

Available online at www.sciencedirect.com



Journal of Computational Physics 205 (2005) 98-107

JOURNAL OF COMPUTATIONAL PHYSICS

www.elsevier.com/locate/jcp

Large-eddy simulation without filter

Bernard Knaepen *, Olivier Debliquy, Daniele Carati

Statistical and Plasma Physics, Université Libre de Bruxelles, CP231, Boulevard du Triomphe, Campus Plaine, 1050 Brussels, Belgium

Received 19 January 2004; received in revised form 22 October 2004; accepted 25 October 2004 Available online 19 December 2004

Abstract

An large-eddy simulation (LES) formalism based on sampling operators instead of filters is developed. The major advantage of this approach is that sampling operators commute with the product and their application to nonlinear terms is not at the origin of any closure problem. In absence of filters that smooth out the small scale structures in the flow, the discretization errors in the LES are expected to be important. They must be modelled. The possible confusion between modelling and discretization errors is however avoided since these two effects are identical in the present formalism. A generalized dynamic procedure is proposed for sampling-based LES which allows for model parameter optimization and does not require a detailed analysis of the discretization error. In addition to its interesting mathematical properties for LES, the velocity obtained by a spatial sampling is much closer to experimental probe data than the filtered velocity field.

© 2004 Elsevier Inc. All rights reserved.

Keywords: LES; Large-eddy simulation; Sampling operator

1. Introduction

The difficulty in designing a suitable model for the unresolved scales in large-eddy simulations (LES) has long been recognized as a complex task because of the interplay between modelling and numerical issues [1–3]. The modelling problem arises when a filter is applied to the Navier–Stokes equations. The presence of an unknown subfilter stress tensor in the LES equations is the direct consequence of the unavoidable non commutation of the product and filter operators. Another closure problem may arise when the filter does not commute with the spatial derivatives. This difficulty can only be avoided by using homogeneous filters, i.e., filters with homogeneous shape and filter width. However, special filters have been studied that are

* Corresponding author.

E-mail address: bknaepen@ulb.ac.be (B. Knaepen).

^{0021-9991/\$ -} see front matter @ 2004 Elsevier Inc. All rights reserved. doi:10.1016/j.jcp.2004.10.037

expected to reduce strongly the effects of the non commutation with the spatial derivatives [4,5]. The difference between the exact and the modelled values of the subfilter terms will be referred to as the subfilter error [6]. The numerical issues may also have different sources. The discretization error made in approximating the differential operators that appear in every term in the LES equations is the most obvious one. It will be referred to as the subgrid scale error. Time stepping errors and aliasing may also affect the performances of the simulation. Providing separate and accurate estimates for both the subfilter and the subgrid errors is only possible using the a priori methods [3] since both effects influence the dynamics of the LES velocity in a complex manner.

A careful analysis of the subgrid errors can be done for direct numerical simulation (DNS). In that case indeed there is no subfilter stress tensor to model. In particular, grid refinement studies have provided estimates for the resolution that is required in a DNS depending on the parameters characterizing the experiment. Similarly, high resolution LES can be used for estimating the accuracy of the subfilter models. It is however more difficult to estimate the subgrid errors since simple exact subfilter models are not available.

The major objective of this study is to propose an LES formalism in which no filter is used. The idea is of course not to advocate the use of unresolved DNS without modelling instead of traditional LES. On the contrary, because the resolution in the LES is by definition lower than in the DNS, the discretization error has to be modelled. A class of operators that have good properties for defining the LES velocity without using filter are the sampling operators. These operators are first introduced for defining the DNS velocity in Section 2. In the context of LES, the sampling operators are shown to eliminate the subfilter closure problem and their properties are discussed in Section 3. A generalized dynamic procedure for these sampling operators is presented in Section 4. It is applied to the decaying turbulence test case in Section 5. A general discussion on the advantages and difficulties expected from the use of this sampling-based LES is given in Section 6.

2. A DNS formalism based on sampling operators

The description of the evolution of a fluid in terms of fields like the velocity, the density or the temperature has proven to be very successful. Obviously, this description cannot be valid for very small scales at which the molecular nature of the medium has to be taken into account. Nevertheless, the description of fluids in terms of continuous media is robust enough to describe accurately most of the phenomena covered by the physics of fluids. The velocity, temperature and density fields are even smooth enough to be compatible with the necessary discretized treatment imposed by the numerical analysis of the governing equations of fluid dynamics. In the remainder of this work we limit our attention to the description of the velocity field u_i . For simplicity, we also assume here that it obeys the incompressible Navier–Stokes equations

$$\partial_t u_i = N_i(u_k) \equiv -\partial_j(u_i u_j) - \partial_i p + v \Delta u_i.$$
⁽¹⁾

These equations must be supplemented by an initial condition and boundary conditions, which will not be discussed in details here. However, it is worth stressing that the spatial dependence of u_i in (1) is defined over a physical domain, denoted $\Omega \subset \mathbb{R}^3$ which is a subset of the three-dimensional space. In a DNS, the situation is obviously different. The DNS velocity, that will be denoted $u_i^{A_0}$, is only defined on a denumerable ensemble of positions in Ω that will be referred to as the grid

$$G^{a_0} = \{\vec{x}_1, \dots, \vec{x}_{N_0}\}, \quad \vec{x}_l \in \Omega.$$
⁽²⁾

Here, N_0 is the number of grid points. In order to emphasize the difference between the field u_i and its numerical version $u_i^{\Delta_0}$, it is convenient to introduce the following two ensembles of applications: (i) the ensemble \mathscr{F} of functions that apply the positions in Ω onto a real value and (ii) the ensemble \mathscr{M}^{Δ_0} of

mappings that apply the grid points in G^{Δ_0} onto a real value. In the following, it will be important to constantly remember that the velocity field u_i corresponds to a vector of elements from \mathscr{F} while the DNS velocity $u_i^{\Delta_0}$ corresponds to a vector of elements from \mathscr{M}^{Δ_0} .

The DNS discretization operator is thus an application from \mathscr{F} to \mathscr{M}^{d_0} . In order to be as explicit as possible, the discretization operators that are considered in the following are systematically sampling operators. They are defined as the application of any function $a \in \mathscr{F}$ on the mapping $a^{d_0} \in \mathscr{M}^{d_0}$ that takes exactly the same value on the grid $a^{d_0}(\vec{x}_n) = a(\vec{x}_n) \forall \vec{x}_n \in G^{d_0}$. It is convenient to introduce the notation

$$u_i^{\Delta_0} = S^{\Delta_0} \star u_i \tag{3}$$

for this sampling discretization operator. It will be shown in the following that this natural choice has some practical advantages.

An obvious consequence of the discretization is the impossibility to apply the spatial differential operators ∂_i on an element of \mathscr{M}^{A_0} , and in particular on $u_i^{A_0}$. Indeed, these operators correspond to applications from \mathscr{F} to \mathscr{F} and they cannot be applied on a mapping from \mathscr{M}^{A_0} . Writing the equations for $u_i^{A_0}$ thus requires a choice on the representation of the differential operators ∂_i in terms of applications from \mathscr{M}^{A_0} into \mathscr{M}^{A_0} . Such a representation is denoted $\partial_i^{A_0}$. In a DNS, the grid G^{A_0} and the operator $\partial_i^{A_0}$ have to be carefully chosen so that the discretization error on the differentiation operator

$$\partial_{i}^{a_{0}} \star S^{A_{0}} \star a - S^{A_{0}} \star \partial_{i}a \tag{4}$$

is reasonably small. The choice for the operator $\partial_i^{A_0}$ implicitly defines the numerical scheme used for the spatial derivatives. A more sophisticated numerical scheme is usually compatible with a coarser grid but, in any case, the number of grid points N_0 required for an accurate numerical description of the velocity field is known to be the bottleneck of the development of DNS, especially for highly turbulent systems. Actually, the exact meaning of "accuracy" for a DNS is not univocally defined. Indeed, the number of required grid points is expected to depend on the type of velocity statistics that is to be predicted. Accurate predictions of high order statistics, especially of the velocity gradients, require a finer mesh than the prediction of the second order Reynolds stress tensor. There is however a fairly large agreement to accept that a DNS focusing on low order statistics of the velocity can be considered as accurate when it captures the small scales down to the dissipation length. This usually does not imply that $u_i^{A_0}$ remains close to u_i .

3. A LES formalism based on sampling operators

The LES approach has been designed for lowering substantially the grid requirement for turbulent flows. At least two viewpoints can be developed regarding the LES. By far, the most widespread formalism assumes that the LES equations have the same status as the Navier–Stokes equations. In particular, the LES velocity field \overline{u}_i is also an element of \mathscr{F} obtained by applying a spatial filter, denoted by the overbar symbol $\overline{\cdots}$ to the actual velocity field u_i . The filtering operator, contrary to the discretization operator, is thus an application from \mathscr{F} into \mathscr{F} . This approach is sometimes referred to as the mathematical LES. Since the equations for \overline{u}_i are defined independently of any numerical approach, we prefer to refer to them as the filtered Navier–Stokes equations (FNS)

$$\partial_i \overline{u}_i = -\partial_j \overline{u}_i \overline{u}_j - \partial_i \overline{p} + v \Delta \overline{u}_i - \partial_j \tau_{ij}.$$
⁽⁵⁾

The hope is that, for a well chosen filter, the accurate numerical treatment of the FNS will require less grid points than the accurate DNS of the same flow. Without discussing the discretization issues related to the numerical treatment of the FNS equations, two consequences of this formalism can already be pointed out. First, the filtering and the product operators do not commute and the FNS equations are not closed. The so-called subgrid scale stress tensor

B. Knaepen et al. | Journal of Computational Physics 205 (2005) 98-107

$$au_{ii} = \overline{u_i u_i} - \overline{u}_i \overline{u}_i,$$

is not expressed in terms of the filtered velocity only and requires a modelling effort. The second unpleasant property of this formalism is the potential difficulty in relating the predictions of the FNS to experimental data. Indeed, because of the filtering, almost all the statistics of \overline{u}_i are different from those of u_i , even the components of the Reynolds stress [7].

An alternate formalism is developed here. The differences with the traditional formalism are fundamental. For instance, no filter is used to damp the smallest structures in the turbulent flow. Also, no model is required for the nonlinearity. The LES velocity is, like the DNS velocity, considered to be obtained by applying a sampling operator on the velocity field u_i . As discussed in the following, the sampling of a product being simply the product of the samplings, the nonlinearity does not cause any closure difficulty in the present formalism. However, discretizing the spatial derivatives does create a closure problem and the modelling effort has to focus entirely on this discretization difficulty. In order to give a precise description of the alternate formalism, the LES grid is defined explicitly by

$$G^{A_1} = \{ \vec{x}_1, \dots, \vec{x}_{N_1} \}, \quad \vec{x}_l \in \Omega.$$
⁽⁷⁾

It is supposed to be significantly coarser $(N_1 \ll N_0)$ than the DNS grid. The ensemble of mappings that apply the grid points in G^{A_1} onto a real value will be denoted \mathcal{M}^{A_1} . Moreover, the LES grid will be assumed to be embedded into the DNS grid $G^{A_1} \subset G^{A_0}$. This is not a very restrictive assumption and it allows to introduce the LES operator S^{A_1} as the product of the discretization operator S^{A_0} that defines the DNS and the coarsening operator C^{A_1,A_0}

$$S^{A_1} = C^{A_1,A_0} \star S^{A_0}.$$
(8)

Hence, the LES operator is an application from \mathscr{F} into \mathscr{M}^{d_1} and the coarsening operator C^{d_1,d_0} is an application from \mathscr{M}^{d_0} into \mathscr{M}^{d_1} . Assuming that the LES is also a sampling operator implies that the coarsening operator is itself a sampling operator: C^{d_1,d_0} applies any mapping $a^{d_0} \in \mathscr{M}^{d_0}$ on the mapping $a^{d_1} \in \mathscr{M}^{d_1}$ that takes exactly the same value on the coarse grid $a^{d_1}(\vec{x}_n) = a^{d_0}(\vec{x}_n), \forall \vec{x}_n \in G^{d_1}$.

Such a definition for the LES operator automatically solves the two aforementioned difficulties of the FNS formalism. First, since the LES velocity $u_i^{A_1}$ is a sampling of u_i on the LES grid, the Reynolds stress for $u_i^{A_1}$ and u_i should be the same. In particular, the comparison between LES and experimental data should be easier [8] since a velocity defined by a spatial sampling is a better numerical estimate of data obtained using a probe than a filtered velocity field. Moreover, there is no commutation error between the product and the discretization operator

$$S^{\Delta_1} \star [u_i u_j](\vec{x}_l) \equiv [u_i u_j](\vec{x} = \vec{x}_l) = u_i (\vec{x} = \vec{x}_l) u_j (\vec{x} = \vec{x}_l) = [S^{\Delta_1} \star u_i](\vec{x}_l) [S^{\Delta_1} \star u_j](\vec{x}_l)$$
(9)

Hence, the term that should be equivalent to the subfilter-scale stress tensor based on the LES operator S^{A_1} , $\tau_{ij} = S^{A_1} \star [u_i u_j] - [S^{A_1} \star u_i] S^{A_1} \star u_j] \equiv 0$, vanishes exactly. The difficulties introduced in using a coarser grid for the LES are thus, in the present formalism, not related to the treatment of the nonlinear terms. There is however a price to pay. In the numerical treatment of the LES based on S^{A_1} , it cannot be pretended that the discretization error is negligible. Writing the equations for $u_i^{A_0}$ also requires a representation of the differential operators ∂_i as an operator $\partial_i^{A_1}$ from \mathcal{M}^{A_1} to \mathcal{M}^{A_1}

$$\hat{o}_{t}u_{i}^{A_{1}} = N_{i}^{A_{1}}(u_{k}^{A_{1}}) + \mathscr{E}_{i}^{A_{1}} \equiv -\hat{o}_{j}^{A_{1}}u_{i}^{A_{1}}u_{j}^{A_{1}} - \hat{o}_{i}^{A_{1}}p^{A_{1}} + \nu\Delta^{A_{1}}u_{i}^{A_{1}} + \mathscr{E}_{i}^{A_{1}}.$$
(10)

If the LES mesh is much coarser than the DNS mesh, the discretization error

$$\mathscr{E}_{i}^{A_{1}} = S^{A_{1}} \bigstar N_{i}(u_{k}) - N_{i}^{A_{1}}(u_{k}^{A_{1}}) \tag{11}$$

is an unknown term that cannot be neglected. The resulting unclosed evolution Eq. (10) define a LES. Closing the LES equations thus requires the modelling of the discretization error of the differentiation

101

(6)

operator $(\mathscr{E}_i^{A_1} \approx M_i^{A_1}[u_k^{A_1}])$ but not of the nonlinear terms. As a matter of fact, aliasing errors are inherently absent in the present formalism because of (9). As a comparison, considering LES based on a spectral representation, the 3/2 aliasing-removal procedure can be seen as the application of an additional Fourier cut-off to the product of filtered velocities. Here, the situation is different since it is not necessary to re-apply a sampling operator on a product to get the proper representation of the sampling values. There is however again a price to pay. The sampled values of a product of velocities "hide" more high frequencies than those of the velocity itself. This has the consequence that the spatial derivatives applied to such products in the convective term will lead to more severe truncation errors than the truncation errors generated by the viscous term (at least for high Reynolds numbers). The nature of this discretization error should not however be very different from the one of the traditional SGS terms.

The pressure p^{A_1} has to be computed using the continuity equation. However, because of the truncation errors, the divergence of the signal $u_i^{A_1}$ is not expected to vanish exactly and an additional model playing the role of a source term in the discretized continuity equation should be introduced

$$\partial_{i}^{A_{1}}u_{i}^{A_{1}} = \mathscr{K}^{A_{1}}.$$

This difficulty is actually also present in traditional LES based on inhomogeneous filters as discussed in [9]. It should be noted that the modelling of \mathscr{K}^{Λ_1} would probably be fairly difficult and might change the nature of the numerical scheme itself since the incompressibility condition is a very strong constraint in most numerical methods. To the best of our knowledge, the commutation error in the incompressibility condition has never been taken into account in more traditional LES in which non-commutative filters are also used. It might turn out that the only practicable strategy will be to ignore this effect, but numerical and theoretical investigations of the commutation error in the incompressibility condition would be welcome.

The above LES viewpoint is very different from the majority of the existing literature on the LES, including some previous publications of the present authors. It must however be acknowledged that the discretization of the Navier–Stokes equations is a problem only because it contains spatial derivatives. Nonlinear terms, without any spatial derivation, would lead to a total decoupling of the different locations. For instance, no discretization issue would ever be raised and no LES problem would ever be defined for an equation like

$$\partial_t a = -\gamma a^2. \tag{13}$$

The leitmotiv that the LES equations are not closed because of the nonlinear term has been introduced because a somewhat misleading comparison has been made with the RANS approach. In that approach indeed, the RANS equations are not closed because of the nonlinear term. It is obvious that the average of a product is usually different from the product of the average and a RANS closure problem would be faced if Eq. (13) is averaged. Similarly, a subfilter closure problem would be faced if Eq. (13) is filtered. The spatial discretization of this equation is however trivial. The numerical treatment of the FNS formalism somewhat mixes the spatial discretization and the ensemble averaging issues, since the filtering operator can be seen as a local averaging procedure. The hope in traditional LES is to use the right combination of: (i) filter, (ii) grid and (iii) model so that the discretization error can be neglected when simulating the FNS.

In the proposed new formalism, the situation is not very different from traditional LES as long as the separation between DNS and LES is concerned. The role of the filtering operator is simply replaced by the coarsening operator. In traditional LES, the DNS limit is obtained when the filter width tends to 0. In that case, the filtering tends to the identity operator. Here, the DNS limit is obtained when, in the coarsening operator C^{Δ_1,Δ_0} , Δ_1 tends to Δ_0 . In that case, the coarsening operator also tends to the identity.

4. Generalized dynamic procedure

A direct consequence of the formalism in terms of sampling operators is that the Germano identity is useless for these LES since $\tau_{ij} = 0$. The idea behind the Germano identity can however still be used. Let us consider a third grid,

$$G^{A_2} = \{ \vec{x}_1, \dots, \vec{x}_{N_2} \}, \quad \vec{x}_l \in \Omega,$$
(14)

that is again embedded in G^{4_1} so that $N_2 < N_1$. Note that the idea of using a sampling operator for the test filter has already been considered recently in [10] and implemented with a Smagorinsky type model for the Burgers equation [11]. Using the same terminology as in the context of the dynamic procedure, it will be referred to as the test-level. The velocity sampled on this coarse grid will be denoted $u_i^{4_2}$. It is a vector of elements in the ensemble \mathcal{M}^{4_2} of mappings that apply the grid points in G^{4_2} onto a real value. A schematic representation of the physical domain Ω and of the three grids is given in Fig. 1.

The equations for $u_i^{\Delta_2}$ are written as

$$\partial_{t}u_{i}^{\Delta_{2}} = N_{i}^{\Delta_{2}}(u_{k}^{\Delta_{2}}) + \mathscr{E}_{i}^{\Delta_{2}} \equiv -\partial_{j}^{\Delta_{2}}u_{i}^{\Delta_{2}}u_{j}^{\Delta_{2}} - \partial_{i}^{\Delta_{2}}p^{\Delta_{2}} + \nu\Delta^{\Delta_{2}}u_{i}^{\Delta_{2}} + \mathscr{E}_{i}^{\Delta_{2}},$$

where

$$\mathscr{E}_{i}^{A_{2}} = S^{A_{2}} \star N_{i}(u_{k}) - N_{i}^{A_{2}}(u_{k}^{A_{2}}).$$
(15)

The equations for $u_i^{\Delta_2}$ are here obtained by applying the discretization operator S^{Δ_2} directly to the Navier–Stokes equations. They can however also be obtained by applying a coarsening operator C^{Δ_2, Δ_1} to the equations for $u_i^{\Delta_1}$ and both versions should be equivalent since $S^{\Delta_2} = C^{\Delta_2, \Delta_1} \star S^{\Delta_1}$

$$\partial_{t} u_{i}^{A_{2}} = C^{A_{2},A_{1}} \star N_{i}^{A_{1}}(u_{k}^{A_{1}}) + C^{A_{2},A_{1}} \star \mathscr{E}_{i}^{A_{1}}.$$
(16)

Comparing the right-hand-side of Eqs. (15) and (16) immediately yields the following identity:

$$\mathscr{E}_{i}^{A_{2}} - C^{A_{2},A_{1}} \bigstar \mathscr{E}_{i}^{A_{1}} \equiv C^{A_{2},A_{1}} \bigstar N_{i}^{A_{1}}(u_{k}^{A_{1}}) - N_{i}^{A_{2}}(u_{k}^{A_{2}}), \tag{17}$$



Fig. 1. The physical domain Ω and the DNS, LES and test-level grids are schematically represented. The sampling operators required for transforming a function defined on Ω into a mapping defined on a grid are mentioned. The coarsening operators used for transforming a mapping defined on a fine grid into a mapping defined on a coarse grid are also indicated.

which can play exactly the same role as the Germano identity for the LES formalism developed here. It can be used following the same strategy as for the traditional dynamic procedure [12–14]. For instance, the discretization error on the LES grid can be modelled by a function of the discretized velocity $u_k^{A_1}$ multiplied by an unknown parameter: $\mathscr{E}_i^{A_1} \approx Cm_i^{A_1}(u_k^{A_1})$. Similarly, the discretization error on the test-level grid can be modelled using the same type of model. Invoking the same scale invariance assumption as in the dynamic procedure, the same parameter *C* could be used on both grids: $\mathscr{E}_i^{A_2} \approx C m_i^{A_2}(u_k^{A_2})$. The optimal value for *C* would thus be given by

$$C = \frac{\langle L_i M_i \rangle}{\langle M_i M_i \rangle},\tag{18}$$

where

$$\begin{split} L_i &= C^{4_2,4_1} \bigstar N_i^{4_1}(u_k^{4_1}) - N_i^{4_2}(u_k^{4_2}), \\ M_i &= m_i^{4_2}(u_k^{4_2}) - C^{4_2,4_1} \bigstar m_i^{4_1}(u_k^{4_1}), \end{split}$$

where the average is taken over the direction of homogeneity. The vector L_i plays the same role as the Leonard tensor in the traditional dynamic procedure. The parameter C given by (18) is only defined on the testlevel grid G^{d_2} . An interpolation, consistent with the numerical scheme used for the derivatives, has to be used to evaluate C on the LES grid G^{d_1} if C is allowed to be inhomogeneous.

Although the modelling of the source term \mathscr{K}^{A_1} appearing in the discretized continuity Eq. (12) is expected to be very challenging, it would also be possible to use a dynamic approach for it. Indeed, two equivalent versions of the discrete continuity equation on the coarser grid G^{A_2} can be written by applying S^{A_2} directly to the continuity equation or by applying C^{A_2,A_1} on Eq. (12). A minimization procedure could then be considered to optimize the parameter appearing in the model for \mathscr{K}^{A_1} .

5. Numerical results

In order to illustrate the possible implementation of these concepts, we have considered the modelling of the discretization error by the Smagorinsky model. In that case, the vector M_i is given by

$$M_{i} = \Delta_{2}^{2} \partial_{i}^{A_{2}} |s^{A_{2}}| s_{ij}^{A_{2}} - S^{A_{2}} \bigstar \Delta_{1}^{2} \partial_{j}^{A_{1}} |s^{A_{1}}| s_{ij}^{A_{1}}.$$
⁽¹⁹⁾

The tensors $s_{ij}^{\Delta_1}$ and $s_{ij}^{\Delta_2}$ represent the strain tensors evaluated on the LES and test grids respectively. The LES and test grid spacings are noted respectively Δ_1 and Δ_2 . It must be acknowledged that the modelling of the discretization error by an eddy viscosity term is questionable. Moreover, a priori test have shown that the correlations between the "exact" unknown term $\mathscr{E}_i^{\Delta_1}$ and its representations in terms of the Smagorinsky model are very poor (about 12%). However, since the dynamic Smagorinsky model has been thoroughly benchmarked and, at the very least, it has the property to be dissipative so that it should stabilize the simulation, there is some rationale to evaluate and test the dynamic procedure for this model in a first step.

This model has been implemented in a pseudo-spectral code with modified wave vectors in order to mimic the behavior of a second-order centered finite difference scheme. Although this method is not computationally optimal, it has the advantage to be very easy to implement both for the DNS and for the LES. The computational domain is a cubic $2\pi \times 2\pi \times 2\pi$ box. The DNS grid, G^{4_0} , corresponds to a 256³ resolution and the modified wave vectors for the finite difference scheme \vec{k}^{FD} are defined by

$$\vec{\mathbf{k}}^{\text{FD}} = (k_x^{\text{FD}}, k_y^{\text{FD}}, k_y^{\text{PD}}) = \frac{1}{\varDelta_0} \left(\sin\left(k_x^{\text{S}} \varDelta_0\right), \sin\left(k_y^{\text{S}} \varDelta_0\right), \sin\left(k_z^{\text{S}} \varDelta_0\right) \right),$$
(20)

B. Knaepen et al. | Journal of Computational Physics 205 (2005) 98-107

$$(k^2)^{\text{FD}} = \frac{4}{\Delta_0^2} \left(\sin^2 \left(\frac{k_x^S \Delta_0}{2} \right) + \sin^2 \left(\frac{k_y^S \Delta_0}{2} \right) + \sin^2 \left(\frac{k_z^S \Delta_0}{2} \right) \right), \tag{21}$$

105

where \vec{k}^{S} is the usual wave vector in the pseudo spectral code. Note that, in the finite difference scheme, the discretization of the second order derivative is not obtained as the "square" of the first order derivative and consequently different definitions are used for the modified wave vectors entering the first and the second order derivatives. The quantity $(k^2)^{FD}$ is only used in the viscous term. In the DNS, the incompressibility condition is enforced by projecting the velocity $\vec{u}(\vec{k}^{FD})$ in the plane perpendicular to \vec{k}^{FD} . The sampling operators S^{A_1} and S^{A_2} are implemented straightforwardly in real space. The LES field is obtained by sampling using S^{A_1} on a 32³ grid. The implementation of the dynamic procedure using the grids G^{A_1} and G^{A_2} is then performed by a simple re-definition of the modified wave vectors (20) and (21) in which Δ_0 is substituted respectively by Δ_1 and Δ_2 .

The preliminary tests, though made with a modified spectral code and a limited resolution, are quite illuminating. First, it shows clearly that a model is required for the decaying turbulence case. The underresolved DNS (LES without model) exhibits an increase of the energy after a short decaying period. The dynamic Smagorinsky model has been implemented in three versions. Indeed, the "Leonard" vector L_i contains two contributions originating respectively from the convective + pressure terms and from the viscous term. In the computation of the dynamic Smagorinsky constant C, the purely convective, the purely viscous and the full Leonard vectors have been implemented. Not surprisingly, the purely viscous version does not perform satisfactorily. It is actually even worse that the no-model case. Also, the purely convective version produces the best agreement with the sampled DNS. The final spectra are also presented. They all exhibit a piling-up of the energy in the high wave vector range. However, the no-model and the purely viscous dynamic model both overpredict the low wave vector energy range, while the dynamic models that account for the convective discretization errors both correctly predict the low k spectrum (see Fig. 2).

Although it would be quite hazardous to make definitive and strong statements on the basis of these preliminary numerical results, they indicate that: (i) the implementation of a dynamic procedure with the sampling operators yields reasonable predictions in the homogeneous decaying turbulence test case and (ii) the Smagorinsky model might be acceptable for modelling the numerical discretization errors on the convective term but not for the viscous term.



Fig. 2. Left: Energy decay. Comparison between the sampled DNS (solid), the LES curves without model (dotted) and with the dynamic Smagorinsky model with the parameter C computed using both convective and viscous contributions (dashed), the convective contribution only (dot-dashed) and the viscous contribution only (double dot-dashed). Right: Energy spectrum at the end of the computation, same symbols.

The treatment of the incompressibility condition deserves some attention. In the present LES, it has been chosen to neglect the source term \mathscr{K}_i in the sampled continuity equation. As previously mentioned, finding a model for \mathscr{K}_i is probably very uneasy. However, neglecting this term implies that the incompressibility has to be enforced by projecting the LES velocity field in the plane perpendicular to the modified wave vectors based on \varDelta_1 . As a consequence of this projection, the definition of $u_i^{\varDelta_1}$ is slightly different from $S^{\varDelta_1} \star u_i$ and $u_i^{\varDelta_0}$ and $u_i^{\varDelta_1}$ do not coincide exactly on the grid G^{\varDelta_1} . The differences are however not very large. Moreover, the combination of the sampling and the incompressibility projection remains nevertheless a projective operator.

6. Discussion

It has been mentioned that the formalism developed here is fundamentally different from the traditional viewpoint on LES. In its implementation however it will have strong similitude with the discrete filtered Navier–Stokes treatment of turbulence. Indeed, both versions of the LES are using a coarse grid. Also, both versions have to rely on a model for taking into account the unresolved scales. Hence, as long as the simulation itself of the LES equations is concerned, the difference might seem quite superficial. Nevertheless, in many other aspects of the LES development, the use of sampling operators to define the LES velocity should have a direct and strong influence.

We have already mentioned that the dynamic procedure can be adapted to this type of operators. In that case, the model has to be understood as a model for the discretization errors and not for the commutation errors between the product and a filtering operator. The structure of the dynamic coefficient as well as the general strategy based on a coarser grid look similar to the traditional dynamic procedure based on the Germano identity. The precise form of the coefficients is however significantly affected by the formalism.

Another domain that is affected by the formalism is the traditional "a priori" technique for estimating the potentialities of a model. Since in the present formalism the model is supposed to represent discretization errors, correlation should be measured with these discretization errors instead of the subgrid-scale stress tensor computed from DNS. It has been mentioned that the Smagorinsky model has a very low correlation with the exact discretization error term $\mathscr{E}_i^{\Delta_1}$.

It is not the purpose of this work to claim that the LES formalism based on the sampling operators solves all the difficulties that are met in developing accurate subgrid-scale models. It indeed eliminates most of the known difficulties but new issues are raised. For instance, the subgrid-scale stress tensor τ_{ij} vanishes but a model is required for the discretization error vector $\mathscr{E}_i^{A_1}$. Also, the statistics of traditional LES velocity are affected by the filter and by the model. Here, this difficulty disappears but statistics of the velocity gradients are also affected by the sampling operator. Finally, one of the difficulty of the traditional dynamic procedure comes from the spatial dependence of the model parameter. Because of the filtering, the optimal parameter should normally be obtained using an integral equation [15,16]. Again, this difficulty seems to disappear here because the sampling of $Cm_i^{A_1}$ is equal to the sampling of C multiplied by the sampling of $m_i^{A_1}$. However, since the model has to be the divergence of a term, there will be discretized differential operators $\partial_i^{A_1}$ and $\partial_i^{A_2}$ applied to the model parameter. Hence, a local version of the dynamic procedure still remains difficult to build starting from clean mathematical principles.

The main purpose of this paper is rather to emphasize that an alternate viewpoint can be consistently developed for the LES. It is motivated by the evidence that nonlinearities are not the source of difficulties when a space-accurate simulation of a partial differential equation has to be designed. The difficulties rather originate from the coupling between different locations induced by the spatial derivatives. The present formalism is also motivated by the total decoupling that it implies between traditional subfilter modelling and numerical errors. Indeed, the subfilter stress tensor vanishes exactly so that the model has to deal with and only with the discretization errors. As a consequence, in this approach, it is not possible to reach a grid

independent LES since the LES operator is directly defined by the grid. Although based on a fairly different viewpoint and using sampling operators, the formalism developed here has the same potentialities as traditional LES in terms of: (i) grid saving, (ii) a priori testing, (iii) possibility of developing a dynamic procedure.

We conclude by emphasizing that the numerical results presented here have not to be considered as an attempt to advocate the use of the Smagorinsky model for the discretization error. The main goal of this study is to be an account on a novel viewpoint on LES that is mathematically well posed. Although the results are encouraging, the tests in Section 5 only prove the numerical feasibility of the proposed method. More extensive a priori and a posteriori tests are definitively required to demonstrate that the present formalism is able to compete with more traditional approaches.

Acknowledgements

The authors are very grateful to Gregory Burton, Yves Dubief, Volker Gravemeier and Alan Wray for fruitful discussions. The numerical results have been obtained during the Center for Turbulence Research summer program 2004 in Stanford University and NASA Ames Research Center. D.C. is a researcher of the Fonds National pour la Recherche Scientifique (Belgium). This work has been supported in part by the Communauté Française de Belgique (ARC 02/07-283) and by the contract of association EURATOM – Belgian state. The content of the publication is the sole responsibility of the authors and it does not necessarily represent the views of the Commission or its services.

References

- [1] S. Ghosal, An analysis of numerical errors in large-eddy simulations of turbulence, J. Comp. Phys. 125 (125) (1996) 187-206.
- [2] Y. Morinishi, O. Vasilyev, Vector level identity for dynamic subgrid scale modeling in large eddy simulation, Phys. Fluids 14 (10) (2002) 3616–3623.
- [3] F.K. Chow, P. Moin, A further study of numerical errors in large-eddy simulations, J. Comput. Phys. 184 (2003) 366-380.
- [4] O. Vasilyev, T. Lund, P. Moin, A general class of commutative filters for LES in complex geometries, J. Comput. Phys. 146 (146) (1998) 105–123.
- [5] A. Marsden, O. Vasilyev, P. Moin, Construction of commutative filters for LES on unstructured meshes, J. Comput. Phys. 175 (175) (2002) 584–603.
- [6] D. Carati, G. Winckelmans, H. Jeanmart, On the modelling of the subgrid-scale and filtered-scale stress tensors in large-eddy simulation, J. Fluid Mech. 441 (2001) 119–138.
- [7] G. Winckelmans, H. Jeanmart, D. Carati, On the comparison of turbulence intensities from large-eddy simulation with those from experiment or direct numerical simulation, Phys. Fluids 14 (2002) 1809–1811.
- [8] S. Cerutti, C. Meneveau, Statistics of filtered velocity in grid and wake turbulence, Phys. Fluids 12 (5) (2000) 1143–1165.
- [9] S. Ghosal, P. Moin, The basic equations for large eddy simulation of turbulent flows in complex geometries, J. Comput. Phys. 118 (1995) 24–37.
- [10] H. Jeanmart, G. Winckelmans, Comparison of recent dynamic subgrid-scale models in turbulent channel flow, in: P. Bradshaw (Ed.), Proceedings of the Summer Program – 2002, Stanford University and NASA Ames Research Center, 2002, pp. 105–116.
- [11] L. Georges, G. Winckelmans, LES deconvolution type terms in second order finite differences: a way to recover energy conserving schemes, Bull. Am. Phys. Soc. 48 (10) (2003).
- [12] M. Germano, U. Piomelli, P. Moin, W. Cabot, A dynamic subgrid-scale eddy-viscosity model, Phys. Fluids A 3 (7) (1991) 1760– 1765.
- [13] M. Germano, Turbulence: the filtering approach, J. Fluid Mech. 238 (1992) 325–336.
- [14] D. Lilly, A proposed modification of the Germano subgrid-scale closure method, Phys. Fluids 4 (1992) 633-635.
- [15] S. Ghosal, T. Lund, P. Moin, K. Akselvoll, A dynamic localization model for large-eddy simulation of turbulent flows, J. Fluid Mech. 286 (1995) 229–255.
- [16] D. Carati, S. Ghosal, P. Moin, On the representation of backscatter in dynamic localization models, Phys. Fluids 7 (1995) 606– 616.