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Ten questions concerning the large-eddy simulation of turbulent flows

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Abstract. In the past 30 years, there has been considerable progress in the development of large-eddy simulation (LES) for turbulent flows, which has been greatly facilitated by the substantial increase in computer power. In this paper, we raise some fundamental questions concerning the conceptual foundations of LES and about the methodologies and protocols used in its application. The 10 questions addressed are stated at the end of the introduction. Several of these questions highlight the importance of recognizing the dependence of LES calculations on the artificial parameter Δ (i.e. the filter width or, more generally, the turbulence resolution length scale). The principle that LES predictions of turbulence statistics should depend minimally on Δ provides an alternative justification for the dynamic procedure.

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Contents

Introduction

There have been many and substantial advances in large-eddy simulation (LES) since the pioneering works of Smagorinsky [1], Lilly [2], Deardorff [3], Schumann [4] and others. Advances have been made in (i) modelling the unresolved processes; (ii) accurate numerical methods on structured and unstructured grids; (iii) detailed comparison of LES calculations with DNS and experimental data in canonical flows; (iv) extensions to include additional phenomena, e.g. turbulent combustion; (v) and in computational power, which has increased by about four orders of magnitude since the 1970s. Expositions on LES are provided by Pope [5] and Sagaut [6]; and reviews at different stages of the development of LES are provided by Rogallo and Moin [7], Galperin and Orszag [8], Lesieur and Métais [9], and Meneveau and Katz [10].

In spite of these advances, there remain fundamental questions about the conceptual foundations of LES, and about the methodologies and protocols used in its application. The purpose of this paper is to raise and to discuss some of these questions.

Before posing the questions to be addressed, it is necessary to introduce the terminology used to describe LES. This needs to be done with some care to include existing divergent views on LES, and to avoid pre-judging some of the questions raised. The fundamental quantity considered in LES is a three-dimensional unsteady velocity field which is intended to represent the larger-scale motions of the turbulent flow under consideration. We refer to this as the *resolved velocity field* and denote it by $\boldsymbol{W}(\boldsymbol{x}, t)$. As discussed at greater length in section 4, we distinguish between *physical LES* and *numerical LES*. The prime example of physical LES is the 'filtering approach' introduced by Leonard [11]. In this approach, $\boldsymbol{W}(\boldsymbol{x}, t)$ is identified as the *filtered velocity field*, denoted by $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$, obtained by applying a low-pass spatial filter of characteristic width Δ to the underlying turbulent velocity field, $\boldsymbol{U}(\boldsymbol{x}, t)$. The effects of the sub-filter scales are modelled, and the resulting evolution equation for $\boldsymbol{W}(\boldsymbol{x}, t)$ is solved numerically on a mesh of spacing h. An example of numerical LES is the 'MILES approach'

advocated by Boris *et al* [12]. In this case, the Navier–Stokes equations are written for $\boldsymbol{W}(\boldsymbol{x}, t)$ and are solved on a mesh of spacing h which is insufficiently fine to resolve the smaller-scale motions, using a numerical method designed to respond appropriately in regions of inadequate spatial resolution. To accommodate all viewpoints we refer to $\boldsymbol{W}(\boldsymbol{x}, t)$ as the *resolved velocity field*, and to Δ as the *turbulence-resolution length scale*, which for numerical LES we define as $\Delta = h$. Turbulent motions that are not resolved are referred to as *residual motions*, and we use the term *residual stress* for the quantity often referred to as the sub-grid scale (SGS) stress, or the sub-filter scale stress.

For a complex flow, an unstructured mesh with non-uniform mesh spacing would normally be used, so that h and Δ are non-uniform, and indeed these scalars provide an incomplete description of the mesh and of the turbulence resolution. For such cases we use $h(\boldsymbol{x})$ and $\Delta(\boldsymbol{x})$, somewhat imprecisely, to characterize the length scales of the numerical and turbulence resolutions.

In addition to introducing terminology, the above discussion draws out the fact that the fundamental quantity in LES—namely the resolved velocity field $\boldsymbol{W}(\boldsymbol{x}, t)$—is an extremely complex object. It is a three-dimensional, time-dependent random field, which has a fundamental dependence on the artificial (i.e. non-physical) parameter Δ, and which (in some approaches) depends also on the mesh spacing h and on the numerical method used. It is not surprising, therefore, that LES raises non-trivial conceptual questions.

In the following sections we address in turn these 10 questions:

1. Is LES the right approach?
2. Can the resolution of all scales be made tractable?
3. Do we have sufficient computer power for LES?
4. Is LES a physical model, a numerical procedure or a combination of both?
5. How can LES be made complete?
6. What is the relationship between $\boldsymbol{U}$ and $\boldsymbol{W}$?
7. How do predicted flow statistics depend on Δ?
8. What is the goal of an LES calculation?
9. How are different LES models to be appraised?
10. Why is the dynamic procedure successful?

The main purpose of this paper is to raise conceptual questions concerning LES which warrant further consideration by the research community. While we offer some answers, they are not intended to be definitive or complete, but rather the primary intention is to stimulate further debate of these questions.

1. Is LES the right approach?

The first point to be made in response to this question is that, given the broad range of turbulent flow problems, it is valuable to have a broad range of approaches that can be applied to study them. There is not one 'right' approach. As discussed more fully elsewhere [5, 13], while the use of LES in engineering applications will certainly increase in the future, the use of simpler Reynolds-averaged Navier–Stokes (RANS) models will be prevalent for some time to come. It is valuable, therefore, to continue to seek improvements to the full range of useful turbulence modelling approaches.

Perhaps the most compelling case for LES can be made for momentum, heat and mass transfer in free shear flows at high Reynolds numbers. For this case, the transport processes of interest are effected by the resolved, large-scale motions; and (in the Richardson–Kolmogorov view at least) there is a cascade of energy, dominantly from the resolved large scales, to the statistically isotropic and universal small scales. There are, therefore, strong reasons to expect LES to be successful, primarily because both the quantities of interest and the rate-controlling processes are determined by the resolved large scales.

In other applications the picture can be quite different. For example, in turbulent combustion at high Reynolds number and Damkohler number, the essential rate-controlling processes of molecular mixing and chemical reaction occur at the smallest scales. In some combustion regimes, these coupled processes occur in reactive–diffusion layers that are much thinner than the resolved scales [14]. Hence the rate-controlling processes do not occur in the resolved large scales, but instead have to be modelled. For such cases, the argument that LES is the 'right' approach is less convincing. While LES may provide a more reliable turbulence model than RANS (especially if there are large-scale unsteady motions) nevertheless the rate-controlling combustion processes require the same modelling as in RANS; indeed, most LES combustion models are derived from RANS models.

A second example is high Reynolds number near-wall flows, the simplest specific case being the turbulent boundary layer on a smooth wall. The wall shear stress—all-important in aerodynamic applications—arises from momentum transfer from the outer flow through the boundary layer to the wall. In the viscous near-wall region, the momentum transfer is effected by the near-wall structures, the length scale of which scales with the tiny viscous length scale. As Bradshaw has succinctly put it: in the viscous near-wall region *there are no large eddies*. But, as has been appreciated at least since Chapman [15], the near-wall motions cannot be resolved in high-Reynolds number LES, but must instead be modelled (to avoid impracticable computational requirements that increase as a power of Reynolds number, as in DNS).

In summary, the arguments in favour of LES are compelling for flows (e.g. free shear flows) in which the rate-controlling processes occur in the resolved large scales. There is the reasonable expectation of LES predictions being accurate and reliable, and of being insensitive to the details of the modelling (provided that Δ is not too large). But for flows in which rate-controlling processes occur below the resolved scales the case is weaker. The rate-controlling processes have to be modelled, and the LES predictions can be expected to have a first-order dependence on these models.

2. Can the resolution of all scales be made tractable?

Following on from the conclusions of the previous section, for flows in which the rate-controlling processes are not confined to the large scales, it is natural to seek methods that resolve all scales in a way that is computationally tractable at high Reynolds number. Is this possible?

Based on the known spacing of near-wall streaks, it can be estimated that there are of order 10^8 streaks on the wings of a Boeing 777 during cruise. In a (hypothetical) DNS of this flow, all 10^8 streaks are resolved, leading to computational intractability, whereas in LES none of the streaks is resolved, so that all of the shear stress at the wall arises from modelled processes. Observations such as these prompt the question raised here. Is it really necessary to represent and resolve all 10^8 streaks? Is it not possible to devise a methodology in which

only a statistically representative sample of these streaks is resolved? Could this be done in such a way that the computation cost increases weakly with Reynolds number, e.g. as ln(Re)? Perhaps the holy grail of turbulence is *the statistical resolution of all scales*—a methodology in which representative samples of motions and processes on all scales are resolved and combined (without empiricism) in a way that remains computationally tractable at large Reynolds number.

Some steps have been made in this direction: we cite two examples.

For simulating homogeneous isotropic turbulence in wavenumber space, Meneguzzi *et al* [16] introduced sparse-mode methods. Based on the wavenumber κ_E characteristic of the energy-containing motions, the wavenumber space is partitioned into shells $2^{m-1}\kappa_E \leqslant |\boldsymbol{\kappa}| < 2^m\kappa_E$, for $m = 1, 2, \ldots$. In the mth shell, only a fraction 2^{-3m} of the Fourier modes are represented. As a consequence, the total number of modes represented increases just as ln(Re).

The second example we cite is the linear eddy model (LEM) [17] and one-dimensional turbulence (ODT) [18], which can be used as SGS models in LES (e.g. [19, 20]). These models fall short of the ideal in that they involve empirical prescriptions, and the computational work increases as a power of Reynolds number (albeit a smaller power than in DNS). Nevertheless, these methods embody the notion of resolving all scales, but only for a small sample of the flow.

These steps notwithstanding, the methodology of the statistical resolution of all scales as described above faces a formidable obstacle: in turbulence there are interactions between the continuous range of length scales—there is no scale separation.

3. Do we have sufficient computer power for LES?

Whatever the situation is today, it is clear that in the early days of LES the available computer power was insufficient for the purpose. It is equally clear that at some time there will be ample computer power. This is an inevitable consequence of the sustained exponential increase of computer power with time, combined with the advances in numerical and computational algorithms, which can yield comparable gains. As sketched in figure 1, there is an inevitable cross-over time after which the available computer power exceeds that needed for LES. When this cross-over occurs depends on the particular flow problem being studied and the computer resources available. The cross-over time (whenever it occurs) divides the development and the use of LES into two eras: the era of insufficient computer power, followed by the era of sufficient computer power. All of this is clear and obvious. The important point to appreciate is that attitudes and practices can be radically different in the two eras.

When there is insufficient computer power, compromise is inevitable, especially on numerical accuracy, the range of scales resolved and testing for numerical and physical accuracies. There is a natural tendency to use all of the available computer power to perform the largest simulation possible. It is generally the case that comprehensive testing requires orders of magnitude more computer time than a single simulation. For example, halving the grid spacing h typically increases the required memory and CPU time by factors of 8 and 16, respectively. Hence, such testing is precluded by the decision to perform the largest simulation possible.

Much of the discussion in the subsequent sections pertains to the second era, when there is ample computer power; and the primary consideration is the best way to perform LES, not what can be afforded.

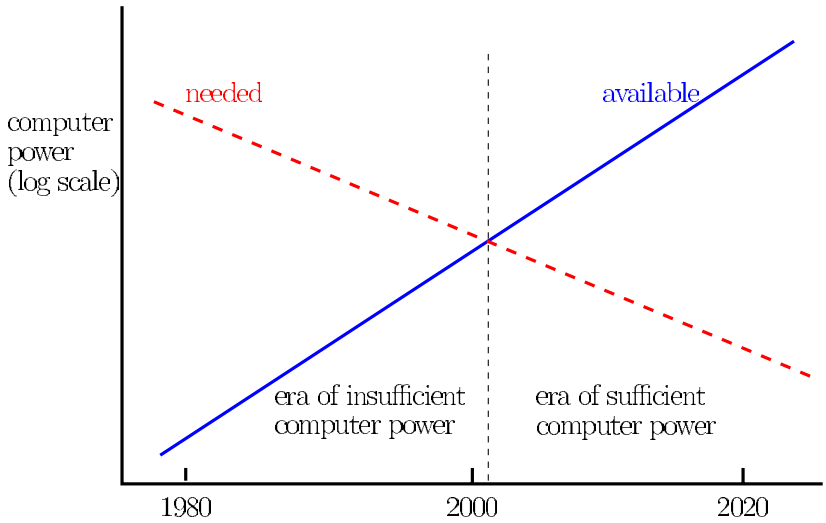

Figure 1. Sketch of the computer power available and that needed for LES as a function of time. The cross-over time is the transition from the era of insufficient computer power to the era of sufficient computer power.

Do we now have sufficient computer power for LES? Arguably we do for simple flows, and for more complex flows that time is fast approaching. Many of the attitudes and practices in the field come from the era of insufficient computer power. In looking to the future of LES, we need to shed these attitudes and practices to realize the greater possibilities that ample computer power offers.

The above notwithstanding, it is inevitable that LES will be applied to ever more challenging flows, with an increased range of length scales to be resolved, and increased complexity of the physical processes (e.g. sprays and granular flows). Hence, for a considerable time to come, there will be insufficient computer power for these most challenging applications of LES.

4. Is LES a physical model, a numerical procedure or a combination of both?

Different approaches to LES provide different answers to this question.

The prevailing opinion expressed by the Stanford/Ames CTR group (see e.g. [21]) is that LES is a physical model. The effects of the residual motions are explicitly modelled, so that the resulting LES model consists of a set of partial differential equations (PDEs), involving Δ, which is sufficient to determine the resolved velocity field $\boldsymbol{W}(\boldsymbol{x}, t)$. For specified Δ, these PDEs are then solved by a numerical method using a mesh spacing h which is sufficiently small to yield numerically accurate solutions. We refer to this as *physical LES* and make the following three observations.

1. Good numerical accuracy comes at a high price. With the numerical methods usually employed, halving the grid spacing increases the computational cost by about a factor of $2^4 = 16$.
2. To show that this approach is indeed being followed, it is necessary to demonstrate that the LES solutions are grid-independent. This is seldom done, the studies of Vreman *et al* [22] and Meyers *et al* [23] being welcome exceptions.

3. For an LES of fixed computational cost (i.e. fixed h), one can consider the optimal value of Δ. A large value of Δ/h corresponds to excellent numerical accuracy, whereas a smaller value corresponds to resolving a greater range of turbulent motions, but with less numerical accuracy. The optimal value depends on the approach and models used; however, by the criteria for comparing models introduced in section 9, it is probable that the optimal value of Δ/h corresponds to non-negligible numerical error. The results of Vreman *et al* [22] and Meyers *et al* [23] support this view.

In view of these considerations, we refine our terminology and define *pure physical LES* to be LES performed with explicit models for the effects of the residual motions and negligible numerical error, whereas in *physical LES* some numerical error may be present.

At the opposite end of the spectrum is *numerical LES*, in which the description of the resolved velocity field $\boldsymbol{W}(\boldsymbol{x}, t)$ and its evolution is fundamentally linked to the numerical method. The representation of $\boldsymbol{W}(\boldsymbol{x}, t)$ is intrinsically discrete—in terms of node, cell or basis-function values—and there is no notion of convergence to the solution of a PDE. Examples of numerical LES are MILES [12], optimal LES [24] and LES using projection onto local basis functions [25]. In MILES, the Navier–Stokes equations are solved numerically on a grid of spacing h which is too large to resolve all of the scales of motion. The numerical method is especially constructed to be stable (and non-oscillatory) in regions of inadequate spatial resolution [12]. In MILES, there is no explicit model for the effects of the residual motions, whereas there is, for example, in optimal LES. Even when there is no explicit model, it should be appreciated that in numerical LES the computed flow fields depend both on the mesh and on the numerical method: the often-used terminology 'no model' is an inadequate description. Indeed, even in physical LES with non-negligible numerical errors, as demonstrated by Vreman *et al* [22] and Kravchenko and Moin [26], the LES results depend on the numerical method used (in addition to h and Δ).

We take the view that pure physical LES, physical LES and numerical LES are all valid approaches, which can be compared as discussed in section 9. When this is done, it seems unlikely that pure physical LES will be advantageous: a non-negligible amount of numerical error is likely to be optimal. In some of the considerations that follow it is necessary to take into account the fact that, except in pure physical LES, the computed LES fields depend on the numerical method and on the grid employed.

5. How can LES be made complete?

A model for turbulent flows is deemed complete if its constituent equations are free from flow-dependent specifications [5]. One flow is distinguished from another solely by the specification of material properties and of initial and boundary conditions. For example, the k–ε model is complete whereas the mixing length model is incomplete, because the mixing length must be specified (as a function of position and time). If two competent practitioners make two independent mixing-length calculation of the same complex flow, the results are bound to differ, because different choices would be made for the specification of the mixing length. Clearly, completeness is highly desirable.

It is important to appreciate that, *as generally practised*, LES is incomplete. The general practice is to generate a computational grid with spacing characterized by $h(\boldsymbol{x})$, say, and then to specify $\Delta(\boldsymbol{x})$ to be proportional (locally) to $h(\boldsymbol{x})$. The turbulence resolution length scale $\Delta(\boldsymbol{x})$ is

a significant parameter in the LES equations, yet it is specified in a flow-dependent, subjective manner. Given this fact, it is regrettable that evaluating the dependence of LES calculations on the value of $\Delta(\boldsymbol{x})$ is not a generally accepted part of LES practice.

LES can be made complete through the use of solution-adaptive gridding: we refer to this as *adaptive LES*. To illustrate this idea, we introduce the following three related quantities:

1. a measure $M(\boldsymbol{x}, t)$ of the turbulence resolution,
2. the turbulence-resolution length scale $\Delta(\boldsymbol{x}, t)$ and
3. a specified turbulence-resolution tolerance ϵ_M.

A conceptually simple measure of turbulence resolution is the fraction of the turbulent kinetic energy in the resolved motions. The evaluation of $M(\boldsymbol{x}, t)$ requires the determination (locally in space and time) of the turbulent kinetic energy of the resolved motions $K(\boldsymbol{x}, t) \equiv \frac{1}{2}\langle(\boldsymbol{W} - \langle\boldsymbol{W}\rangle) \cdot (\boldsymbol{W} - \langle\boldsymbol{W}\rangle)\rangle$, and that of the residual motions $k_r(\boldsymbol{x}, t)$. Then we define

$$M(\boldsymbol{x}, t) \equiv \frac{k_r(\boldsymbol{x}, t)}{K(\boldsymbol{x}, t) + k_r(\boldsymbol{x}, t)}. \tag{1}$$

Thus the value of M is between 0 and 1: $M = 0$ corresponds to DNS and $M = 1$ to RANS. Smaller values of M correspond to the resolution of more of the turbulent motions. (Although this definition of M is conceptually simple, in LES, the approximation of means, denoted here by angled brackets $\langle\ \rangle$, is non-trivial and a methodology to estimate k_r is required.)

The turbulence resolution length scale $\Delta(\boldsymbol{x}, t)$ can also be viewed as the turbulence resolution control parameter. The smaller the value of Δ, the greater the fraction of the energy that is resolved and, hence, the smaller the value of M. Thus, the value of M can be controlled by varying Δ. (To some extent this control is non-local: $M(\boldsymbol{x}, t)$ is affected by the value of Δ at other locations and at earlier times.) If the ratio h/Δ is fixed, then varying Δ is accomplished by varying the mesh spacing $h(\boldsymbol{x})$.

In adaptive LES, a value of the turbulence-resolution tolerance ϵ_M is specified, e.g. $\epsilon_M = 0.2$ corresponds to the resolution of 80% of the kinetic energy. The LES is then performed with adaptive gridding (i.e. the adjustment of $\Delta(\boldsymbol{x}, t)$ via $h(\boldsymbol{x}, t)$) to maintain

$$M(\boldsymbol{x}, t) \leqslant \epsilon_M. \tag{2}$$

In regions where M exceeds ϵ_M the grid is refined; where M is much smaller than ϵ_M the grid is coarsened.

For a given flow, the turbulence statistics computed by adaptive LES should be assumed to depend on ϵ_M, until the contrary is demonstrated. Consequently, ϵ_M is part of the model specification. While different implementations of adaptive LES using different numerical methods may produce somewhat different results (for the same value of ϵ_M), nevertheless, this approach goes a good way towards removing the subjectivity and incompleteness of the standard approach.

Needless to say, even though solution-adaptive gridding is increasingly available in computational fluid dynamics (CFD) codes, there are several implementation challenges to be overcome to implement adaptive LES. However, only by a methodology such as this can LES be made complete.

6. What is the relationship between *U* and *W*?

To clarify the question posed in the heading, we recall that $\boldsymbol{U}(\boldsymbol{x}, t)$ denotes the velocity field in the turbulent flow under consideration, and $\boldsymbol{W}(\boldsymbol{x}, t)$ denotes the 'resolved velocity field' obtained from LES. It is easier to say what the relationship between $\boldsymbol{U}$ and $\boldsymbol{W}$ is *not* than to say what it is! As explained below, the conventional view that $\boldsymbol{W}(\boldsymbol{x}, t)$ is the spatially filtered value of $\boldsymbol{U}(\boldsymbol{x}, t)$ is not sustainable.

To clarify the issues involved, it is necessary to introduce a more precise notation than is conventionally used. First, it is essential to distinguish between physical and modelled quantities. We illustrate this in the simpler context of the k–ε model. The turbulent kinetic energy is defined as

$$k(\boldsymbol{x}, t) \equiv \tfrac{1}{2}\langle u_i(\boldsymbol{x}, t) u_i(\boldsymbol{x}, t)\rangle, \tag{3}$$

where

$$\boldsymbol{u}(\boldsymbol{x}, t) \equiv \boldsymbol{U}(\boldsymbol{x}, t) - \langle \boldsymbol{U}(\boldsymbol{x}, t)\rangle \tag{4}$$

is the fluctuating velocity field, and the dissipation is defined by

$$\varepsilon \equiv 2\nu\langle s_{ij} s_{ij}\rangle, \tag{5}$$

with ν the kinematic viscosity and

$$s_{ij} \equiv \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{6}$$

the fluctuating rate of strain. We denote by $k_m(\boldsymbol{x}, t)$ and $\varepsilon_m(\boldsymbol{x}, t)$ the quantities considered in the k–ε model. It is important to appreciate that k_m and ε_m are not defined by equations (3) and (5): instead, they are defined as the solutions to the k–ε model equations (with the appropriate initial and boundary conditions). As is well accepted, the k–ε model is far from perfect, and so k_m does not equal k, and ε_m does not equal ε. Instead, k_m is a *model* for k. At the same time, these considerations identify the goal for turbulence modelling in this context: a perfect k–ε model (if one exists) yields solutions k_m and ε_m which are equal to k and ε.

In the LES context, it should be appreciated that fundamentally $\boldsymbol{W}(\boldsymbol{x}, t)$ is defined as the solution to the LES equations, not as the spatially filtered value of $\boldsymbol{U}(\boldsymbol{x}, t)$, which we denote by $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$.

However, we may ask, is it possible (in principle) to have a perfect LES model such that $\boldsymbol{W}(\boldsymbol{x}, t)$ equals $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$? The answer is *no*; the reason being that $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$ is a random field, whose future evolution is not determined by its current state. Thus, while we may impose $\boldsymbol{W}(\boldsymbol{x}, 0) = \overline{\boldsymbol{U}}(\boldsymbol{x}, 0)$ as an initial condition, for $t > 0$, $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$ has a statistical distribution, and hence there is no value of $\boldsymbol{W}(\boldsymbol{x}, t)$ which equals $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$. This argument is developed more fully in section 13.5.6 of Pope [5].

Clearly, therefore, the relationship between $\boldsymbol{U}$ and $\boldsymbol{W}$ can only be statistical. Hence, among other consequences, *a priori* testing as it is usually practiced is highly dubious, since it compares LES quantities with the corresponding quantities obtained from a particular realization of $\boldsymbol{U}(\boldsymbol{x}, t)$. Similar arguments and conclusions are given by Lesieur [27], Langford and Moser [24] and Sagaut [6].

From the statistical viewpoint which is appropriate to these considerations, an LES procedure consists of the following components:

(i) A set of model evolution equations for the resolved velocity field $\boldsymbol{W}(\boldsymbol{x}, t)$ and possibly also for some statistics of the residual motions, denoted by $\boldsymbol{R}(\boldsymbol{x}, t)$, such as the residual kinetic energy or stresses. In physical LES these equations involve $\Delta(\boldsymbol{x}, t)$.

(ii) For a given flow, a specification of $\Delta(\boldsymbol{x}, t)$ and a stochastic procedure for specifying initial and boundary conditions on $\boldsymbol{W}$ and $\boldsymbol{R}$.

(iii) A procedure for generating, from $\boldsymbol{W}$ and $\boldsymbol{R}$, estimates of statistics of the velocity field $\boldsymbol{U}(\boldsymbol{x}, t)$.

To expand on the last component, let Q denote a statistic of $\boldsymbol{U}(\boldsymbol{x}, t)$ that is of interest, and let $\mathcal{Q}$ denote the operation performed on $\boldsymbol{U}(\boldsymbol{x}, t)$ to obtain it, i.e.

$$Q = \mathcal{Q}\{\boldsymbol{U}(\boldsymbol{x}, t)\}. \tag{7}$$

For example, for the two-point (one-time) velocity correlation, we would have

$$Q_{ij}(\boldsymbol{x}, t, \boldsymbol{r}) = \langle U_i(\boldsymbol{x}, t) U_j(\boldsymbol{x} + \boldsymbol{r}, t)\rangle. \tag{8}$$

In the last of the three components of the LES, there is a procedure or operation, denoted by $\mathcal{Q}^m(\boldsymbol{W}, \boldsymbol{R}, \Delta)$, which yields an estimate Q^m for the statistic Q. It is useful to decompose the model as

$$Q^m = Q^w + Q^r, \tag{9}$$

where Q^w is a component determined solely by $\boldsymbol{W}$, whereas Q^r is a model for the residual contribution which may depend on $\boldsymbol{W}$, $\boldsymbol{R}$ and Δ. (This decomposition may not be unique.) Thus, for the example of the two-point correlation, the contribution from the resolved velocity is

$$Q^w_{ij}(\boldsymbol{x}, t, \boldsymbol{r}) = \langle W_i(\boldsymbol{x}, t) W_j(\boldsymbol{x} + \boldsymbol{r}, t)\rangle_N, \tag{10}$$

where $\langle\ \rangle_N$ denotes an ensemble average over N LES simulations. (For flows in which it is possible, time and spatial averaging can be used in place of, or in addition to, ensemble averaging. It should be noted that, even with averaging, Q^w, Q^r and Q^m are random variables used to estimate the value of the non-random statistic Q.)

The 'perfect' LES procedure is therefore one in which, for all statistics Q of interest, the LES estimates Q^m (or at least $\langle Q^m\rangle$) are equal to Q. Hence, our answer to the question 'What is the relationship between $\boldsymbol{U}$ and $\boldsymbol{W}$?' is that it can only be statistical: for the statistics of interest, the estimates Q^m obtained from $\boldsymbol{W}$ and $\boldsymbol{R}$ are models for the corresponding statistics Q of the turbulent velocity field.

Another possible answer to the question—one frequently given—is that the statistics of $\boldsymbol{W}$ model the statistics of the filtered velocity field $\overline{\boldsymbol{U}}$. While this is a tenable position, we make the following observations.

1. $\overline{\boldsymbol{U}}$ is a non-physical quantity, dependent on the filter type and filter width.
2. In applications it is the statistics of $\boldsymbol{U}$ that are relevant: a knowledge of the statistics of $\overline{\boldsymbol{U}}$ is not necessarily sufficient.

3. Component (iii) (the estimation of statistics of $\boldsymbol{U}$) is an important ingredient in an LES procedure, which arguably has not received the attention it deserves, because it is not needed if attention is confined to statistics of $\boldsymbol{W}$ and $\overline{\boldsymbol{U}}$.
4. For an LES methodology to model successfully the statistics of $\boldsymbol{U}$, it is not *necessary* for the statistics of $\boldsymbol{W}$ to correspond to those of $\overline{\boldsymbol{U}}$.

In the filtering approach and in optimal LES, the aim of the modelling is to yield resolved fields $\boldsymbol{W}(\boldsymbol{x}, t)$ whose statistics correspond to those of $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$. But in other approaches (e.g. MILES) as stated above, requiring such a correspondence is not necessary, and may not be useful.

7. How do predicted flow statistics depend on Δ?

As in the previous section, we consider a general statistic of the turbulent flow (denoted by Q), and the corresponding estimate of Q (denoted by Q^m) obtained from the LES. The value of Q^m depends on two artificial parameters; the turbulence resolution length scale Δ and the numerical resolution h. These are artificial parameters in the sense that, while they affect Q^m, they have no impact on the underlying velocity field $\boldsymbol{U}(\boldsymbol{x}, t)$, and hence they have no effect upon Q.

We focus attention on the influence of Δ by considering the ratio h/Δ to be fixed. In pure physical LES, provided that h/Δ is sufficiently small, the solutions are numerically accurate and hence the dependence on h is negligible. (Test calculations by Vreman *et al* [28] and Chow and Moin [29] show that this requirement is $h/\Delta \leqslant \frac{1}{4}$ for a scheme with second-order spatial accuracy, and $h/\Delta \leqslant \frac{1}{2}$ for sixth-order accuracy.) For numerical LES, the eddy resolution is determined directly by the grid: the parameter Δ does not appear explicitly in the equations, and hence we can simply define $\Delta = h$, yielding $h/\Delta = 1$. Physical LES involving some numerical error is generally performed with $h/\Delta = 1$ or $h/\Delta = \frac{1}{2}$. Thus, we treat h/Δ as a secondary parameter, which is fixed for the sake of the current discussion.

We consider the simplest case of a free shear flow in which the energy-containing motions are characterized by an integral length scale L, and the Reynolds number is extremely large so that the Kolmogorov scale η (which characterizes the smallest motions) is very small compared with L. The statistic obtained from the LES is denoted by $Q^m(\Delta)$ to show explicitly its dependence on Δ—and it is this dependence which is examined in this section. Essentially, the same considerations apply to the dependence of Q^m on ϵ_M in adaptive LES.

For generality we consider a statistic Q which has contributions from both the energy-containing and dissipative scales, and we speculate that $Q^m(\Delta)$ varies with Δ as depicted qualitatively in figure 2. (Such a statistic can be formed, for example, as the sum of a statistic dominated by the energy-containing range and a statistic dominated by the dissipation range.) In addition to L and η, the figure shows the length scales ℓ_{EI} and ℓ_{DI} which demarcate the inertial subrange from the energy-containing range and from the dissipation range, respectively. As Δ is reduced from order L to ℓ_{EI}, more and more of the energy-containing motions are resolved. Hence, more of the energy-containing contribution to Q is represented directly through $\boldsymbol{W}$, and less is modelled. As Δ is further decreased towards ℓ_{DI}, an intermediate asymptote, denoted by Q_I^m, is approached. This corresponds to Δ being in the inertial subrange. Nearly all of the energy-containing contribution to Q is represented directly in terms of $\boldsymbol{W}$, whereas nearly

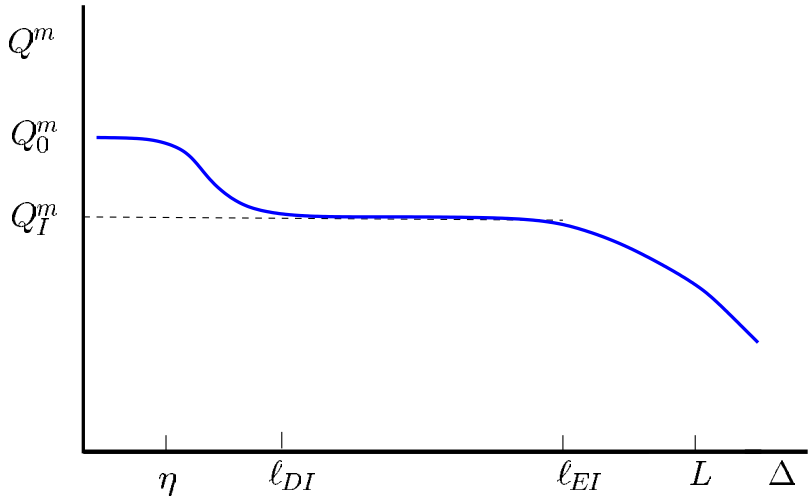

Figure 2. Variation of the model Q^m for that statistic Q as a function of the turbulence resolution length scale Δ (on a log scale): Q_0^m is the DNS limit as Δ tends to zero; Q_I^m is the intermediate asymptote in the inertial subrange.

all of the dissipation-range contribution is modelled. As Δ is further reduced, eventually the DNS asymptote Q_0^m is reached in which $Q^m(\Delta)$ tends to Q as all of the scales are resolved. The achievement of this asymptote depends on the LES model appropriately reverting to the Navier–Stokes equations as Δ tends to zero—which we assume to be the case for all models considered here.

It is emphasized that the existence of this intermediate asymptote is a hypothesis, in need of testing for different statistics, and its existence certainly depends upon the LES model being consistent with inertial-range scaling. If other processes are involved (e.g. combustion or mixing at large or small Schmidt number), then transitions may occur around the values of Δ corresponding to the resolution of those processes.

To expand on this picture, figure 3 shows the two contributions to Q^m, i.e. the contribution Q^w solely from $\boldsymbol{W}$ and the model Q^r for the residual contribution (which depends on $\boldsymbol{W}$, $\boldsymbol{R}$ and Δ; see equation (9)). The behaviour of Q^w is simple: as Δ decreases from $\Delta \approx L$, the resolved contribution Q^w increases until it approaches the asymptote Q_I^w (around $\Delta \approx \ell_{EI}$), corresponding to the contribution to Q from the energy-containing motions, which are well resolved for $\Delta \leqslant \ell_{EI}$. As Δ decreases through the inertial sub-range from ℓ_{EI} to ℓ_{DI}, Q^w changes little, since it contains essentially all of the contributions from the energy-containing motions, but none from the dissipative motions. However as Δ decreases beyond ℓ_{DI} towards η and towards zero, more and more of the dissipative contribution is directly resolved by Q^w, which tends to Q_0^m.

The behaviour of Q^r is a little more complicated. For $\Delta \approx L$, Q^r models both the contribution to Q from the dissipative scales, and also the contribution from the unresolved large-scale motions. As Δ decreases towards ℓ_{EI}, this latter contribution decreases towards zero. In the inertial subrange, Q^r models the contribution from the dissipation scales, and its value is essentially constant. In this range, $\boldsymbol{W}$ and $\boldsymbol{R}$ vary with Δ, and hence the constancy of Q^r depends on the model satisfying the correct inertial-range scaling. As Δ decreases from ℓ_{DI} to zero, all of the dissipative motions become resolved, and hence any reasonable model ensures that Q^r tends to zero.

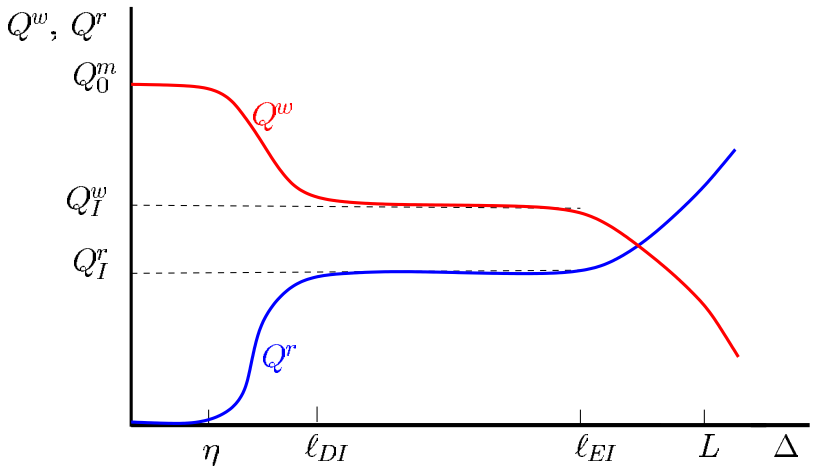

Figure 3. The contributions to the modelled statistic Q^m from the resolved motions Q^w and from the residual model Q^r as a function of the turbulence resolution length scale Δ. In the inertial subrange, Q^w and Q^r approach the intermediate asymptotes, Q_I^w and Q_I^r.

This idealized picture calls for several qualifications, but also leads to important conclusions.

(i) Figures 2 and 3 pertain to unrealistically high Reynolds number at which the intermediate asymptote is clear. At moderate Reynolds numbers, the intermediate asymptote may not be discernible.

(ii) The computational cost of the LES varies approximately as $(L/\Delta)^4$, and hence it is not feasible to perform simulations with $\Delta \ll \ell_{EI}$. With $\Delta \approx \eta$, the computational cost is comparable with DNS, and hence is not feasible beyond moderate Reynolds numbers.

(iii) If the statistic Q in question contains a significant contribution from the dissipative scales (as assumed in figures 2 and 3), then it is important to recognize

  (a) that the convergence for Δ in the inertial subrange ($\ell_{DI} < \Delta < \ell_{EI}$) is to the intermediate asymptote Q_I^m, not to the true value of Q;
  (b) for practical values of Δ (e.g. $\Delta \geqslant \ell_{EI}$) the LES prediction $Q^m(\Delta)$ has an order-one contribution from the modelled term Q^r.

(iv) In contrast with the previous case, if the statistic Q in question *and the processes affecting it* pertain solely to the energy-containing range, then it is reasonable to suppose that there is a single asymptote (i.e. $Q_I^m = Q$), and hence $Q^m(\Delta)$ converges to Q as Δ/ℓ_{EI} becomes small. This situation is depicted in figure 4. Since the earliest days, this has been the promise of LES.

Note that, in item (iv) above, the qualification '... and processes affecting it ...' is necessary. Consider, for example, a statistic Q pertaining to the large scales of the composition field in turbulent combustion. Even though the statistic pertains to the large scales, the rate-controlling processes of molecular mixing and chemical reaction occur on the smallest scales. Hence, $Q^m(\Delta)$ cannot be assumed to converge to Q unless these small scales are resolved. So the picture remains that of figure 2 with $Q_I^m \neq Q$.

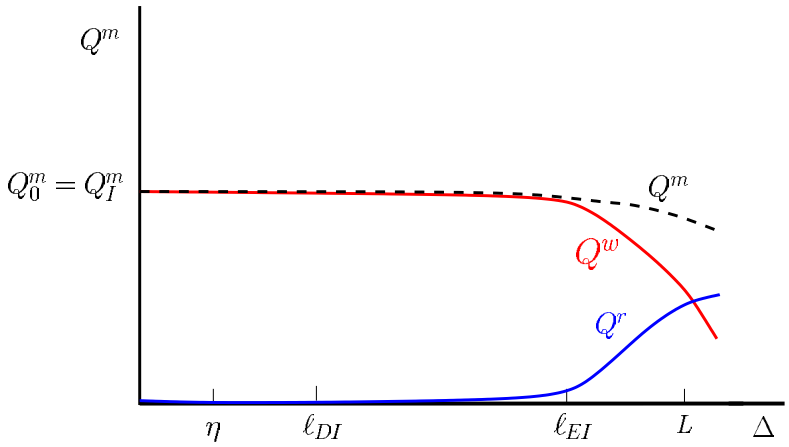

Figure 4. The modelled statistic Q^m and its components Q^w and Q^r against the turbulence resolution length scale Δ for the case in which the statistic Q and the processes affecting it are confined to the energy-containing scales.

We have considered here Q^m as a function of Δ. For adaptive LES (as described in section 5), Q^m can be considered as a function of the turbulence resolution tolerance ϵ_m, and the picture is essentially the same for $Q^m(\epsilon_m)$ as it is for $Q^m(\Delta)$.

8. What is the goal of an LES calculation?

For a given flow and a given LES model, what is the goal of the calculations performed? This superficially naive question is prompted by the fact that, as discussed above, statistics $Q^m(\Delta)$ obtained from LES depend on the artificial parameter Δ. It is intrinsically unsatisfactory to accept $Q^m(\Delta)$ (for some value of Δ) as a prediction for Q—for $Q^m(2\Delta)$ or $Q^m(\frac{1}{2}\Delta)$, for example, may yield substantially different predictions.

A more satisfactory answer can be provided in the idealized case (considered in the previous section) of very high Reynolds number free shear flow. The goal of the LES calculation can be to estimate the intermediate asymptotic value Q_I^m (see figure 2), which is independent of Δ. This can be achieved by performing LES with several (at least three) different values of Δ, so that the intermediate asymptote can be estimated by extrapolation to $\Delta = 0$.

At moderate Reynolds number, and in more complex flows, a completely satisfactory answer is more elusive. However it should surely be an essential part of the LES methodology to perform simulations over a range of Δ to assess the sensitivity of $Q^m(\Delta)$ to Δ. If the sensitivity is large over the whole range investigated, what can be concluded about the flow statistic Q?

9. How are different LES models to be appraised?

Given two LES models, which we refer to as model A and model B, what criteria are to be used to assess their relative merits? In the broader context of turbulence modelling

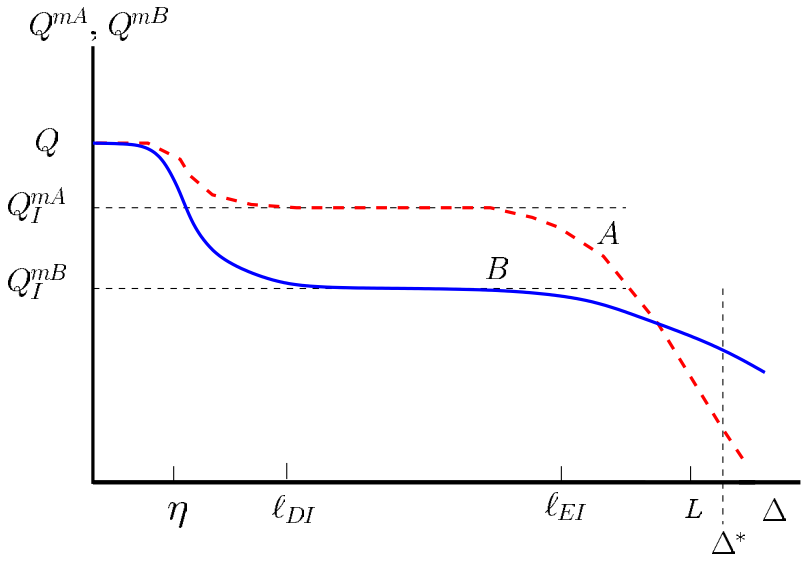

Figure 5. The predictions $Q^{mA}(\Delta)$ and $Q^{mB}(\Delta)$ of the statistic Q obtained from LES models A and B as functions of the turbulence resolution length scale Δ for the case in which Q has contributions from both energy-containing and dissipative scales.

(including LES), Pope [5] suggests five criteria:

(i) level of description
(ii) completeness
(iii) cost and ease of use
(iv) range of applicability, and
(v) accuracy.

Completeness is the topic of section 5. Here we first discuss accuracy, and then cost (in conjuction with accuracy). For LES, an additional criterion, which we assume to be satisfied by the models considered, is convergence to DNS in the limit at Δ/η tends to zero.

Considering again the very high-Reynolds number flow of the previous two sections, figure 5 is a sketch of $Q^m(\Delta)$ given by models A and B. It shows that the two models have different intermediate asymptotes, denoted by Q_I^{mA} and Q_I^{mB}, respectively. Recalling that the ideal goal of an LES calculation is to estimate this intermediate asymptote, for the case depicted in figure 5, model A clearly has superior accuracy, since Q_I^{mA} is closer to Q than is Q_I^{mB}. Note that if LES calculations were performed at the single value $\Delta = \Delta^*$ then the contrary conclusion would incorrectly be drawn.

Figure 6 depicts the situation in which the statistic Q of interest pertains solely to the energy-containing motions and both models asymptote to Q (for $\Delta/\ell_{EI} \ll 1$). As a consequence, each model becomes as accurate as desired as Δ/ℓ_{EI} decreases, and the criterion of accuracy alone does not favour one model over the other.

The second criterion to consider is the computational cost, most simply measured in CPU time, T, and most simply approximated as $T_A = c_A(L/\Delta)^4$ and $T_B = c_B(L/\Delta)^4$, for models A and B respectively, where c_A and c_B are model-dependent constants. Obviously the CPU time increases as Δ decreases. Figure 7 is a sketch of $Q^m(\Delta)$ as a function of CPU time for the

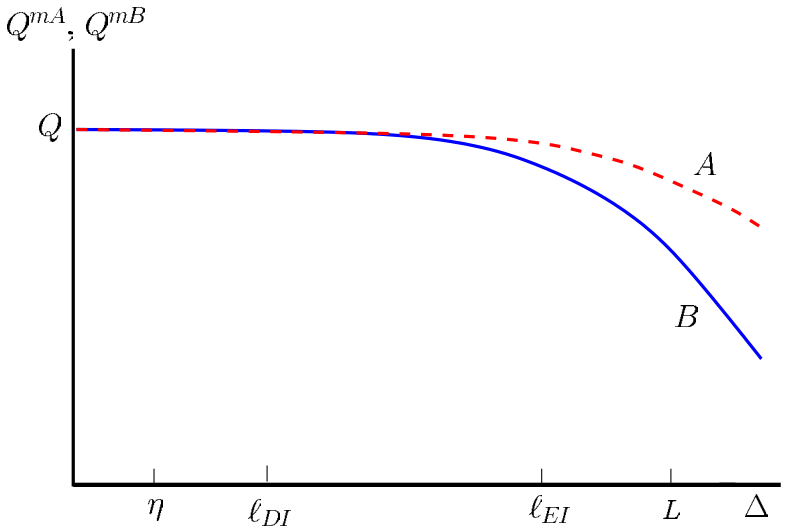

Figure 6. The predictions $Q^{mA}(\Delta)$ and $Q^{mB}(\Delta)$ of the statistic Q obtained from LES models A and B as functions of the turbulence resolution length scale Δ for the case in which Q and the processes affecting it are confined to the energy-containing range.

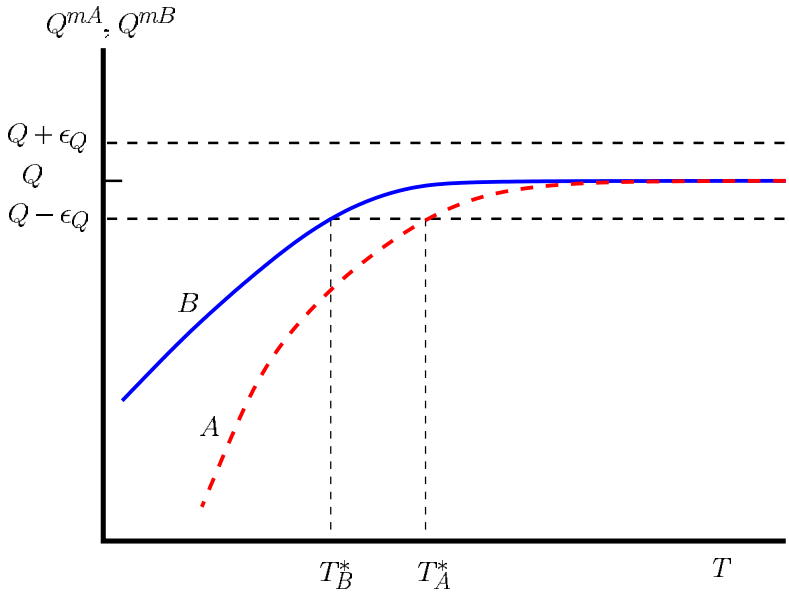

Figure 7. For the case depicted in figure 6, Q^{mA} and Q^{mB} plotted against CPU time T. The horizontal dashed lines show the interval of acceptable accuracy.

two models for the same case as is shown in figure 6. An error tolerance ϵ_Q is specified so that the calculation $Q^m(\Delta)$ is acceptably accurate if it lies in the range $[Q-\epsilon_Q, Q+\epsilon_Q]$. For the case depicted in figure 7, model B is superior since it achieves the required accuracy in time T_B^* which is less than T_A^*.

Evidently, for this case, c_A is much larger than c_B, i.e. for given Δ/L, method A is much more expensive. From figure 6 it is evident that, compared with method A, method B requires a smaller value of Δ to achieve acceptable accuracy, yet it requires less CPU time (figure 7).

Thus, the principal criteria to appraise LES models are (intermediate) asymptotic accuracy, and computational cost to achieve acceptable accuracy. It is important to appreciate that such an appraisal cannot be made without characterizing the Δ dependence of the models. In particular, comparing models based on calculations with a single value of Δ can be extremely misleading.

10. Why is the dynamic model successful?

The dynamic model was proposed by Germano *et al* [30], with important modifications and extensions provided by Lilly [31] and Meneveau *et al* [32]. The model has proved quite successful, and the same procedure has been applied in several other contexts.

The dynamic model is usually motivated by notions of scale similarity, although this rationale is not explicitly stated in the original paper. If the turbulent motions possess scale similarity, then a model that respects this scale similarity should be applicable at different scales (i.e. for different values of Δ); and this principle can be used to determine the numerical coefficients in the model. The most well-known application is to the Smagorinsky model, in which the dynamic procedure is used to determine the appropriate value of the Smagorinsky coefficient c_s.

Several observations cast doubt on this rationale for the dynamic Smagorinsky model:

(i) Turbulence at high Reynolds number can reasonably be assumed to possess scale similarity, but only over length scales corresponding to the inertial subrange. In the inertial subrange, the Smagorinsky model is, by construction, consistent with the known inertial-range scaling laws, and the appropriate value of the Smagorinsky coefficient is uniquely determined (for given filter type) by the analysis developed by Lilly [2]. In this circumstance there is, therefore, neither need for nor benefit from the dynamic model.

(ii) It is reasonable to suppose that the Smagorinsky model yields accurate predictions of energy-containing statistics in high Reynolds number free flows, provided that Δ is well within the inertial subrange. These statistics will be insensitive to a further reduction in Δ. In the Smagorinsky model, the coefficient c_s appears only in the product $c_s\Delta^2$: hence decreasing Δ is equivalent to decreasing c_s. If energy-containing statistics are insensitive to Δ, they are, therefore, also insensitive to c_s, again negating the value of the dynamic procedure.

(iii) The dynamic procedure has been most successful in remedying the standard Smagorinsky model's serious deficiencies in laminar flows, transitional flows and in the viscous near-wall region. In none of these circumstances is scale similarity plausible.

(iv) Based on similar considerations, Jiménez and Moser [33] conclude that 'the physical basis for the good *a posteriori* performance of the dynamic-Smagorinsky subgrid models in LES ... appears to be only weakly related to their ability to correctly represent the subgrid physics'.

Since the dynamic model *does* appear to be successful, it is natural to ask: why? The behaviour of the dynamic Smagorinsky model has been studied by Meneveau and Lund [34] for the case in which Δ approaches η, and hence scale similarity does not hold. At the other limit, Porté-Agel *et al* [35] introduce a *refined* dynamic procedure to produce scale-dependent coefficients for the case in which Δ approaches L. In the remainder of this section, we offer an alternative principle to motivate both the standard and refined dynamic procedures.

As discussed in section 7, the LES prediction $Q^m(\Delta)$ of a turbulent-flow statistic Q pertaining to the energy-containing range (in a high-Reynolds number free flow) can be supposed to vary with Δ as illustrated in figure 6. The figure shows $Q^m(\Delta)$ given by two different models, A and B, both of which converge to Q as Δ/ℓ_{EI} tends to zero. If the computational cost (at fixed Δ) is the same for both models, then clearly model A is superior, since it approaches the asymptote, Q, sooner as Δ decreases.

Another view of the same observation is provided by the identity

$$Q^m(\Delta) - Q = [Q^m(\Delta_I) - Q] + \int_{\Delta_I}^{\Delta} \frac{\mathrm{d}Q^m(\Delta)}{\mathrm{d}\Delta}\,\mathrm{d}\Delta, \tag{11}$$

which follows from the fundamental theorem of calculus (for any differentiable function $Q^m(\Delta)$). The left-hand side represents the error in the LES prediction as a function of Δ, which we require it to be as small as possible (in magnitude). The first term on the right-hand side represents the error in the prediction for $\Delta = \Delta_I$, and we take Δ_I to be sufficiently small for this error to be negligible. Thus the error (at scale Δ) is essentially given by the last term; and, roughly speaking, the smaller the derivative $|\mathrm{d}Q^m(\Delta)/\mathrm{d}\Delta|$, the smaller the error. As may be seen from figure 6, the derivative $|\mathrm{d}Q^m(\Delta)/\mathrm{d}\Delta|$ is smaller for method A compared with method B.

Based on this observation, it is natural to seek an LES model which has the following properties (with respect to statistics $Q^m(\Delta)$ of interest pertaining to the energy-containing motions in a high-Reynolds number flow):

(a) for $\Delta = \Delta_I$ well within the inertial subrange, the LES predictions are accurate,

(b) for $\Delta > \Delta_I$, the predicted statistics vary as weakly as possible with Δ.

We suppose that (a) is satisfied by any reasonable model that has the correct inertial-range scaling (e.g. the Smagorinsky model), and so we focus on property (b).

The dynamic model is based on filtering. Specifically, it is based on quantities filtered with respect to one filter of width $\overline{\Delta}$, and a second filter of somewhat larger width $\widetilde{\overline{\Delta}}$. Quantities so filtered are denoted by, for example, $\overline{\boldsymbol{U}}$ and $\widetilde{\overline{\boldsymbol{U}}}$, respectively. The LES model Q^m for the statistic Q of interest can be evaluated based on $\overline{\boldsymbol{U}}$ and $\overline{\Delta}$, i.e.

$$Q^m(\overline{\Delta}) = Q^w(\overline{\boldsymbol{U}}) + Q^r(\overline{\boldsymbol{U}}, \overline{\Delta}), \tag{12}$$

where Q^w denotes the contribution from the resolved motions (determined solely from $\overline{\boldsymbol{U}}$), and Q^r is the model for the contribution from the residual motions. For the *same* statistic Q, the LES model can also be applied based on $\widetilde{\overline{\boldsymbol{U}}}$ and $\widetilde{\overline{\Delta}}$, i.e.

$$Q^m(\widetilde{\overline{\Delta}}) = Q^w(\widetilde{\overline{\boldsymbol{U}}}) + Q^r(\widetilde{\overline{\boldsymbol{U}}}, \widetilde{\overline{\Delta}}). \tag{13}$$

To fulfil condition (b), we introduce the following principle: *the LES model coefficients should be chosen to minimize the difference between* $Q^m(\overline{\Delta})$ *and* $Q^m(\widetilde{\overline{\Delta}})$.

As depicted in figure 4, as Δ decreases from $\Delta \approx L$, Q^w increases, whereas Q^r decreases. The magnitude of Q^r is typically proportional to a model constant, c_Q, say. An interpretation of the above principle is that c_Q should be chosen so that the decrease in $Q^r(\Delta)$ as Δ decreases from $\widetilde{\overline{\Delta}}$ to $\overline{\Delta}$ should be balanced by the corresponding increase in $Q^w(\Delta)$. Figure 8 illustrates

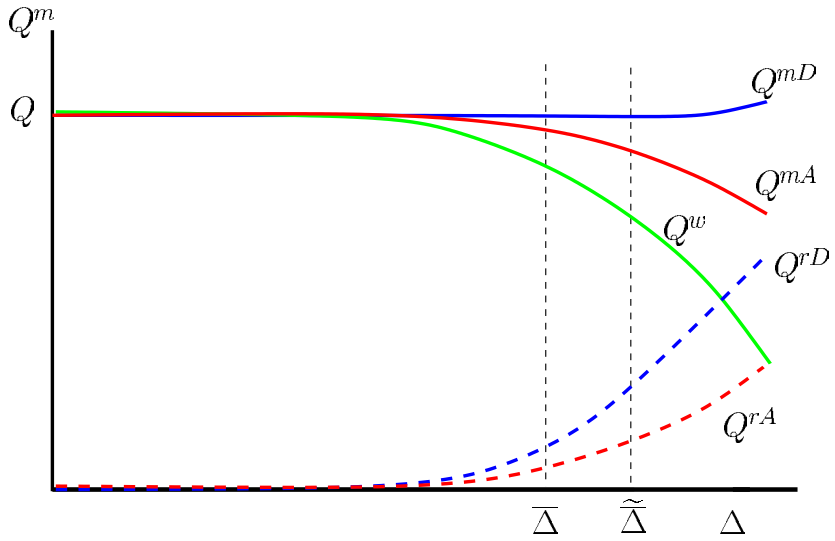

Figure 8. For the given model A, and the dynamic model D, a sketch of the resolved contribution $Q^w(\Delta)$ and of the modelled residual contributions $Q^{rA}(\Delta)$ and $Q^{rD}(\Delta)$ to the model predictions $Q^{mA}(\Delta)$ and $Q^{mD}(\Delta)$ of a large-scale statistic Q. The dynamic model selects the model coefficient c_Q so that $Q^{mD}(\widetilde{\overline{\Delta}})$ equals $Q^{mD}(\overline{\Delta})$.

these ideas for a model denoted by A with a fixed value of c_Q, and for the dynamic model denoted by D. (For simplicity, the resolved contribution Q^w is taken to be the same for both models.) As may be seen from the figure, for model A, the decrease in Q^r, i.e. $Q^{rA}(\widetilde{\overline{\Delta}}) - Q^{rA}(\overline{\Delta})$ is less than the increase in Q^w, i.e. $Q^w(\overline{\Delta}) - Q^w(\widetilde{\overline{\Delta}})$, and consequently the model prediction $Q^{mA}(\widetilde{\overline{\Delta}})$ is less than $Q^{mA}(\overline{\Delta})$. According to the above principle, the value of c_Q is too small in model A. The dynamic procedure selects c_Q so that $Q^{mD}(\overline{\Delta})$ equals $Q^{mD}(\widetilde{\overline{\Delta}})$.

We now apply this principle to the Smagorinsky model and show that it yields essentially the same specification for the Smagorinsky coefficient c_s as the dynamic procedure. The LES equations incorporating the Smagorinsky model are solved with $\Delta = \overline{\Delta}$. The resolved velocity field $\boldsymbol{W}(\boldsymbol{x}, t)$ is deemed to model the filtered velocity field $\overline{\boldsymbol{U}}(\boldsymbol{x}, t)$.

The LES field $\boldsymbol{W}$ is filtered with a filter of width $\widetilde{\Delta}$, so that $\widetilde{\boldsymbol{W}}$ corresponds to the doubly filtered velocity field $\widetilde{\overline{\boldsymbol{U}}}$. The filter width $\widetilde{\overline{\Delta}}$ is that corresponding to filtering by $\overline{\Delta}$ and then by $\widetilde{\Delta}$: for a Gaussian filter the relation is $\widetilde{\overline{\Delta}} = [\overline{\Delta^2} + \widetilde{\Delta}^2]^{1/2}$. Thus, it is assumed (as in the standard dynamic model) that the statistics of the LES fields $\boldsymbol{W}$ and $\widetilde{\boldsymbol{W}}$ are the same as those of the filtered fields $\overline{\boldsymbol{U}}$ and $\widetilde{\overline{\boldsymbol{U}}}$.

We consider the quantity

$$Q_{ij}(\boldsymbol{x}, t, \overline{\Delta}) \equiv \overline{U_i U_j} - \tfrac{1}{3}\overline{U_k U_k}\delta_{ij}, \tag{14}$$

defined at the $\overline{\Delta}$ filter level. The corresponding quantity at the $\widetilde{\overline{\Delta}}$ filter level is consistently defined by

$$Q_{ij}(\widetilde{\overline{\Delta}}) \equiv \widetilde{\overline{U_i U_j}} - \tfrac{1}{3}\widetilde{\overline{U_k U_k}}\delta_{ij}, \tag{15}$$

where the dependence on $\boldsymbol{x}$ and t is no longer shown explicitly. It is readily observed that these two quantities are related by

$$Q_{ij}(\widetilde{\overline{\Delta}}) = \widetilde{Q_{ij}(\overline{\Delta})}. \tag{16}$$

The Smagorinsky model for $Q_{ij}(\overline{\Delta})$, denoted by $Q^m_{ij}(\overline{\Delta})$, can be written as

$$Q^m_{ij}(\overline{\Delta}) = Q^w_{ij}(\overline{\Delta}) + Q^r_{ij}(\overline{\Delta}), \tag{17}$$

where

$$Q^w_{ij}(\overline{\Delta}) \equiv \overline{U}_i\overline{U}_j - \tfrac{1}{3}\overline{U}_k\overline{U}_k\delta_{ij} \tag{18}$$

is the contribution that is known from the resolved field, and

$$Q^r_{ij}(\overline{\Delta}) \equiv -2c_s(\overline{\Delta})\overline{\Delta^2}\overline{\mathcal{S}}\,\overline{S}_{ij} \tag{19}$$

is the Smagorinsky model for the residual contribution. Here $c_s(\overline{\Delta})$ is the Smagorinsky coefficient at scale $\overline{\Delta}$; $\overline{S}_{ij}$ is the filtered rate of strain

$$\overline{S}_{ij} \equiv \frac{1}{2}\left(\frac{\partial\overline{U}_i}{\partial x_j} + \frac{\partial\overline{U}_j}{\partial x_i}\right), \tag{20}$$

and $\overline{\mathcal{S}}$ is the filtered rate-of-strain invariant

$$\overline{\mathcal{S}} \equiv [2\overline{S}_{ij}\overline{S}_{ij}]^{1/2}. \tag{21}$$

The same model applied at the $\widetilde{\overline{\Delta}}$ filter level is

$$Q^m_{ij}(\widetilde{\overline{\Delta}}) = Q^w_{ij}(\widetilde{\overline{\Delta}}) + Q^r_{ij}(\widetilde{\overline{\Delta}}), \tag{22}$$

where $Q^w_{ij}(\widetilde{\overline{\Delta}})$ and $Q^r_{ij}(\widetilde{\overline{\Delta}})$ are defined analogously to equations (18) and (19), with the latter involving the coefficient $c_s(\widetilde{\overline{\Delta}})$.

In view of the identity, equation (16), these model equations provide two estimates of $Q_{ij}(\widetilde{\overline{\Delta}})$: the first is directly in terms of $\widetilde{\overline{\boldsymbol{U}}}$ from equation (22); the second is from filtering equation (17) which is based on $\overline{\boldsymbol{U}}$, i.e.

$$\widetilde{Q^m_{ij}(\overline{\Delta})} = \widetilde{Q^w_{ij}(\overline{\Delta})} + \widetilde{Q^r_{ij}(\overline{\Delta})}. \tag{23}$$

We are now in a position to state, in this context, the alternative principle that leads to the dynamic model. This principle is: *the model coefficient c_s should be chosen to minimize the mean-square difference between the model's prediction of $Q_{ij}(\widetilde{\overline{\Delta}})$ based on $\widetilde{\overline{\boldsymbol{U}}}$, equation (22), and that based on $\overline{\boldsymbol{U}}$, equation (23)*. Note that there is no appeal to the scale similarity.

Rather, the aim is to select c_s so that the statistics predicted *at a single filter level* (i.e. $Q_{ij}(\widetilde{\overline{\Delta}})$) depend as little as possible on the level of the filtered velocity field (i.e. $\overline{\boldsymbol{U}}$ or $\widetilde{\overline{\boldsymbol{U}}}$) on which the prediction is based.

The difference to be minimized is

$$\delta Q_{ij}^m \equiv \widetilde{\overline{Q_{ij}^m(\overline{\Delta})}} - Q_{ij}^m(\widetilde{\overline{\Delta}}). \tag{24}$$

This is obtained by subtracting equation (23) from equation (22), and in the notation of Pope [5] the result is

$$\delta Q_{ij}^m = \mathcal{L}_{ij}^d - c_s(\widetilde{\overline{\Delta}})M_{ij}, \tag{25}$$

with the definitions

$$\mathcal{L}_{ij}^d \equiv (\widetilde{\overline{U_i}\,\overline{U_j}} - \tfrac{1}{3}\widetilde{\overline{U_k}\,\overline{U_k}}\delta_{ij}) - (\widetilde{\overline{U}_i}\,\widetilde{\overline{U}_j} - \tfrac{1}{3}\widetilde{\overline{U}_k}\,\widetilde{\overline{U}_k}\delta_{ij}), \tag{26}$$

$$M_{ij} \equiv 2\gamma\widetilde{\overline{\Delta^2\mathcal{S}}\,\overline{S}_{ij}} - 2\widetilde{\overline{\Delta}}^2\widetilde{\overline{\mathcal{S}}}\,\widetilde{\overline{S}}_{ij} \tag{27}$$

and

$$\gamma \equiv c_s(\overline{\Delta})/c_s(\widetilde{\overline{\Delta}}). \tag{28}$$

(As in the usual derivation of the dynamic model, equation (25) involves the approximation that, when equation (19) is filtered, $c_s(\overline{\Delta})$ is taken to be spatially uniform.)

The unknown parameter γ is unity if scale similarity prevails, and is close to unity otherwise. For the usual case $(\widetilde{\overline{\Delta}})/\overline{\Delta} = 2$, the second term in equation (27) is approximately 4 times the first term, and hence the value of $c_s(\widetilde{\overline{\Delta}})$ is insensitive to γ. Thus, the standard practice of setting $\gamma = 1$ is a reasonable first approximation, even when scale similarity does not hold.

The mean-square difference between the two predictions of $Q_{ij}^m(\widetilde{\overline{\Delta}})$ is

$$\chi \equiv \langle \delta Q_{ij}^m \delta Q_{ij}^m \rangle. \tag{29}$$

It follows simply from equation (25) that the value of $c_s(\widetilde{\overline{\Delta}})$ which minimizes χ is

$$c_s^* \equiv \langle \mathcal{L}_{ij}^d M_{ij} \rangle / \langle M_{ij} M_{ij} \rangle. \tag{30}$$

This is just the standard formula for c_s used in the dynamic model, except that some practical form of averaging is used, rather than using expectations.

As observed by Porté-Agel *et al* [35], this dynamic procedure yields (to a first approximation) the value of the Smagorinsky coefficient $c_s(\widetilde{\overline{\Delta}})$ at the scale $\widetilde{\overline{\Delta}}$, whereas, to perform the LES, the value of $c_s(\overline{\Delta})$ is required. Hence a refined procedure, such as that advanced by Porté-Agel *et al* [35], provides an estimate of γ to be used in equation (27), and, more importantly, so that c_s at the required scale is obtained as $c_s(\overline{\Delta}) = \gamma c_s(\widetilde{\overline{\Delta}})$.

For the simplest case of high-Reynolds number homogenous isotropic turbulence, the dynamic procedure can be applied to determine c_s^* as a function of $\widetilde{\overline{\Delta}}$ (for fixed $\widetilde{\overline{\Delta}}/\overline{\Delta}$). For $\widetilde{\overline{\Delta}}$

in the inertial subrange, one expects c_s^* to be independent of $\widetilde{\overline{\Delta}}$, and equal to the value given by the Lilly analysis. But as $\widetilde{\overline{\Delta}}$ increases beyond ℓ_{EI} towards the integral scale L, the expectation is that c_s^* decreases. Thus, in the inertial subrange the Smagorinsky length scale ℓ_s, defined by $\ell_s^2 \equiv c_s^* \widetilde{\overline{\Delta^2}}$, varies as $\widetilde{\overline{\Delta}}$ in accord with inertial range scaling; however, for larger values of $\widetilde{\overline{\Delta}}$, ℓ_s increases more slowly than $\widetilde{\overline{\Delta}}$ (as c_s^* decreases).

In summary, it has been shown that both the standard and refined dynamic procedures can be derived from the principle that the model coefficients should be chosen (as functions of Δ) to minimize the dependence of relevant turbulence statistics on Δ. In particular, for the Smagorinsky model, the coefficient $c_s(\widetilde{\overline{\Delta}})$ is chosen to minimize the difference between $Q_{ij}(\widetilde{\overline{\Delta}})$, equation (15), evaluated based on $\overline{\boldsymbol{U}}$ and on $\widetilde{\overline{\boldsymbol{U}}}$. If scale similarity holds then γ is unity, and the procedure yields the standard result for $c_s(\overline{\Delta}) = c_s(\widetilde{\overline{\Delta}})$. If scale similarity does not hold, then (setting $\gamma = 1$), the procedure yields a reasonable approximation to $c_s(\widetilde{\overline{\Delta}})$. In a refined procedure, the value of γ is estimated so as to provide an improved estimate of $c_s(\widetilde{\overline{\Delta}})$ and, more importantly, of $c_s(\overline{\Delta}) = c_s(\widetilde{\overline{\Delta}})$.

11. Conclusions

As we enter the era in which there is sufficient computer power for LES, it is useful to re-examine both the conceptual foundations of the approach and the methodologies and protocols generally employed.

For flows in which rate-controlling processes occur below the resolved scales (e.g. near-wall flows and combustion), LES calculations have a first-order dependence on the modelling of these processes. Approaches that include a statistical resolution of all scales provide a more fundamental description of the rate-controlling processes; however, it remains a challenge to devise such approaches that are computationally tractable and free of empiricism.

The relationship between the resolved LES velocity field $\boldsymbol{W}(\boldsymbol{x}, t)$ and the turbulent velocity field $\boldsymbol{U}(\boldsymbol{x}, t)$ can only be statistical. Corresponding to a turbulence statistic Q, the LES provides a model Q^m for Q of the form

$$Q^m = Q^w + Q^r, \tag{31}$$

where Q^w is the contribution from the resolved motions (which is obtained directly from $\boldsymbol{W}$) and Q^r is the modelled contribution from the residual motions.

In LES, the turbulence resolution length scale $\Delta(\boldsymbol{x})$ is an artificial parameter of prime importance. As a rule, as Δ decreases, Q^w increases and Q^r decreases. Unless demonstrated otherwise, there is every reason to suppose that LES predictions Q^m depend (maybe strongly) on Δ. As a consequence, characterizing the dependence of predictions on Δ must be part of the overall LES methodology.

As currently practised, LES is incomplete because the turbulence resolution length scale $\Delta(\boldsymbol{x})$ is specified subjectively in a flow-dependent manner. It can be made complete through adaptive LES. The variation of $\Delta(\boldsymbol{x}, t)$ is controlled (by grid adaption) so that a measure $M(\boldsymbol{x}, t)$ of turbulence resolution (e.g. the fraction of the turbulent kinetic energy in the resolved motions) is everywhere below a specified tolerance ϵ_M.

In a high-Reynolds-number turbulent flow, as Δ is decreased into the inertial subrange, it can be supposed that Q^w and Q^r approach an intermediate asymptote (provided that the model is consistent with inertial-range scaling). As Δ is decreased through the dissipation range, Q^m approaches the correct value Q (provided that the model appropriately reverts to the Navier–Stokes equations in this limit). The most that an LES calculation can hope to achieve, is to obtain an accurate estimate of the intermediate asymptote Q_I^m. This asymptote may or may not be equal to Q depending upon whether or not Q and the processes affecting it depend solely on the energy-containing scales.

With respect to the criteria 'accuracy' and 'cost', the relative merits of different LES models can be appraised only when the dependence of their predictions on Δ has been characterized. If the intermediate asymptote Q_I^m differs from the turbulence statistic Q, then the model whose value of Q_I^m is closest to Q is to be preferred, based on the criterion of accuracy. If several models have Q as their intermediate asymptote, then the model which achieves acceptable accuracy with the least computational cost is to be preferred. By this criterion, it is highly probable that the optimal model contains non-negligible numerical errors.

An alternative principle is advanced to justify the dynamic procedure, namely, the LES model coefficients should be chosen to minimize the difference between $Q^m(\overline{\Delta})$ and $Q^m(\widetilde{\overline{\Delta}})$ (where $\overline{\Delta}$ is the value of Δ used in the LES and $\widetilde{\overline{\Delta}}$ is somewhat larger). It is shown that this principle applied to the Smagorinsky model results in essentially the same formula for the coefficient c_s (i.e. equation (30)) as the standard dynamic model. As previously observed by Porté-Agel *et al* [35], if scale similarity does not hold, then the coefficient obtained is an approximation to the appropriate value at scale $\widetilde{\overline{\Delta}}$, not at the required scale $\overline{\Delta}$.

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