Is LES ready for complex flows?

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Abstract

Recent developments in LES modelling, combined with further advances in capabilities of computers and numerical methods, provide a strong incentive to apply LES to complex flows. This brings to focus a number of issues in the development of LES that are not yet fully resolved. These include modelling and numerical elements, their respective errors, and the potential for interaction between these two sources of error. We discuss the relative importance of some of the errors that can arise in simple as well as complex flows and give global criteria and guidelines that can be helpful in order to arrive at a form of LES that is robust and accurate.

1 Introduction

The intricate nature of high Reynolds number turbulent flow has to date proven to defy detailed rigorous or direct numerical analysis and, consequently, has given rise to a number of modelling strategies. Such strategies are aimed at reducing the complexity of the underlying system of equations while retaining sufficient information to reliably predict the flow phenomena of interest

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in an application. These two conflicting requirements are prominent in large-eddy simulation (LES).

In recent years there has been a significant interest and associated development in large-eddy simulation (LES) which raises the question whether the LES approach can already be applied to flows of engineering interest and consequently move away from academic problems. To address this question objectively in this generality is quite difficult. Instead, we will focus on some outstanding open problems that need to be confronted in order to develop LES, in particular for complex flows. While there has undeniably been considerable progress in LES concerning modelling and numerical issues which has resulted in a number of large-scale complex flow predictions by a large number of different research groups using LES, the significance of some of the not yet resolved problems suggests that both a 'yes' and a 'no' answer are still possible for the question raised. In particular, as we discuss below, the answer strongly depends on the type of information one wants to predict.

One can choose between the 'implicit' and the 'explicit' filtering approach to LES [10]. We adopt here the explicit filtering approach because it is more amenable to analysis and allows for a separation of issues related to modelling and numerical treatment. In this approach a spatial filter is applied to the Navier-Stokes equations. The reduction of the flow complexity and information contents that is achieved in this way depends strongly on the type and the width of the adopted filter. At one extreme, the width of the applied filter may be so large that virtually all information contained in the solution is removed while, at the other extreme, a very small filter-width may be adopted which does not reduce the complexity at all. Subsequently, the filtered equations need to be closed by the introduction of a model for the sub-grid stresses and finally the resulting system of equations is treated numerically. These elements of LES, i.e. the information retained in the filtered field, the suitability of and the need for accurate subgrid modelling, and the role of and contamination arising from the numerical treatment will be focused upon. In view of the desired strong reduction in computational effort compared to direct numerical simulation (DNS), these various sources of error can be quite significant [9, 8] and can lead to intricate interactions with some unexpected consequences.

The large-eddy modelling of incompressible flow includes filtering of the convective terms which leads to the turbulent stress tensor τ

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j \quad ; \quad i,j = 1,2,3 \tag{1}$$

as the major so-called subgrid term. This expression contains contributions from the filtered ($\overline{u}_i$) and the unfiltered (u_i) velocity fields and cannot, in practice, be expressed in terms of the filtered solution alone. Various modelling strategies have been proposed, some of which find their origin in physical arguments while others start from rigorous information about properties of the stress tensor. We consider some recent modelling strategies which aim at optimising the use of the scales that are available in an LES in order to arrive at improvements in the subgrid model. This 'inverse modelling' [5] or 'approximate deconvolution' [2, 19] can give rise to models that combine high correlation with suitable transfer of energy from the resolved to the unresolved scales.

For geometrically complicated flows the use of a convolution filter, i.e. the use of a constant filter-width, may not be desirable. In such flows one may observe regions of high turbulence intensity with many small-scale contributions next to regions of weakly turbulent flow with predominantly large-scale components in the solution or next to regions of little interest such as the far wake of a bluff-body flow. An efficient LES of such situations calls for spatial filters with nonuniform width. This, however, gives rise to additional terms that contribute to inter-scale energy-transfer in a specific way depending directly on the non-uniformity of the filter-width. This type of contribution has largely been left unstudied in literature even though its order of magnitude may be comparable to contributions from the turbulent stress tensor.

In order to arrive at a slightly more quantitative approach to the question of adequacy of LES it is important to incorporate the type of information one wants to extract from the simulation. Since this differs widely in the various application areas the capabilities of present-day LES can already be of some or even sufficient use in certain areas while the same LES capabilities provide insufficient accuracy in other applications, e.g. due to restricted computational resources and numerical capabilities. To quantify this somewhat, we consider the prediction of a quantity q, which has an exact value q_e. If we want to predict q and allow an error ε then accurate predictions of only a certain range of scales in the flow are required. We denote $q(n)$ the value of q evaluated with the first n modes of the largest scales. The requirement $|q(n) - q_e| < \varepsilon$ specifies the necessary number of modes $n_q(\varepsilon)$ for the quantity q. If in an LES one can provide $n_q(\varepsilon)$ modes with sufficient accuracy then the quantity q is adequately predicted. Clearly, a decrease in ε will lead to a (strong) increase in $n_q(\varepsilon)$ and, moreover, different quantities q will require possibly very different values of $n_q(\varepsilon)$ in order to yield the desired accuracy.

However, the number of modes given by $n_q(\varepsilon)$ is ideal assuming modelling errors and numerical errors are negligible. Thus a central question is how LES should be designed to arrive at an accurate prediction of at least these first $n_q(\varepsilon)$ modes. Because of these two types of errors any LES aiming at an adequate prediction of the quantity q should involve $N_{LES} > n_q(\varepsilon)$ modes. The success of LES clearly depends on how much larger N_{LES} needs to be, compared to the absolute minimum $n_q(\varepsilon)$. One might expect 'good' subgrid models as well as 'good' numerics to lead to a (slight) decrease in N_{LES}. The latter will be illustrated in this paper. Other factors may, however, lead to an increase in the required N_{LES}. For example, a somewhat higher 'numerical' value for the minimal resolution may exist, e.g., in order to provide a stable treatment of flow near walls or interfaces or to provide enough resolution to generate a stable solution in case inflow and outflow boundaries are introduced such as in spatially developing flows. It is clear that the lower limit $n_q(\varepsilon)$ needs to be respected in any LES and this may well explain some of the reported failures of LES in predicting certain quantities in complex flows. A number of test-cases have been studied with LES by a large number of groups in recent years (see e.g. ref. [18] for a detailed account of one of these cases) and several appear very illustrative in relation to the failure to reach the lower value $n_q(\varepsilon)$.

For a strict DNS the number of modes N_{DNS} that needs to be incorporated is related to the reciprocal Kolmogorov length. Of course the main virtue of LES is that N_{LES} is related to the reciprocal filter-width, i.e. $1/\Delta$ so that N_{LES} can be much lower than N_{DNS}. At the same time the desire to predict q with an accuracy ε implies that $N_{LES} > n_q(\varepsilon)$ which therefore provides a strict upper-bound for Δ. Stated differently, there is an obvious limit to the amount of information that can be 'filtered away' if one insists in maintaining a minimal accuracy for the prediction of some flow property. In order to have some independent control over the interaction between numerical and modelling errors in the subsequent LES the resolution should be fine enough. In particular this implies that the mesh-size h has to be sufficiently smaller than Δ. Appropriate values for the ratio Δ/h depend on the spatial discretization scheme that is used but should be at least larger than 2 or 4 for fourth- or second-order methods, respectively. We will illustrate this below. In total, the desired accuracy with which q needs to be predicted fully controls an upper-bound for the mesh-size. Actual LES is flawed and constrained in many ways compared to the 'optimal efficiency LES' which would need only $n_q(\varepsilon)$ modes. Thus the actual number of modes used, N_{LES}, must be larger than $n_q(\varepsilon)$ and the corresponding filter-width and resolution, h, need to be smaller. Better numerics and modelling can help to increase acceptable values of Δ and h and vice versa, but never beyond bounds set by $n_q(\varepsilon)$.

The organisation of this paper is as follows. In section 2 we briefly formulate the filtering approach to LES and identify some basic properties of the LES modelling problem that deserve to be incorporated into any modelling attempt. Recent developments in subgrid modelling which aim at incorporating information from the scales that are directly available in an LES will be considered. Section 3 describes additional complications to the LES equations that arise from extension to complex flows. This involves the use of nonuniform filters and gives rise to additional terms in the filtered equations which have a specific contribution to the inter-scale energy transfer that will be interpreted and estimated. The numerical treatment of the LES equations is another source of unavoidable and sometimes surprising errors. Section 4 is devoted to some unexpected consequences and paradoxes associated with the interaction of numerical and modelling errors. All sources of error in LES can be controlled to some degree at the expense of adding to the computational effort. Some guidelines for LES which aim at keeping the mixture of errors within reasonable bounds will be suggested in section 5 where we also collect some concluding remarks.

2 The filtering and inversion approach to LES

In this section we briefly introduce the filtering of the Navier-Stokes equations to derive the governing equations for large-eddy simulation. Some properties of the filtered equations will be mentioned which all have consequences for the underlying modelling problem. As an illustration, algebraic properties of the turbulent stress tensor will be considered in more detail as well as the use of approximate inversion techniques and dynamic modelling.

The starting point in the filtering approach is the introduction of the filter operator L which is used to filter the Navier-Stokes equations. The filter considered in this section is a convolution filter and in 1d this is defined by

$$\overline{u}(x,t) = L(u) = \int_{-\infty}^{\infty} G(x-\xi)u(\xi,t)d\xi \tag{2}$$

where G denotes the normalised filter-kernel. In three spatial dimensions we consider the application of 'product filters' which are defined by $\overline{u}(\mathbf{x},t) \equiv L(u) = L_1(L_2(L_3(u)))$ where each of the one-dimensional filter-operations L_j corresponds to one of the Cartesian coordinates and can be written in a way similar to eq. (2). The filter-kernel G used in LES typically has most of its 'weight' concentrated around the origin in a bounded domain of size Δ which we refer to as the filter-width. It can be shown that the application of this convolution filter commutes with partial derivatives that occur in the Navier-Stokes equations, i.e. $L(\partial_t u) = \partial_t(L(u))$ and similarly $L(\partial_j u) = \partial_j(L(u))$ where ∂_t and ∂_j denote partial differentiation with respect to time t and spatial coordinate x_j respectively. The filter operator does not commute with the product operator $S(u_i,u_j) = u_i u_j$ and as is well known the filtering of the nonlinear terms in the convective flux gives rise to the turbulent stress tensor τ_{ij}^L where we explicitly use the label 'L' to emphasise the role of the filter. In incompressible flows and in case convolution filters are used, this is the only new term that arises in the filtered equations and can be expressed in the following way:

$$\begin{aligned} \tau_{ij}^L &= \overline{u_i u_j} - \overline{u}_i \overline{u}_j \\ &= L(S(u_i,u_j)) - S(L(u_i),L(u_j)) \\ &= [L,S](u_i,u_j) \end{aligned} \tag{3}$$

Here we introduced the commutator of the filter L with the product operator S for later convenience. This relation shows that the basic modelling problem in LES is completely identified with properties of the commutator $[L,S]$. The filtered Navier-Stokes equations take on the same form as the unfiltered equations with the exception that the divergence of the turbulent stress tensor appears as an extra term in the filtered equations. With the unfiltered equations written as $NS(u) = 0$ with NS a symbolic notation for the 'Navier-Stokes' operator, the filtered equations can be written as $NS(\overline{u}) = -\partial_j \tau^L_{ij}$. In this way the divergence of the turbulent stress tensor appears as a 'source-term' for the evolution of the filtered solution. In practice it cannot be expressed in terms of the filtered solution alone and ideally would require full knowledge of the unfiltered solution. Thus the closure problem in LES is to find suitable expressions for τ^L in terms of $\overline{u}$ alone. This modelling process is central in LES and can be guided by incorporating any sound physical properties of small-scale phenomena in turbulent flow or by taking into account the mathematical structure of the filtered equations. We illustrate some of the latter possibilities next.

The filtered equations have a number of rigorous properties which can be used to assist in the modelling process. There are several symmetries of the filtered equations known, such as translational and rotational symmetry, Gallilean invariance and scale invariance [10]. Similarly the realisability requirements for the turbulent stress tensor [22] can be used to restrict the multitude of possibilities for modelling τ^L. We will not consider these properties here but instead turn to algebraic properties of τ^L and their use in subgrid modelling. The commutator defining the turbulent stress tensor τ^L shares a number of properties with the Poisson-bracket in classical mechanics. An important property of Poisson-brackets is in the context of LES known as Germano's identity [3]

$$[\mathcal{L}_1\mathcal{L}_2, S] = [\mathcal{L}_1, S]\mathcal{L}_2 + \mathcal{L}_1[\mathcal{L}_2, S] \quad i.e. \quad \tau^{\mathcal{L}_1\mathcal{L}_2} = \tau^{\mathcal{L}_1}\mathcal{L}_2 + \mathcal{L}_1\tau^{\mathcal{L}_2} \tag{4}$$

where $\mathcal{L}_1$ and $\mathcal{L}_2$ denote any two filter operators and $\tau^K = [K, S]$ is the turbulent stress tensor associated with a filter K. Similarly Jacobi's identity holds for S, $\mathcal{L}_1$ and $\mathcal{L}_2$:

$$[\mathcal{L}_1, [\mathcal{L}_2, S]] + [\mathcal{L}_2, [S, \mathcal{L}_1]] = -[S, [\mathcal{L}_1, \mathcal{L}_2]] \quad i.e. \quad [\mathcal{L}_1, \tau^{\mathcal{L}_2}] - [\mathcal{L}_2, \tau^{\mathcal{L}_1}] = \tau^{[\mathcal{L}_1, \mathcal{L}_2]} \tag{5}$$

This formulation of the Jacobi identity holds for general filters. In case convolution filters are considered the right hand side in eq. (5) is zero. The expressions in eq. (4) and eq. (5) provide relations between the turbulent stress tensor corresponding to different filters and can be used to dynamically model τ^L. The success of models incorporating eq. (4) is by now well established and applied in many different flows. In the traditional formulation one selects $\mathcal{L}_1 = \mathcal{H}$ and $\mathcal{L}_2 = L$ where $\mathcal{H}$ is the so called test-filter. In this case one can specify Germano's identity as

$$\tau^{\mathcal{H}L}(u) = \tau^{\mathcal{H}}\left(L(u)\right) + \mathcal{H}\left(\tau^L(u)\right) \tag{6}$$

The first term on the right hand side involves the operator $\tau^{\mathcal{H}}$ acting on the resolved LES field $L(u)$ and during an LES this is known explicitly. The remaining terms need to be replaced by a model. In the dynamic modelling approach the next step is to assume a base-model m^K corresponding to the filter-level K and optimise any coefficients in it in accordance with e.g. an optimal compliance with the Germano identity in a least squares sense [14]. Several choices for the base model have been used varying from the Smagorinsky eddy-viscosity model to mixed versions consisting of similarity models, e.g. Bardina's model or the tensor-diffusivity model, combined with an eddy-viscosity term. The first base model gives rise to the dynamic model and the second option to what is known as the dynamic mixed models. In actual simulations this approach has proven to be very successful, mainly because these models avoid excessive dissipation in relatively quiescent regions of the flow whereas appropriately high values of eddy-viscosity arise in regions with large turbulent intensity. In implementations of the dynamic procedure shortcomings of the assumed base model can require some technical adjustments. As an example, the use of dynamic eddy viscosity is not guaranteed to yield positive and relatively smoothly varying dynamic coefficients. This could lead to numerical instabilities and for that reason 'clippling' and averaging over suitable parts of the flow domain are introduced. The self-adjusting property of the model-parameters proceeds dynamically in accordance with the local instantaneous flow properties and does not require ad hoc parameters other than in specifying the test-filter $\mathcal{H}$. In addition, the dynamic modelling is appealing in many applications because it displays a self-restoring feedback mechanism. In fact, an under-prediction of the dynamic eddy viscosity typically tends to lead to a slight increase of small scale components of sizes comparable to the filter-width which in turn will increase the eddy viscosity and thus remove some of the newly arisen small scale components. This feedback has several appealing consequences for applications of LES. A quite complete comparison of a large number of subgrid models, combining the ideas of energy-dissipation, similarity and Germano's identity for turbulent flow in a temporal mixing layer can be found in ref. [27]. Recently, the use of inverse modelling approaches has been developed which gives rise to a further development of dynamic mixed subgrid models. We give a brief illustration of this next.

The operator formulation allows to readily identify 'generalised' similarity models which involve approximate inversion defined by $\mathcal{L}^{-1}(L(x^k)) = x^k$ for $0 \leq k \leq N$ [5]. With this operation it is possible to partially reconstruct the unfiltered solution u from the filtered solution $\overline{u}$ and use this information in the definition of a subgrid model. Without any inversion the original similarity model by Bardina [1] can be written as $m_B = [L, S](L(u))$, i.e. applying the definition of the turbulent stress tensor directly to the available filtered field. A direct generalisation of this arises from $m_{GB} = [L, S]\left(\mathcal{L}^{-1}(L(u))\right)$ using the approximate inversion. This model was analysed in a kinematic simulation as well as for single Fourier modes. Compared to the original Bardina similarity model the generalised model showed to combine high correlation with improvements in dissipative properties while retaining the possibility to represent backscatter of energy. More recently the approximate inversion was combined with dynamic modelling [11]. This was based on the choice $\mathcal{L}_1 = \mathcal{H}$ and $\mathcal{L}_2 = \mathcal{H}^{-1}L$ for which Germano's identity can be specified to

$$\tau^L(u) = \tau^{\mathcal{H}}\left(\mathcal{H}^{-1}L(u)\right) + \mathcal{H}\left(\tau^{\mathcal{H}^{-1}L}(u)\right) \tag{7}$$

Compared to the traditional formulation which involves the modelling of terms which correspond to length scales Δ_L and $\Delta_{\mathcal{H}L}$ this extension which incorporates the (approximate) inverse of the test-filter $\mathcal{H}^{-1}$ requires modelling of terms on the scale of Δ_L as before and $\Delta_{\mathcal{H}^{-1}L}$. Since $\Delta_{\mathcal{H}^{-1}L} \leq \Delta_L \leq \Delta_{\mathcal{H}L}$ the terms that require modelling are smaller and at the same time it is easier to maintain modelling assumptions, e.g. involving properties of an inertial range. Dynamic models based on the above have been applied successfully. A further extension involving repeated application of $\mathcal{H}^{-1}$ is also possible formally. However, since (approximate) inversion is not a very well behaved operation for the smaller scales, in actual applications one faces the risk of reconstructing small scale contributions which have been contaminated with possible numerical artifacts. Therefore there is a clear practical upper-bound to the number of times $\mathcal{H}^{-1}$ can be used beneficially and from recent experience 3 or 4 appears a definite upper-bound.

Another way of optimising the use of the information contained in an LES which is more implicit gives rise to the 'tensor-diffusivity' or 'gradient' model. Again, the basis for this model is, essentially, approximate deconvolution. Consider, for example, the Gaussian filter

$$G(z) = \frac{exp(-z^2/\sigma^2)}{\sqrt{\pi}\sigma} \tag{8}$$

For such a filter we find that the commutator τ^L is given by

$$\overline{uv} - \overline{uv} = \sum_{k=1}^{\infty} \left(\frac{\sigma^2}{2}\right)^k \frac{1}{k!} \frac{\partial^k \overline{u}}{\partial x^k} \frac{\partial^k \overline{v}}{\partial x^k} \tag{9}$$

The full infinite series above is equivalent to deconvolving $\overline{u}$ and $\overline{v}$ (clearly a singular operation) then forming the product uv and then applying the filter operation. Taking only the first term in the series above as a subgrid model we have in d dimensions

$$\overline{uv} - \overline{u}\,\overline{v} \approx \frac{\sigma^2}{2} \frac{\partial \overline{u}}{\partial x_\ell} \frac{\partial \overline{v}}{\partial x_\ell} \tag{10}$$

where repeated indicies are summed and $\ell = 1, 2, .., d$. Use of this approximation on the filtered, constant density, incompressible momentum equation for $\overline{u}_i$ yields the following subgrid force on the RHS

$$\frac{-\sigma^2}{2} \overline{S}_{jk} \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_k} \tag{11}$$

where $\overline{S}_{jk}$ is the strain-rate tensor of the filtered velocity field. Hence the term 'tensor diffusivity' model which dates back to [12]. Similarly one could arrive at this model using a Taylor expansion on the Bardina model. A direct application of this model in LES can lead to an ill-behaved system of equations as was analysed in [26]. However, the appealing property of being able to represent backscatter, without the need of an additional filtering, can be retained if this base model is combined with a dynamic eddy-viscosity. In that case a computationally efficient and competitive subgrid model is arrived at [27, 13]

3 Non-uniform filters and LES of complex flows

The desire to extend LES to complex flows in an efficient way implies that one typically encounters situations in which the turbulence intensities vary considerably within the flow domain. In certain regions of the flow a nearly laminar, smoothly evolving flow may arise while a lively, fine scale turbulent flow can be present in another region. This calls for a filtering approach involving a filter with a non-uniform filter-width. Here we will study some consequences of applying such filters and in particular identify and estimate the additional terms that arise from using a variable filter-width.

We consider the effect of applying a general, compact support filter which is defined by $u \to \overline{u}$:

$$\overline{u}(x,t) \equiv L(u) = \int_{x-\Delta_-(x)}^{x+\Delta_+(x)} \frac{H(x,\xi)}{\Delta(x)} u(\xi,t)d\xi \tag{12}$$

where $\Delta_+,\ \Delta_- \geq 0$ denote the x-dependent upper - and lower 'bounding functions' of the filter. The filter domain can also be represented by the filter-width $\Delta = \Delta_+ + \Delta_-$ and the 'skewness' $\sigma = \Delta_+ - \Delta_-$ which together with the 'normalised kernel' H specify the properties of the filter. We can derive the LES equations for nonuniform filters and identify a 'mean' term associated with the Navier-Stokes operator acting on the filtered solution and several new terms which are related to commutators containing the filter L as was sketched in the previous section. Incompressible flow is governed by the Navier-Stokes equations subject to the constraint of divergence free velocity fields. In dimensionless form this system of equations can be written in conservation form as

$$\partial_j u_j = 0 \quad ; \quad \partial_t u_i + \partial_j(u_i u_j) + \partial_i p - \frac{1}{Re}\partial_{jj} u_i = 0 \quad ; \quad i = 1,2,3 \tag{13}$$

where p denotes the 'pressure', Re the Reynolds number and the summation convention is adopted. If we apply the filter to the system of equations in (13) commutators of L with partial derivatives and multiplication arise. After some manipulation we find:

$$\partial_j \overline{u}_j = -[L, \partial_j](u_j) \tag{14}$$

This shows that application of a non-convolution filter to the continuity equation gives rise to terms which in general violate the local conservation form. Filtering the Navier-Stokes equations yields

$$\partial_t \overline{u}_i + \partial_j(\overline{u}_i\overline{u}_j) + \partial_i\overline{p} - \frac{1}{Re}\partial_{jj}\overline{u}_i =$$
$$- \Big([L,\partial_i](p) - \frac{1}{Re}[L,\partial_{jj}](u_i) + [L,\partial_j](S(u_i,u_j)) + \partial_j([L,S](u_i,u_j))\Big) \quad (15)$$

in which the 'Navier-Stokes' operator applied to the filtered field is identified on the left hand side. The first three terms on the right hand side are related to commutators of L and partial derivatives ∂_j which as before implies violation of the conservation property in general. The turbulent stress tensor arises in the last term on the right hand side. It is the only filter-term in case convolution filters are adopted while more general filters yield the full system of equations (14) and (15). The central modelling problem for the continuous formulation and general filters is now extended to approximations modelling commutators like $[L,\partial_x]$, $[L,\partial_{xx}]$ and $[L,S]$ in terms of operations on $\overline{u}$. A mathematically consistent modelling can be arrived at using approximate inversion [5] which can be extended to non-uniform filters in a consistent way with the help of symbolic manipulation software such as maple. The new terms that have arisen can be shown to obey the same algebraic identities as put forward in relation to $[L,S]$. These identities can be used e.g. in a dynamic modelling of the commutators of non-uniform filtering and partial derivatives which need to be taken into account for complex flows.

In order to establish the importance of these new commutators in relation to the regular filter terms $[L,S]$ and to interpret in what way these terms contribute to the inter-scale energy transfer we analyse the commutators for general high order filters acting on sufficiently smooth signals [6]. Such N-th order filters are defined by requiring the first N moments to be invariant, i.e. $L(x^k) = x^k$ for $k = 0,1,...,N-1$. In the following we will apply such filters and retain only the leading order terms assuming sufficiently smooth signals for the moment. In 1d one may readily show that

$$\overline{u}(x) = u(x) + \Big(\Delta^N(x)M_N(x)\Big)\, u^{(N)}(x) + \cdots \quad (16)$$

for N-th order filters. Here $M_N \sim L(x^N)$ is the N-th order moment. If we turn to the decomposition of a typical term

$$\overline{\partial_x(u^2)} = \partial_x(\overline{u}^2) + \partial_x([L,S](u)) + [L,\partial_x](S(u)) \quad (17)$$

one observes the commutators $[L,S]$ and $[L,\partial_x]$ to arise naturally. As derived in detail e.g. in [6, 8] one finds corresponding expressions for these commutators given by:

$$\begin{aligned}
[L,\partial_x](S(u)) &= A(x)\Big(\Delta^{N-1}\Delta' M_N\Big) + B(x)\Big(\Delta^N M_N'\Big) + \cdots \\
\partial_x([L,S](u)) &= a(x)\Big(\Delta^{N-1}\Delta' M_N\Big) + b(x)\Big(\Delta^N M_N'\Big) \\
&+ c(x)\Big(\Delta^N M_N\Big) + \cdots
\end{aligned}$$

where A, B, a, b and c are smooth functions containing combinations of derivatives of the solution u. From this we infer that a constant filter-width implies $[L, \partial_x] = 0$ and the leading order term of the turbulent stress tensor equals $[L, S] \sim \Delta^N$ for N-th order filters. However, non-uniform filters clearly give rise to contributions to the commutators which are a priori of equal order of magnitude. From this we infer, unlike findings in [21, 20] that it is not possible to remove the commutators $[L, \partial_x]$ by a careful selection of the filter. In fact, all filters that would reduce this commutator are of higher order and consequently will also reduce the usual term $[L, S]$. The only possibility to control $[L, \partial_x]$ independently is by reducing non-uniformity of the filter-width, e.g. by keeping grid-nonuniformity, which usually defines local filter-widths, small. We will quantify this to some extent next and illustrate the dynamic effect associated with the new commutators.

A detailed analysis of the new commutators can be obtained e.g. in a single-wave analysis in which we assume a solution $u = \sin(kx)$. For illustration purposes we consider a symmetric top-hat filter for which one has $[L, \partial_x](\sin(kx)) = -\mathcal{A}' \sin(kx)$. Since $\mathcal{A} = \sin(k\Delta(x)/2)/(k\Delta(x)/2)$ depends on x through Δ we observe the importance of maintaining smooth and comparably slow spatial variations in Δ. In particular

$$\mathcal{A}' = \left[\frac{\cos(k\Delta/2) - 2\sin(k\Delta/2)}{(k\Delta/2)}\right]\frac{\Delta'}{\Delta} = -\frac{1}{24}((k\Delta)^2)' + \frac{1}{1920}((k\Delta)^4)' + \ldots \tag{18}$$

In order to appreciate the magnitude of this commutator compared to $[L, S]$ in a dynamic context we recall that $[L, \partial_x](S(u))$ needs to be compared to $\partial_x([L, S](u))$. After some manipulation we find

$$[L, \partial_x](S(u)) + \partial_x([L, S](u)) = C(k\Delta(x))\{k\sin(2kx) + \frac{\Delta'(x)}{\Delta(x)}(\cos(2kx) - 1)\} \tag{19}$$

where the characteristic flux function C for this filter is given by

$$C(z) = \frac{z\sin(z) - 2 + 2\cos(z)}{z^2} = -\frac{1}{12}z^2 + \frac{1}{180}z^4 + O(z^6) \tag{20}$$

The two contributions to the flux have a ‘weight’ k and (Δ'/Δ) respectively from which we infer that if variations in Δ are sufficiently slow, i.e. $|\Delta'| \ll |k\Delta|$ then filter-width non-uniformity can be disregarded. We infer that the dynamic effect of the new commutator is related to the sign of Δ'. One may interpret this as follows. A decreasing filter-width contributes to the backscatter of energy; in particular it appears that subgrid contributions tend to become resolved and thus shift to the grid-scale modes. Conversely an increase in filter-width is associated with extra dissipation since resolved scales which are convected into such regions tend to become subgrid contributions. In a priori estimates of these terms based on DNS of temporal boundary layer flow [7] it appeared that close to solid walls the flux contribution from the commutators $[L, \partial_j]$ is about half as large as that arising from $[L, S]$ and hence one cannot avoid modelling the new commutators near walls since at high Reynolds numbers these are automatically associated with strong grid clustering. Likewise, a high correlation of the new commutators and (generalised) similarity models was observed which suggests efficient and accurate ways to model these contributions.

4 Interaction between numerical and modelling errors

From the filtering of the equations in the previous sections it has become clear that a large number of subgrid terms arise which need to be modelled and subsequently treated numerically. If the ratio of the filter-width to the grid-spacing of the LES-grid is too small then significant numerical errors can occur and interact with the modelling errors discussed above. We will illustrate some consequences of the implicit filtering approach in which the filter-width Δ and grid-spacing h are identified and confront this with the explicit filtering approach in which the ratio Δ/h is chosen larger than 1. The implicit filtering approach has the benefit of computational efficiency in relation to the amount of information contained in the solution but this benefit can be obscured completely by an adverse interaction between the different errors which can contaminate much larger scales. Such an interaction between errors can be controlled in the explicit filtering approach but leads to an increase in computational effort. In actual LES a suitable balance, expressed partly by an appropriate ratio between Δ and h should therefore be used.

We consider the numerical effects by tracing the operations on a representative contribution for a convolution filter. This allows the comparison of different spatial discretization methods, filter-widths and filter implementations which are the main sources of local error. We focus on filtering $\partial_j(u_i u_j) + \partial_i p$ in the Navier-Stokes equations and find

$$\begin{aligned} \partial_j(\overline{u_i u_j}) + \partial_i \overline{p} &= [\delta_j(\overline{u}_i \overline{u}_j) + \delta_i \overline{p} + \mathcal{D}_i] + \partial_j \tau_{ij} \\ &= [\delta_j(\overline{u}_i \overline{u}_j) + \delta_i \overline{p} + \mathcal{D}_i] + [\partial_j m_{ij} + \mathcal{R}_i] \\ &= \delta_j(\overline{u}_i \overline{u}_j) + \delta_i \overline{p} + \delta_j m_{ij} + [\mathcal{D}_i + \mathcal{D}_i^{(m)} + \mathcal{R}_i] \qquad (21) \end{aligned}$$

where $\mathcal{D}_i$ denotes the discretization error arising from application of a spatial discretization method δ_j to the convective terms, $\mathcal{D}_i^{(m)}$ is the error when implementing the model m_{ij}, e.g. filtering as well as discretization errors and $\mathcal{R}_i = \partial_j(\tau_{ij} - m_{ij})$ is the total 'model-residue' associated with m_{ij}. This term can only be determined in *a priori* evaluations and is of course unknown during an actual LES. So, whereas formally $\partial_j(\overline{u_i u_j}) + \partial_i \overline{p}$ is needed in an LES strictly speaking only $\delta_j(\overline{\overline{u}_i\overline{u}_j}) + \delta_i\overline{p}$ is directly available and two main sources of discrepancy can be identified. Whereas the subgrid-term $\partial_j\tau_{ij}$ is usually modelled with a subgrid-model, the discretization error $\mathcal{D}_i$ is not taken into account. The first question is whether this is justified and for this purpose an *a priori* comparison of different spatial discretization methods and filter-widths was made for turbulent flow in a mixing layer [24, 25]. The magnitude and ratio of the discretization error $\mathcal{D}_i$ and the flux due to the turbulent flux $\partial_j\tau_{ij}$ determines in large part the reliability of LES predictions. We evaluated these terms for a well developed flow and evaluated the errors associated with a second and a fourth order finite volume discretization operator δ_j. It was shown that if $\Delta = h$, the discretization error $\mathcal{D}_i$ is larger than the subgrid term for both methods and in this case LES predictions would not be reliable even with a perfect subgrid-model for τ. If Δ is sufficiently larger than h, i.e. smoother fields are represented on the same grid, the contribution of $\partial_j\tau_{ij}$ is considerably larger than $\mathcal{D}_i$. In this regime the second-order method shows only a relatively small decrease of $\mathcal{D}_i$ for increasing Δ, whereas the fourth-order method shows a rapid decrease of $\mathcal{D}_i$. This was observed for both fine and very coarse LES-grids and can serve as a guidance in selecting Δ for a specific discretization method on a given grid. An interesting related study can be found in [15] in which the Smagorinsky constant was varied at fixed grid resolution. When Δ is large the filtered fields become smoother which reduces the discretization error at the expense of containing only little information about the smaller scales. A good compromise appears the choice $\Delta = 2h$ for the fourth order method while a second order method requires a higher value of Δ/h. In that case fourth order discretizations are more efficient than second order ones.

The second question we address is how the different errors $\mathcal{D}_i$, $\mathcal{D}_i^{(m)}$ and $\mathcal{R}_i$ interact dynamically. We consider the dynamic mixed model in combination with the discretization schemes used above as well as a pseudo-spectral method. Discrepancies between LES and filtered DNS results arise mainly from shortcomings of the model and from numerical discretization on a relatively coarse grid. In LES these sources of error interact which complicates testing, since separation of subgrid-modelling and numerical effects is difficult [16]. We propose approximate separation of the effects of modelling and discretization error by incorporating LES at higher resolution. We consider the evolution of the total kinetic energy E:

$$E = \int_\Omega \frac{1}{2}\overline{u}_i\overline{u}_i d\mathbf{x} \tag{22}$$

where Ω is the flow domain. As a function of time E displays a gradual decrease. Variations in spatial discretization method show variations in the predictions for E whose magnitude is of the same order as would arise when changing from a dynamic subgrid model to e.g. the Bardina similarity model. These effects of the errors increase considerably if we use $\Delta = h$ instead of $\Delta = 2h$. We can approximately separate the modelling and discretization effects and focus on their interaction by incorporating a fine-grid LES. The discretization error in LES will become smaller if the resolution is increased at constant Δ. The discretization error in such a 'fine-grid LES' will be considerably smaller and we can obtain LES predictions with negligible discretization error effects. The difference between these two large-eddy simulations can then give an indication of the effect of the discretization error: $\varepsilon_d = E_{\text{LES}} - E_{\text{fine-grid LES}}$ whereas the difference between the fine-grid LES and the filtered DNS measures the effect of the modelling error: $\varepsilon_m = E_{\text{fine-grid LES}} - E_{\text{filtered DNS}}$.

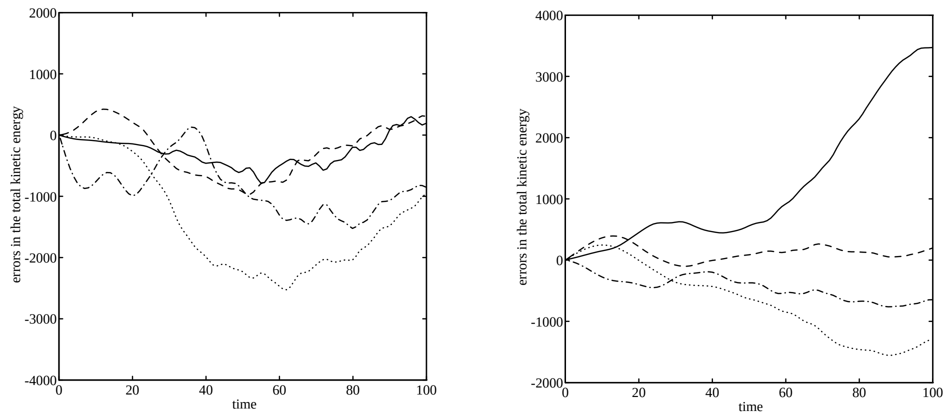

Figure 1: Error decomposition with modelling error (solid) and discretizations error effect for the three discretization methods: dashed (second order), dash-dotted (spectral) and dotted (fourth order). Left figure $\Delta = h$ and right figure $\Delta = 2h$.

We calculated these errors for the turbulent flow in a mixing layer on a representative grid which is about six times coarser in each direction than required for DNS. The corresponding fine-grid LES has been performed with the ratio between Δ and h in the fine-grid LES sufficiently large, i.e. the fields are quite smooth on grid-scale and discretization errors will be considerably reduced. The quantities ε_d and ε_m are shown in figure 1. The discretization error effects are smaller than the modelling error only if $\Delta \geq 2h$ whereas with implicit filtering ε_d is even larger than ε_m. The second-order scheme is observed to give the smallest discretization error effect. This does not imply that the discretization error itself is small, but only its effect on the evolution of the total kinetic energy. For the fourth order and pseudo-spectral methods the discretization error and modelling error effect have opposite sign, which implies that the discretization error assists the subgrid-model in the representation of this quantity: the total error is considerably smaller than the modelling error. These observations suggest that e.g. for the spectral scheme, improvement of the subgrid-model (decrease of the modelling error) is expected to give worse results, since the total error will increase. Likewise one can infer that an increase in the resolution may result in worse predictions. All these errors and their interactions can be extremely disturbing for more complex flows for which no proper separation is available and one has to rely on intuition and previous experience in order to judge and justify the outcome of a particular simulation. Since in the past this has proven to be a very underdeveloped area, we list some (hopefully) useful guidelines in the next section.

5 Some guidelines for predictable LES

In this section we will formulate some general guidelines which can enhance the credibility of a flow simulation within the LES approach. Since there has been a large development in the capabilities of computers and numerical methods, it has become possible to use some of these capabilities to systematically vary certain numerical elements within a 'reference' LES and monitor the sensitivity of the predictions. Since LES is in many respects close to a direct numerical simulation, several of the guidelines are of relevance for numerical reasons only whereas certain suggestions are more specific to the LES context. The following list which compiles the guidelines is necessarily incomplete and somewhat biased given the fact that LES is still a lively and rapidly developing field of research. Moreover, we have put forward some guidelines which may add too much to the computational cost; however, we have taken the liberty to formulate an LES approach focusing more on reliability than on strict saving of computational effort. Eventually, LES can offer an expensive and reliable answer irrespective of the quality of the subgrid model and in part also quite independent of the quality of the numerical methods involved, provided the subgrid contributions are sufficiently reduced. This 'escape-route', however, would be virtually identical to a well resolved DNS and be not very practical in most cases. However, the fact that LES has this limit build into it can be used also to infer about the reliability of any given 'reference' LES.

The list of guidelines presented below has been split into mainly numerical, mainly modelling and interaction issues. There can be a strong interaction and interdependence between modelling and numerics and for that reason some points are described under more than one topic. As a whole, an LES is as strong as its weakest element (as are many other approaches).

- Numerical guidelines:

— *Use smooth grids with low stretching and skewness and 'equal' resolution in each direction.* This is of importance since the formal as well as the attained accuracy of spatial discretization schemes can be considerably affected by either shortcoming of the grid. Moreover, the resolution should be comparable in each of the coordinate directions in order to avoid contamination of the solution in an under-resolved direction through 'folding back' of energy contained in modes which are well resolved in another coordinate direction.

— *Avoid numerical dissipation.* In particular for turbulent flow the presence of some numerical dissipation can cover shortcomings e.g. in resolution, grid properties or modelling used in the approach. Although this may appear helpful in cases in which the resolution is too low anyway, it adds to the unreliability of LES and can seriously affect the predictions, in particular if the same approach would be used for other flows, at other resolutions or for other flow conditions.

— *Validate your code.* In order to eliminate as much as possible numerical artifacts and remaining uncertainties regarding resolution, inflow and outflow conditions, geometrical description of the flow domain etc. validation is essential. This could incorporate comparison with simpler theories, e.g. using linear stability theory, checking whether basic symmetries of the equations are also contained in the numerical formulation, using experimental data if available and comparison with available filtered DNS data in case validation for simple flows is included. It is sensible to have some discipline of version management of the software.

— *Vary numerical parameters.* In any numerical study a certain number of relevant numerical parameters appear and basically no physically relevant prediction should depend on any of these parameters. Variations in resolution, definition of geometry, inflow/outflow boundaries, numerical method and method of evaluation of the simulation results should be considered for LES as well as DNS.

— *Incorporate LES predictions at different filter-width to mesh-size ratios into a flow analysis.* As was illustrated in the previous section a carefully selected set of LES predictions can be used to appreciate the influence of some of the errors involved and to some extent one could estimate these errors from the combined LES predictions. With present day computers it is now feasible to conduct several LES investigations of one flow and from it extract a quantitative appreciation of the reliability of the predictions.

- Modelling guidelines:

— *Use dynamic modelling.* Dynamic modelling is appealing since it does not add any ad hoc parameters to the modelling other than properties of the test-filter. The approach has proven to be quite robust and possesses a self-restoring property if the resolution is sufficiently high.

Moreover, at suitable resolution it avoids the introduction of special wall treatment. Both properties give rise to a prediction of the large-scale flow which is quite robust, suitable for transitional and turbulent flow and can be used in quite general inhomogeneous flows.

— *Use explicit filtering approach.* In contrast to the implicit filtering setting of LES the explicit filtering offers independent control and treatment of the various steps relevant within LES. Using all available resolution aimed only at predicting small scale properties of the flow can lead to considerable unreliability and contamination of much of the predictions of all the other scales. In the explicit filtering some of the resolution can be used to increase the reliability with which the smaller scales are predicted.

— *Incorporate similarity and dissipation into modelling.* Both these properties arise naturally from spectral considerations of LES; similarity is an inertial range property of the turbulent stress tensor itself and the required energy transfer to smaller scales is efficiently represented by dissipation although more refined ways of energy transfer may be required if other elements in the LES approach become more refined.

— *Use smooth grids with low stretching and skewness and 'equal' resolution in each direction.* For modelling this point is relevant since high stretching and skewness give rise to significant additional terms in the equations which require to be modelled. Similarly, unevenness in the grid can lead to sizeable effects in the implementation and evaluation of the actual model and obscure many of the model's potential.

— *Incorporate LES predictions at different filter-width to mesh-size ratios into a flow analysis.* From a carefully designed set of LES predictions one could infer errors arising from the subgrid modelling.

— *Vary numerical parameters.* The influence of the subgrid model can be controlled to some extent by a suitable change in the numerical parameters. Moreover, several models require additional filtering and differentiation and the number of points available to do this is usually quite restricted and hence can make the implemented model appear to have different properties compared to the continuum formulation.

— *Optimise use of scales available in LES.* The options for LES modelling offered by inverse modelling, approximate deconvolution and/or subgrid estimation have not been fully exploited and can be beneficial to LES.

- Restricted interaction guidelines:

— *Choose Δ/h appropriately.* The ratio of the filter-width Δ to (local) mesh-size h is an important parameter in LES. If it is large then the LES prediction will appear smooth on grid-scale and the quality of the prediction will be mainly restricted by the quality of the subgrid model. Conversely, if this ratio is small then the effects of numerics will be large. In practice a ratio $\Delta/h \geq 2$ appears adequate when fourth order methods are employed but this ratio should be increased to 4 if second order methods are used.

— *Incorporate LES predictions at different filter-width to mesh-size ratios into a flow analysis.* As before, this step involves performing a number of large-eddy simulations for the same flow from which an approximate error appreciation can be inferred.

In order to develop LES for general complex flows the treatment of the near wall region is crucial and not yet well developed in LES. Similarly, if shocks or detailed capturing of chemistry is required also including multi-phase flows then a proper modelling of this 'near interface' region is vital. Finally, an appreciation and possibly an estimate of the error in the LES predictions should be aimed at. For this purpose the use of approximate inversion of the filtering, the compliance with algebraic properties and other rigorous characteristics of the subgrid terms and a systematic variation of e.g. the resolution, independent of the filter width should be developed. The filter-width Δ (with suitable h) and a certain subgrid model imply a certain number of modes N_{LES} to be involved which should at any rate be sufficiently larger than the number of modes $n_q(\varepsilon)$ needed to predict a quantity q with a desired level of accuracy. It appears relevant to quantify suitable numbers n_q and corresponding N_{LES} for several geometrically simple flows which are well documented and allow for a fully resolved DNS as well in order to provide a well controlled point of reference. From an estimate of N_{LES} for these flows and a number of subgrid models and numerical methods it would be possible to formulate more general selection and design rules for reliable LES in the future. For the modelling process it is advisable to respect rigorous guidelines (e.g. symmetries, realisability, algebraic properties, inequalities) and to formulate some error monitoring and control aiming at the prediction of an 'error-bar' during a simulation.

Acknowledgements

Stimulating and inspiring discussion with several participants in the turbulence programme of the Isaac Newton Institute has been much appreciated and helpful. One of us (BJG) would like to thank the European Science Foundation for supporting part of this work.

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