0$ and without any model for $\tilde{\bar{\mathscr{A}}}_{ij}$. Different initial velocity fields $\tilde{\bar{u}}_i^0$ have been used in $t = 0$ (figure 3). The LES equations are then solved numerically until $t = t^*$ where the simulation is stopped and the sign of the velocity field is flipped. In each case, at time $t = 2t^*$, the initial condition has been recovered with a flipped sign ($\tilde{\bar{u}}_i(2t^*) = -\tilde{\bar{u}}_i^0$). Two reversible models $\tilde{\mathscr{B}}_{ij}^M$ have been used for the filtered-scale stress tensor. First, the dynamic Smagorinsky model with volume averaging which is shown to be reversible in § 8. Secondly, the leading term of the expansion (3.11), the so-called tensor diffusivity model:

$$\tilde{\mathscr{B}}_{ij}^M = \Delta^2 (\widetilde{\partial_k \bar{u}_i \, \partial_k \bar{u}_j}). \tag{7.2}$$

We used a fully de-aliased pseudospectral code with 32^3 modes. The LES filter is Gaussian in both cases, with $\Delta = \Delta_{\text{grid}}/\sqrt{2}$. Hence, at the maximum wavenumber of the numerical grid, $k_{\max} = \pi/\Delta_{\text{grid}}$, the LES filter is $G(k_{\max}) = \exp(-\frac{1}{4}\pi^2) = 0.085$; the grid size thus captures well the range where the filter is significant, while not over-killing it. Several statistical quantities have been recorded during the simulation. At $t = 2t^*$, the even moments of the velocity (such as the energy) are recovered exactly while the odd moments (such as the skewness) are recovered with a change of sign. The slight differences in the energy are only due to the explicit time integration; indeed, the Smagorinsky coefficient is computed dynamically at the beginning of the timestep, even when time is reversed. Notice that, in the case of the Smagorinsky model, the second part of the simulation corresponds to effective negative viscosity everywhere (figure 4).

The influence of the initial condition has been tested. In figure 3, we compare the results of the free decay of turbulence with zero molecular viscosity for four different initial conditions with the same spectrum. The first velocity field is generated according to the procedure proposed by Rogallo (1981). This leads to random phases and the initial dissipation vanishes (solid lines). Once the velocity is flipped, the energy increases and reaches exactly the initial level before starting a new decay. In the second simulation, the same initial field is used in a ten timestep simulation. After these ten timesteps, the Fourier modes of the velocity are all rescaled so that

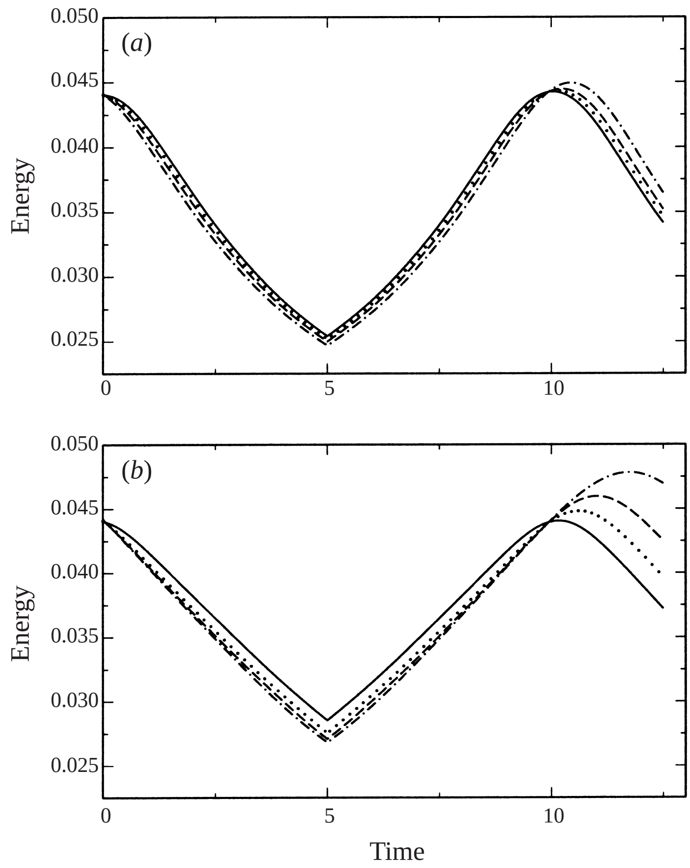

FIGURE 3. Comparison in the LES energy decay with zero molecular viscosity and without a model for the subgrid-scale stress tensor $\mathscr{A}_{ij}$ for (*a*) the dynamic Smagorinsky model with volume average and (*b*) the tensor diffusivity model. Initial conditions correspond to ———, a randomly generated isotropic velocity field, and of velocity fields obtained from the successive rescalings to the initial spectrum after pre-simulations of ten timesteps each (· · · · · ·, 1×10; – – – –, 2×10; —·—·—, 4×10). In all cases, the velocity is flipped at $t = t^* = 5$. Clearly, the initial energy is recovered at $t = 2t^*$ independently of the initial condition and for both models.

the initial spectrum is recovered. This provides the second initial condition (dotted lines). Of course, the phases in this second initial condition are not random anymore and should correspond to a more realistic turbulent field. As a consequence, the initial dissipation is now non-zero and positive. When the field is flipped, the energy increases and reaches its initial level at time $2t^*$. However, reversibility also implies that the dissipation, here represented by the transfer of energy from the filtered scales to the large scales, will be reversed if the sign of the large-scale velocity field is changed. Indeed, the net energy flux, defined as

$$\epsilon = -\langle \tilde{\mathscr{B}}_{ij} \tilde{\tilde{S}}_{ij} \rangle, \tag{7.3}$$

changes sign with the LES velocity. Hence, the dissipation at time $t = 2t^*$ will be recovered with the opposite sign and the energy now goes over the initial level before starting a new decay. This is the signature that ten timesteps were used in a pre-simulation in order to build up the phases. The same simulation has been redone

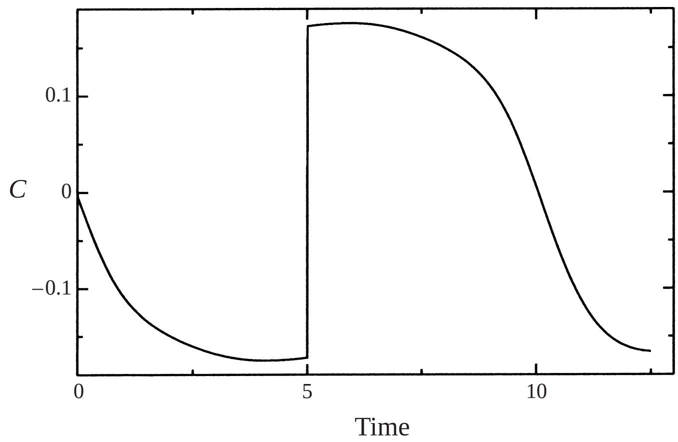

FIGURE 4. Evolution of the model coefficient for the simulation using the dynamic Smagorinsky model. The conditions of the simulation are the same as in figure 3 with the random Gaussian initial conditions.

with two and four times a ten timestep pre-simulation with rescaling and the effect is made even clearer.

The fact that the local dissipation defined by (7.3) can become locally negative and represent local inverse energy flux is well known. Modelling backscatter is thus usually considered as an important issue in LES (see, e.g. Leith 1990; Mason & Thomson 1992; Carati, Ghosal & Moin 1995; Borue & Orszag 1998; Winckelmans *et al.* 1998, 2001; Leonard & Winckelmans 1999). The stochastic modelling of backscatter has been envisaged by most of these authors. It should be noted, however, that the stochastic representation of the backscatter is only compatible with the modelling of the scales that are lost owing to discretization (modelling of $\mathscr{A}_{ij}$). Indeed, the backscatter represented by the filtered-scale stress tensor is expressed exactly in terms of the LES velocity $\tilde{\bar{u}}_i$ and is deterministic in nature. Finally, we remark that, contrary to the usual belief, even the global effect of the filtered scales cannot always correspond to dissipation. Indeed, the expansion (3.11) shows that $\epsilon[\tilde{\bar{u}}_l] = -\epsilon[-\tilde{\bar{u}}_l]$. However, for a reasonable large-scale velocity field (corresponding to the filtering of real turbulence), the net effect when using the leading term in the expansion is dissipative. The mean model dissipation defined by (7.3) is then (Leonard 1997):

$$\epsilon \approx -\langle \tilde{\mathscr{B}}_{ij} \tilde{\bar{S}}_{ij} \rangle = -\Delta^2 \langle (\widetilde{\partial_k \tilde{\bar{u}}_i \, \partial_k \tilde{\bar{u}}_j}) \tilde{\bar{S}}_{ij} \rangle, \tag{7.4}$$

which is a measure of the opposite of the skewness of the velocity. This quantity is known to be negative in real turbulent flows and their DNS. It is also found to be negative in LES of real turbulent flows. Thus, if the skewness of the large-scale velocity field remains negative, global dissipation is indeed ensured for the tensor diffusivity model (7.2). The reversibility of this model for the filtered-scale stress tensor is thus not problematic since its contribution is generically dissipative for LES of real turbulence. Right after t^*, the dissipation is negative (figure 5). Indeed, the transformation $\tilde{\bar{u}}_i \to -\tilde{\bar{u}}_i$ modifies an infinite number of velocity moments and represents a major change in $\tilde{\bar{u}}_i$. In particular, the reversed velocity field now has positive skewness, a state that would never be observed in LES of real turbulence.

The important property discussed here shows that, for a wide class of filters, the filtered-scale stress tensor alone will never introduce irreversibility in the LES

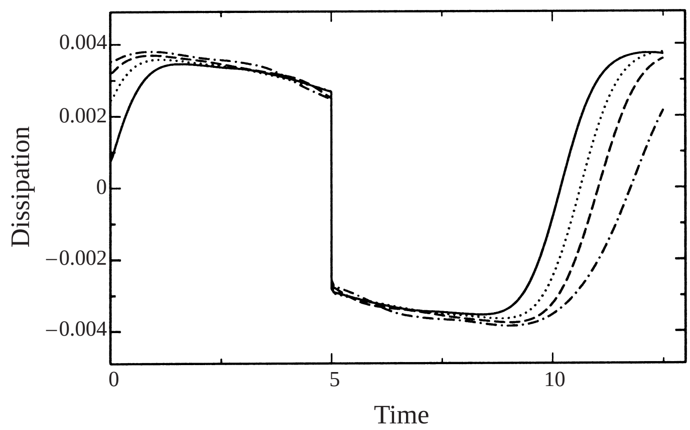

FIGURE 5. LES dissipation as expressed by the right-hand side of (7.4). The conditions of the simulations are the same as in figure 3.

equations. This unexpected property also shows that the discretization operator should not be neglected since it is, with the molecular viscosity, the only source of irreversibility.

8. Reversibility in existing models

Although the usually accepted phenomenology for the filtered-scale model has almost always assumed that the small scales induce an irreversible dissipation at the large-scale level, some reversible models have been proposed and are actually used in the LES community. We have already mentioned models built from the truncation, to one or more terms, of the expansion (3.11).

The Bardina's scale-similarity model $\mathcal{T}^M_{ij} = \overline{u_i^A u_j^A} - \bar{u}_i^A \bar{u}_j^A$ is another reversible model. It is interesting to notice that the Bardina model can also be expanded in terms of the derivatives of u_i^A. For the one-dimensional case, this expansion is written:

$$\overline{\bar{a}\bar{b}} - \bar{\bar{a}}\bar{\bar{b}} = \sum_{rs} d_{rs}\, \partial_x^r \bar{a}\, \partial_x^s \bar{b}, \tag{8.1}$$

where the coefficients d_{rs} are derived from a generating function which is reminiscent of (3.7): $H(\phi, \psi) = G(\mathrm{i}(\phi + \psi)) - G(\mathrm{i}\phi)\, G(\mathrm{i}\psi)$. This property is not interesting in practice since the Bardina model is obviously already written in terms of $\tilde{\bar{u}}_i$. However, it can be used to prove that the first term in the expansion of the Bardina model coincides with the leading term (3.10) in the expansion (3.4). This largely explains why the Bardina model is also highly correlated with the exact $\mathcal{T}_{ij}$.

We have also mentioned the dynamic Smagorinsky model. Here, we show that the dynamic procedure systematically yields reversible models when no clipping is used (including the case of the Smagorinsky model). The dynamic procedure (Germano *et al.* 1991; Germano 1992; Lilly 1992; Moin & Jimenéz 1993) is a recently developed method designed to compute rather than prescribe the unknown coefficient that appears in the models for the filtered-scale stress tensor. The main ingredient in the dynamic procedure is an identity derived by Germano (1992) between filtered-scale stress tensors obtained using the same filter with two different widths: Δ and $\alpha\Delta$ with $\alpha > 1$ (typically chosen equal to 2). The dynamic procedure has often been used together with the Smagorinsky model. However, it can be implemented with any model. For that reason, we here assume that the model is fully determined by the large-scale velocity field, up to a multiplicative constant:

$$\tau_{ij}^{M} = Cm_{ij}[\bar{u}_l], \tag{8.2}$$

$$T_{ij}^{M} = Cm_{ij}[\widehat{\bar{u}}_l], \tag{8.3}$$

where $T_{ij} \equiv \widehat{\overline{u_i u_j}} - \widehat{\bar{u}}_i\widehat{\bar{u}}_j$. Since the discretization operator is usually not introduced when considering the dynamic procedure, our starting point is here the standard LES equation (1.2). The filter $\widehat{\ldots}$ is the additional test filter applied to the $\overline{\ldots}$ quantities. It is fully determined by the requirement that the convolution of the LES filter of width Δ with the test filter produces the LES filter of width $\alpha\Delta$ (Carati & Vanden Eijnden 1997). Both models for τ_{ij}^M and T_{ij}^M are assumed to have the same functional dependence on $\bar{u}_i$ and $\widehat{\bar{u}}_i$. This is a similarity hypothesis. We also define:

$$L_{ij} = \widehat{\bar{u}_i\bar{u}_j} - \widehat{\bar{u}}_i\widehat{\bar{u}}_j, \tag{8.4}$$

$$M_{ij} = \widehat{m_{ij}[\bar{u}_l]} - m_{ij}[\widehat{\bar{u}}_l]. \tag{8.5}$$

The dynamic procedure is based on satisfying Germano's identity, $(T_{ij}^M - \widehat{\tau}_{ij}^M) - L_{ij} = 0$, in the least-squares sense (Lilly 1992). Defining the error $E_{ij} = CM_{ij} - L_{ij}$, the minimizing of $E_{ij}E_{ij}$ leads, for flows with one or more homogeneous direction(s), to the following prediction for C (Lilly 1992; Ghosal *et al.* 1995):

$$C = \frac{\langle M_{ij}L_{ij}\rangle}{\langle M_{kl}M_{kl}\rangle}, \tag{8.6}$$

where the brackets stand for averaging over the homogeneous direction(s).

As expressed by (8.6), the dynamic procedure relates the model coefficient directly to the large-scale velocity field: $C = C[\bar{u}_l]$. The remarkable property of the expression (8.6) is that the computed $C[\bar{u}_l]$ always has the same parity as the tensor $m_{ij}[\bar{u}_l]$. Hence, the total model is always invariant under the change of sign of $\bar{u}_l$:

$$C[\bar{u}_l]m_{ij}[\bar{u}_l] = C[-\bar{u}_l]m_{ij}[-\bar{u}_l], \tag{8.7}$$

satisfying automatically the constraint (2.8). We stress again that this property is independent of the model used in (8.2) and (8.3). If a model without dynamic procedure satisfies the constraint (2.8), then its dynamic version will preserve this property. If, as for the Smagorinsky model, the model with a fixed coefficient is not invariant under the change $\bar{u}_l \leftrightarrow -\bar{u}_l$, then a dynamic version of the model will restore the invariance. For instance, the dynamic prediction for the effective viscosity in the Smagorinsky model, $\nu_e = C[\bar{u}_l]\Delta^2(2\bar{S}_{kl}\bar{S}_{kl})^{1/2}$, will change sign when reversing the large-scale velocity field.

This property of the dynamic procedure has caused some troubles in the early stages of its development. Indeed, when local versions of the dynamic model (with $C = C(\boldsymbol{r}, t)$) were developed and tested together with the Smagorinsky model (Ghosal *et al.* 1995), it appeared that C was locally very often negative, even though its space-average was positive. As a consequence, numerical instabilities were observed in the LES runs. The practitioners solved the problem by introducing a cutoff at $C = 0$ (clipping procedure), keeping only the positive values of the Smagorinsky coefficient, and thus introducing irreversibility. The clipping clearly removes the possible numerical instabilities. However, it is usually considered as a non-desirable artifact which is imposed by numerical stability constraints and is not motivated by any modelling considerations. This has prompted the development of a new dynamic model (Ghosal *et al.* 1995) in which the eddy viscosity is based on the subgrid-scale energy. In this case, the eddy viscosity can become negative but no clipping is required since the instabilities are saturated when the subgrid-scale energy vanishes. However, in its basic formulation and without clipping, the dynamic procedure always leads to reversible filtered-scale models. Finally, it is important to notice that this assertion is also true for mixed models of the form:

$$\tau_{ij}^M = n_{ij}[\bar{u}_l] + Cm_{ij}[\bar{u}_l], \tag{8.8}$$

$$T_{ij}^M = n_{ij}[\hat{\bar{u}}_l] + Cm_{ij}[\hat{\bar{u}}_l], \tag{8.9}$$

where the first term, n_{ij}, is reversible. Example of such models are the mixed model: 'Bardina model + dynamic Smagorinsky term' (Zang, Street & Koseff 1993), or the newly developed mixed model: 'tensor diffusivity model + dynamic Smagorinsky term' (Vreman *et al.* 1996, 1997; Winckelmans *et al.* 1998). In these mixed approaches, the first term (Bardina model or truncation of the exact expansion) represents the filtered-scale stress tensor, while the second term models the subgrid-scale stress tensor. In these mixed models, defining

$$P_{ij} = L_{ij} + (\widehat{n_{ij}[\bar{u}_l]} - n_{ij}[\hat{\bar{u}}_l]), \tag{8.10}$$

the dynamic procedure leads to

$$C = \frac{\langle M_{ij} P_{ij} \rangle}{\langle M_{kl} M_{kl} \rangle}. \tag{8.11}$$

Again, the total model is invariant when changing the sign of the large-scale velocity. As discussed in § 4, the additional eddy viscosity should be understood as a model for the subgrid-scale stress tensor $\bar{\tilde{\mathscr{A}}}_{ij}$. The fact that this term also appears to be reversible when computed dynamically should be seen as a pathology of the dynamic procedure which does not influence the results when volume or surface averaging can be used.

9. Conclusion

A decomposition of the total additional stress that appears in the LES equations into a term mainly due to discretization and a term mainly due to filtering has been proposed. The discretization operator is usually not precisely determined and no exact result can be derived for the modelling of the related subgrid-scale stress tensor. However, the discretization is generically responsible for some loss of information and irreversible models such as the eddy viscosity term are expected to give a reasonable picture of its effect on the LES field. On the contrary, the filter can be defined without ambiguity. It has been proved that the related filtered-scale stress tensor can be expressed exactly in terms of the LES field for a wide class of filters. This exact expression shows that the filtering is generically not responsible for any information loss and that, consequently, the filtered-scales stress does not introduce any irreversibility effect in the LES equations. The combination of the two terms strongly motivates the modelling of the total LES stress tensor in terms of mixed models in which the reversible part can be derived from the expansion proposed in § 3.

It must be acknowledged here that the derivation of the mathematical expansion of the filtered-scale stress tensor is not valid for completely general filters. Also, the use of the Fourier representation for proving the expansion assumes homogeneity. The derivation of the expansion proposed in § 3 is thus strictly valid only for homogeneous flows. However, these assumptions should not lead to the conclusion that these results have no relevance for moderately inhomogeneous flows (requiring moderately inhomogeneous filters). In particular, the effect of a filter that does not remove information from the field but only attenuates the energy contained in the small-scale range should be similar in homogeneous and inhomogeneous flows. In this last case, it should still be possible to derive a reconstruction procedure, even if it might be appreciably different from the exact expansion proposed in § 3. Also, the filtered-scale stress tensor which has been shown to lead to reversible dynamics for homogeneous filters is not expected to lead to purely irreversible effects when slightly inhomogeneous filters are used. For instance, the mixed model (tensor-diffusivity model supplemented by a dynamic Smagorinsky term) has been used, with good success, in LES of channel flow using an explicit Gaussian filter that is homogeneous in the planes parallel to the wall but not in the wall normal direction. Also, the introduction *ab initio* of two operators – discretization and filtering – for defining the LES field makes the assumption on the filter not very restrictive. Indeed, the combination of a smooth filter G and a very general discretization operator $\mathscr{D}$ should cover a wide range of practical LES cases.

It must be stressed that for any practical application, both operators G and $\mathscr{D}$ are essential. The filtering allows the influence of the small scales to diminish, but does not remove any information for the velocity field. Alone, it will only correspond to a change of basis in which the LES should be exactly equivalent to the DNS. The discretization is precisely the operation which removes some information and which makes the LES less time- and memory-consuming than the DNS. However, alone the discretization would remove scales that might contain an appreciable amount of energy and would require a very good model to guarantee the success of the LES. The combination of two operators allows for time and memory savings in passing from the DNS to the LES and implies that the discretization only affects a small fraction of the energy contained in the filtered field. For the 128^3 DNS, the reduction to a 32^3 LES can be obtained from a discretization operator given by a sharp cutoff at $k = 16$. For the fields used in the *a priori* tests, this operation only cuts 2% of the total energy whereas the filtering removes between 5 and 50% of the energy, depending on the filter width.

Finally, we conclude by mentioning two other approaches in which the LES stress tensor is reconstructed instead of being purely modelled. Domaradski & Saiki (1997) recently proposed a technique in which the unresolved velocity u^C is reconstructed by using the nonlinear interaction term in the resolved Navier–Stokes equations. Closer to the present approach, the iterative deconvolution procedure used by Stolz & Adams (1999) leads to an approximate reconstruction of the filtered-scale stress tensor which also assumes that the filter is invertible within the resolution domain of the LES.

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