AIAA JOURNAL
Vol. 37, No. 4, April 1999

Mathematical and Physical Constraints on Large-Eddy Simulation of Turbulence

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Recent progress in the theoretical foundations of large-eddy simulation is reviewed. Most of the work reported is motivated by conceptual difficulties encountered in applying the large eddy simulation method to inhomogeneous complex geometry flows. Among the topics covered are the problem of the lack of commutation between filtering and derivative operators for inhomogeneous flows, the issues of enforcing symmetry and realizability conditions in subgrid modeling, and the problem of unacceptably high numerical errors in large eddy simulation implementations with finite difference methods.

I. Introduction

IN direct numerical simulation (DNS) of Navier–Stokes (NS) turbulence, the numerical resolution is sufficiently fine so as to resolve all scales of motion that carry significant energy. It is well known that such resolution requirements make DNS prohibitively expensive for many aerospace applications. The Reynolds-averaged Navier–Stokes (RANS) approach is much cheaper computationally but require nonuniversal closure models, which are often difficult to construct, especially in problems involving complicated geometry and flow separation. An intermediate approach is large-eddy simulation (LES), where one only seeks to resolve those eddies that are large enough to contain information about the geometry and dynamics of the specific problem under investigation and to regard all structures on a smaller scale as universal following the viewpoint of Kolmogorov. The difficulty of this approach is there is no real separation between the large and small scales; the division is merely a convention. This prevents a systematic approximate solution of the closure problem along the lines, e.g., of the Chapman–Enskog development for Boltzmann's equation. In the latter example, there exists a regime of interesting problems where the scale of variation of hydrodynamic variables is much larger than the molecular mean free path. Such a scale separation is not possible in the case of LES.

There are two possible approaches to thinking about LES. In the first, for every dynamical variable f, e.g., pressure, one explicitly defines a smoothed or filtered variable $\bar{f}$ defined as an appropriate local average of f, so that $\bar{f}$ is a smoother function that only follows the large-scale structure of f and lacks the small-scale fluctuations. One then derives from the NS equations a set of equations satisfied by the corresponding filtered variables. These equations are exact because no approximation has been made so far. However, the LES equations are unclosed. At this stage, an approximate model is chosen for the unclosed terms to give a set of model LES equations. These equations are then solved numerically.

A second possible approach is to simply discretize the NS equations, using some appropriately chosen numerical scheme, on a grid that is too coarse to allow for any sensible resolution of the fine structure generated by the exact NS equations. One then tries to account for any problems created by this lack of resolution by adding additional terms or modifying the numerical scheme itself to fix these problems (such as insufficient energy dissipation). Examples of this approach are simulations that do not use any subgrid models at all but rely on the inherent dissipation of numerical schemes to mimic transfer of energy to smaller scales through triad interactions.

The main advantage of the first approach is that it enables one to address the issues of subgrid modeling and numerical methods separately, thereby enabling one to deal with two very difficult problems one at a time. This has a distinct advantage for any theoretical analysis of either subgrid modeling or numerical errors. The second approach may be cheaper (no overheads for subgrid models) when it works. However, when it does not, it is more difficult to determine exactly what went wrong, e.g., trying to improve grid resolution to resolve mean variables may trigger an instability because of decreased numerical dissipation. In this paper we will assume the former approach to LES simply because it is more structured and, therefore, is more amenable to theoretical analysis. There exists a not too precisely stated hope that when one solves the NS equations on a discrete grid with a dissipative scheme perhaps one obtains exactly the solution of a set of LES equations with some combination of filtering and subgrid model that is implicit. That is, we do not know exactly what the filtering scheme and subgrid models are, but there exists a scheme and a model such that the corresponding LES equations when solved would give the numerical solution exactly. This belief, however, is not true, as has been pointed out in the literature.[1,2]

In the next section, we discuss the basic equations for the filtered variables. In the case of inhomogeneous flows, there is a closure problem that arises not due to the nonlinearity of the NS equations but because of the failure of the derivative operator to commute with the filtering operation and/or because of the presence of finite boundaries. The various approaches for dealing with this problem are discussed. In Sec. III we discuss the issue of subgrid modeling and the constraints imposed on the subgrid model by the mathematical structure of the NS equations. In Sec. IV, we discuss the issue of discretization errors in LES. Because of the presence of a continuum of spatial scales, a new approach to error analysis is required with errors being characterized by their power spectra rather than single numerical values. The power spectra depend on both the numerical method as well as the energy spectrum, but may be expressed in separable form. The principal results are summarized in Sec. V.

For simplicity, and due to limitations of space and the author's expertise, discussion will be limited to incompressible turbulence. However, many of the results are easily extendible to the general case of compressible flows.

II. Basic Equations of LES

We will follow the index notation for tensors with the summation convention. The NS equations are, therefore, written as follows:

$$\partial_t u_i + u_k \partial_k u_i = -(1/\rho)\partial_i p + \nu \partial_{kk} u_i \tag{1}$$

$$\partial_i u_i = 0 \tag{2}$$

where ν and ρ are the (constant) kinematic viscosity and density, respectively, u_i is the velocity, and p is the pressure. For any dynamical field $f(\boldsymbol{x}, t)$ the corresponding LES field is defined as

Received May 13, 1998; presented as Paper 98-2803 at the AIAA 29th Fluid Dynamics Conference, Albuquerque, NM, June 15–18, 1998; revision received Nov. 23, 1998; accepted for publication Nov. 29, 1998.

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$$\bar{f}(\boldsymbol{x},t) = \int f(\boldsymbol{y},t) G\left(\frac{\boldsymbol{x}-\boldsymbol{y}}{\Delta}\right) \mathrm{d}\boldsymbol{y} \tag{3}$$

where G is some function (the filter) with an effective width of the order of unity and Δ is the filter width. On applying the operation (3) to Eqs. (1) and (2), we derive the basic equations of LES:

$$\partial_t \bar{u}_i + \bar{u}_k \partial_k \bar{u}_i = -(1/\bar{\rho})\partial_i \bar{p} + \nu \partial_{kk} \bar{u}_i - \partial_j \tau_{ij} \tag{4}$$

$$\partial_i \bar{u}_i = 0 \tag{5}$$

where

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j \tag{6}$$

is the (unclosed) subgrid stress. Note that the first term on the right-hand side of Eq. (4) is a consequence of the constancy of ρ.

A. Problems with Inhomogeneous Flows

The derivation of Eqs. (4) and (5) are valid provided all of the differentiation operators commute with the filtering operator, that is, if the following is true for any function $f(\boldsymbol{x})$:

$$\overline{\frac{\partial f}{\partial x_i}} = \frac{\partial \bar{f}}{\partial x_i} \tag{7}$$

It is easily verified that Eq. (7) is true if the filter width Δ in Eq. (3) is a constant. However, for a wall-bounded flow, if the distance from the wall is less than $\Delta/2$ one will need to truncate the filter function G, or do something similar for the filtering operation (3) to be well defined. Thus, either Δ must be variable or the functional form of G itself must change as one approaches walls. This is entirely consistent with the definition of LES because the length scale below which eddies can be regarded as universal decreases as one approaches walls. For the same reason, a variable filter width is also essential for the proper formulation of LES in inhomogeneous flows (of which wall-bounded flows represent a special case). That variable filter widths result in a violation of Eq. (7) invalidating the basic equations (4) and (5) was recognized early.[3] The problem, however, has been largely ignored until recently, perhaps as a result of being overshadowed by more serious problems related to numerical methods. It was hoped that any errors that result in ignoring this problem would perhaps be comparable to other sources of errors, viz., errors due to the subgrid closure, truncation errors, aliasing errors, and time-stepping errors. Whereas such an approach might have been not entirely unreasonable at the time, the rapid advancement[4,5] of LES in recent years has necessitated a more careful examination of this issue.

B. NS Acquires Extra Terms

A systematic analysis of this commutation error may be undertaken along the following lines[6]:

We consider the one-dimensional case of a dynamical variable $u(x)$; the generalization to three dimensions is obvious. A one-to-one transformation from an infinite domain $-\infty < \xi < +\infty$ to a finite domain $a < x < b$ may be affected through a monotonic function

$$\xi = f(x) \tag{8}$$

such that $f(a) = -\infty$ and $f(b) = +\infty$. In the ξ space there are no boundaries so that filtering with a uniform filter width Δ is easily defined as in Eq. (3). Filtering in physical space x is then defined as follows. 1) Transform variables $x \to \xi$ in $u(x)$. 2) Filter $u[f^{-1}(\xi)]$ the usual way. 3) Transform back $\xi \to x$ to get filtered field. Mathematically, this operation amounts to the following definition:

$$\begin{aligned}\bar{u}(x) &= \frac{1}{\Delta}\int_{-\infty}^{+\infty} G\left(\frac{\xi-\eta}{\Delta}\right) u[f^{-1}(\eta)]\,\mathrm{d}\eta \\ &= \frac{1}{\Delta}\int_a^b G\left[\frac{f(x)-f(y)}{\Delta}\right] u(y) f'(y)\,\mathrm{d}y\end{aligned} \tag{9}$$

It is easy to show that away from boundaries Eq. (9) is approximately equal to filtering with the kernel G but with a variable filter width $\delta(x) = \Delta/f'(x)$, that is,

$$\begin{aligned}&\frac{1}{\Delta}\int_a^b G\left[\frac{f(x)-f(y)}{\Delta}\right] u(y) f'(y)\,\mathrm{d}y \\ &\quad \approx \frac{1}{\delta(x)}\int_{-\infty}^{+\infty} G\left[\frac{x-y}{\delta(x)}\right] u(y)\,\mathrm{d}y\end{aligned} \tag{10}$$

It should be noted that in definition (9), due to the function f approaching $\pm\infty$ for x approaching boundaries, the integrand never becomes undefined. However, if the right-hand side of Eq. (10) were used to define the filtering operation, the integrand would become undefined near boundaries and one would have to restrict the integration to a finite domain thereby creating additional boundary terms. This difficulty is avoided in definition (9) by transforming away all boundaries to infinity. (An alternate approach that explicitly retains the boundary terms has been proposed by Fureby and Tabor.[7]) Filter (9) actually differs markedly from approximate form (10) near boundaries, as the kernel becomes visibly asymmetric.[6] Note that the requirement that the filter width in the wall normal direction, δ, should approach zero near boundaries does not mean that the grid spacing h should also approach zero (which is impossible to meet with finite computing resources). In LES, one seeks to resolve the large structures that depend on detailed geometry of the specific problem and use a model for the collective effect of the universal small scales. This is no longer feasible, however, very near a wall, where the relevant length scale is the thickness of the viscous boundary layer ℓ and the dynamics at this scale cannot be captured by any universal turbulence model but should be computed explicitly. Therefore, very near a wall, ideally, one ought to have $h \sim \ell$ or smaller, whereas far from the the wall, the corresponding requirement is $h \sim \delta$. This ideal resolution, $h \sim \ell$, though nonzero, is still very small, and often practical constraints on computing resources preclude reaching this level of resolution. In such cases one either needs to consider avoiding computing very close to the wall by resorting to some model of the near-wall region to provide boundary conditions at the top of the wall layer (see Ref. 8 and the references therein) or one simply accepts that resolution close to the wall is less than the ideal requirement and hopes that this does not have an adverse impact on the rest of the computation.

An expression for the commutation error can easily be written down using definition (9),

$$\begin{aligned}\mathcal{C}[u] \equiv \overline{\frac{\mathrm{d}u}{\mathrm{d}x}} - \frac{\mathrm{d}\bar{u}}{\mathrm{d}x} &= \frac{1}{\Delta}\int_a^b G\left[\frac{f(x)-f(y)}{\Delta}\right] \\ &\times u'(y) f'(y)\left[1 - \frac{f'(x)}{f'(y)}\right]\mathrm{d}y\end{aligned} \tag{11}$$

If G is symmetric (as with most commonly used filters), then it is easily shown using Taylor series analysis that $\mathcal{C}[u] = c_2(x)\Delta^2 + \cdots$, where $c_2(x)$ is a coefficient independent of Δ and proportional to the second moment of G. Because the filter width and the grid spacing are usually of comparable magnitude, the error made in assuming that the derivative and filtering operations commute is of the same order as the truncation error of a second-order finite difference scheme. In turbulence computations, high-order methods, such as spectral methods[9] and more-recently compact schemes,[10] are usually preferred over second-order schemes. This could be especially important in LES because the high-order modes near the limit of resolution could have significant amplitudes. Therefore, the commutation error can be a serious threat to the accuracy of turbulence computations, degrading the resolution of a high-order method to no more than a second-order scheme. The following estimate for the subgrid stress, $|\tau_{ij}| \sim \Delta^{2/3}$, is well known. Therefore, the commutation error, which is $\sim\Delta^2$, is perhaps a correction compared to the modeled subgrid term for the low-order modes, but may be more significant for the smaller scales near the grid resolution. Estimates for the relative magnitude of the commutation error in LES have been provided earlier by Fureby and Tabor.[7]

One method of correcting for the commutation error is to approximate $\mathcal{C}[u]$ by a linear combination of derivatives $\bar{u}''(x)$, $\bar{u}''''(x), \ldots,$ and choose the coefficients such that the residual error is less than any desired order (in practice the same order as the truncation error).

The following approximation, for example, has fourth-order accuracy:

$$\overline{\frac{\mathrm{d}u}{\mathrm{d}x}} = \frac{\mathrm{d}\bar{u}}{\mathrm{d}x} - \alpha\delta^2\left(\frac{\delta'}{\delta}\right)\frac{\mathrm{d}^2\bar{u}}{\mathrm{d}x^2} + \mathcal{O}(\delta^4) \tag{12}$$

where $\delta(x) = \Delta/f'(x)$ is the local filter width introduced earlier and $\alpha = \int \zeta^2 G(\zeta)\,\mathrm{d}\zeta$. Expansion (12) can be applied to derivatives in each direction in the NS equations, and the equations for the filtered field $\bar{u}$ can be written down. They are the usual LES equations augmented by the higher-order derivative terms[6]

$$\partial_t \bar{u}_i + \mathcal{D}_j(\bar{u}_i\bar{u}_j) = -\mathcal{D}_i\bar{p} - \mathcal{D}_j\tau_{ij} + Re^{-1}\mathcal{D}_k\mathcal{D}_k\bar{u}_i \tag{13}$$

$$\mathcal{D}_i\bar{u}_i = 0 \tag{14}$$

where the operator $\mathcal{D}_i$ has the asymptotic expansion

$$\mathcal{D}_i = \partial_i - \alpha\Delta^2\Gamma_{ijk}\partial_j\partial_k + \cdots \tag{15}$$

where Δ is the filter width, Γ_{ijk} are known coefficients describing the manner in which the computational grid is stretched and distorted, and α is the second moment of the filter kernel defined earlier. A similar set of modified LES equations have been derived by Fureby and Tabor.[7]

The physical meaning of the additional terms may be easily understood. For this, consider a Gaussian wave packet $u(x)$ traveling from left to right according to the evolution equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \tag{16}$$

Suppose that the physical space filter width $\delta(x)$ is increasing monotonically from left to right. Then as the wave travels, it would encounter ever increasing filter widths so that $\bar{u}$ would have a decreasing peak and broadening width as it propagates to the right even though $u(x)$ travels unchanged in form. On applying Eq. (12) to Eq. (16), we find

$$\frac{\partial\bar{u}}{\partial t} + \frac{\partial\bar{u}}{\partial x} = \nu\frac{\partial^2\bar{u}}{\partial x^2} \tag{17}$$

where $\nu = \alpha\delta^2(\delta'/\delta)$ is positive. The term on the right-hand side of Eq. (17) is a diffusion term, which causes the necessary spreading of the wave packet $\bar{u}$. The interpretation can be confirmed by exactly evaluating $\bar{u}$ and comparing with the prediction of Eq. (17) for a simple choice of $\delta(x)$. The opposite effect is observed for a wave packet moving from right to left. In this case the diffusion term is replaced by an antidiffusion term, so that the wave packet increases in amplitude and becomes more and more confined. However, for such a wave, if the domain of x is $(-\infty, +\infty)$ the wave packet would diverge like a delta function due to the antidiffusion term. This is clearly an incorrect prediction because $\bar{u}(x)$ should clearly converge to $u(x)$ as the wave moves to the left and the filter width approaches zero. This difficulty arises because as the profile of $\bar{u}$ becomes sharper its higher-order derivatives become larger and ultimately the correction term on the right of Eq. (17) becomes of the same order as the neglected terms invalidating the approximation unless further correction terms are brought to play on the right-hand side of Eq. (17). For a semibounded domain (a, ∞) (or bounded domain), which is a more realistic situation, the divergence does not occur because a wave moving to the left, though initially amplifying, is ultimately reflected on reaching the boundary and subsequently travels to the right with decaying amplitude.

Though the effect of the correction term is easy to understand in this simple situation, its effect in the context of the full NS equations is unknown because LES with the correction terms has never been done. An interesting model problem to study may be LES of the collision of a vortex with a wall, where one should be able to observe the creation (destruction) of fine structure brought about by the additional terms as the vortex moves toward (away) from the wall (the zone of finest resolution).

A question that immediately comes to mind is whether boundary conditions in addition to the usual no-slip ones are needed for the LES equations near rigid walls because by adding the extra terms we have increased the order of the basic equations. To examine this question let us consider the simplest of boundary value problems:

$$\frac{\mathrm{d}u}{\mathrm{d}x} = 0 \tag{18}$$

with the boundary condition

$$u(0) = 1 \tag{19}$$

The solution is clearly

$$u(x) = 1 \tag{20}$$

which implies

$$\bar{u}(x) = 1 \tag{21}$$

Now let us see what is needed to recover this solution from the equation for $\bar{u}$ obtained by applying the filtering operation to Eq. (18) and using Eq. (12):

$$\frac{\mathrm{d}\bar{u}}{\mathrm{d}x} = \nu\frac{\mathrm{d}^2\bar{u}}{\mathrm{d}x^2} \tag{22}$$

Let us choose as an example the mapping $f(x) = \log x$, so that $\nu = \alpha\delta^2(\delta'/\delta) = \alpha\Delta^2 x$. Thus, the equation for $\bar{u}$ in this elementary example is

$$\frac{\mathrm{d}\bar{u}}{\mathrm{d}x} = \alpha\Delta^2 x\frac{\mathrm{d}^2\bar{u}}{\mathrm{d}x^2} \tag{23}$$

which has the general solution

$$\bar{u}(x) = 1 + Cx^{1+\alpha^{-1}\Delta^{-2}} \tag{24}$$

given the boundary condition $\bar{u}(0) = 1$. It is clear that Eq. (21) cannot be derived as the unique solution to Eq. (23) no matter what boundary condition is specified for $\mathrm{d}\bar{u}/\mathrm{d}x$. This is because Eq. (23) is singular at $x = 0$ due to vanishing of the coefficient of the second derivative, and the uniqueness theorem for solutions of second-order differential equations do not hold for solutions through $x = 0$.

The correct condition needed to recover Eq. (21) is the boundedness condition

$$\lim_{\Delta\to 0}\bar{u}(x, \Delta^2) \tag{25}$$

which should be finite if the limit is taken with fixed x. Applying Eq. (25) to Eq. (24) readily implies $C = 0$ and Eq. (21) follows. A more practical way of enforcing Eq. (25) is to look for an asymptotic solution in the form

$$\bar{u} = \bar{u}_0 + \Delta^2\bar{u}_1 + \cdots \tag{26}$$

which from the start rules out solutions that are singular as $\Delta \to 0$. On substituting Eq. (26) in Eq. (23) we have the following chain of equations:

$$\frac{\mathrm{d}\bar{u}_0}{\mathrm{d}x} = 0 \tag{27}$$

$$\frac{\mathrm{d}\bar{u}_n}{\mathrm{d}x} = \alpha x\frac{\mathrm{d}^2\bar{u}_{n-1}}{\mathrm{d}x^2} \qquad (n = 1, 2, \ldots) \tag{28}$$

Because $\bar{u} \to u$ as $x \to 0$, we have the boundary conditions $\bar{u}_n(0) = 1$ if $n = 0$ and $\bar{u}_n(0) = 0$ otherwise. Thus, at each step we have a differential equation of the same order as the original one, and no additional boundary conditions are required. The procedure has been worked out in detail by Ghosal and Moin[6] for the incompressible NS equations. However, the authors present the asymptotic method as an alternative to introducing additional boundary condition. This, however, is incorrect. As noted earlier, additional boundary conditions do not determine the solution uniquely and are not needed. The correct condition is the requirement (25), which is enforced through the asymptotic expansion (26). The procedure does involve added computational cost because each time step would require one or more additional evaluations of terms on the right-hand side, and additional storage may also be required. Therefore, it is attractive to examine whether it is possible to choose the filter function G cleverly, so that the filtering and differentiation do commute with an error not greater than that the truncation error, and so that the additional terms are ignorable. This is discussed in the following section.

C. Eliminating Extra Terms

Van der Ven[11] proposed a form of the filter function G such that the commutation error is made as small as desired. Van der Ven worked with the filtering definition

$$\bar{u}(x) = \frac{1}{\delta(x)} \int_{-\infty}^{+\infty} G\left[\frac{x-y}{\delta(x)}\right] u(y)\,\mathrm{d}y \tag{29}$$

where $\delta(x)$ is the space-dependent filter width. As pointed out earlier, this definition is approximately the same as definition (9) away from boundaries, but near boundaries the integrand becomes undefined, or, if the integration is stopped at the domain boundaries, boundary terms arise as a consequence of integration by parts. Van der Ven noted this difficulty but left the problem open for future investigation. If we ignore this boundary problem for the time being, the commutation error may be written as follows:

$$\mathcal{C}[u] = \frac{\delta'(x)}{\delta(x)} \int_{-\infty}^{+\infty} [G(\zeta) + \zeta G'(\zeta)] f[x - \zeta\delta(x)]\,\mathrm{d}\zeta \tag{30}$$

Van der Ven[11] observed that, if G is chosen as the solution of the equation

$$G(\zeta) + \zeta G'(\zeta) = \epsilon G^{(n)}(\zeta) \tag{31}$$

where ϵ is arbitrary, then the right-hand side of Eq. (30) may be written after n integration by parts as follows:

$$\mathcal{C}[u] = \epsilon\delta'(x)\delta^{n-1}(x)\overline{u^{(n)}(x)} \tag{32}$$

Thus, the commutation error can be made arbitrarily small. Equation (31) is easily solved by taking Fourier transforms. In particular, if $n = 2m$ (a positive natural number) and if $\epsilon = (-1)^m\alpha$ $(\alpha > 0)$, then one obtains the two parameter family of filters $G_m(\alpha, \zeta)$ defined through the Fourier transform

$$\hat{G}_m(k; \alpha) = \exp[-(\alpha/2m)k^{2m}] \tag{33}$$

In particular, $m = 1$ corresponds to a Gaussian filter. For all of these filters, the commutation error $\sim\delta'(x)\delta^{2m-1}(x)$.

Van der Ven's analysis has recently been generalized by Vasilyev et al.[1] so as to contain the earlier work of Ghosal and Moin[6] and Van der Ven[11] as special cases. Vasilyev et al. use the filtering definition (9), with $f(a) = \alpha$ and $f(b) = \beta$, but G is allowed to be a function of $(\eta - \xi)/\Delta$ as well as ξ separately. They are able to write the commutation error in the following form:

$$\mathcal{C}[u] = \sum_{k=1}^{+\infty} A_k M_k(\xi)\Delta^k + \sum_{k=0}^{+\infty} B_k \frac{\mathrm{d}M_k}{\mathrm{d}\xi}\Delta^k \tag{34}$$

where the moment M_k is defined as

$$M_k(\xi) = \int_{\xi-\alpha/\Delta}^{\xi-\beta/\Delta} \zeta^k G(\zeta, \xi)\,\mathrm{d}\zeta \tag{35}$$

If the filter is chosen so that $M_0(\xi) = 1$ and $M_k(\xi) = 0$ for $k = 1, 2, \ldots, n-1$, then from Eq. (34) it follows that $\mathcal{C}[u] \sim \Delta^n$. There exists a wide class of such filters with $n-1$ vanishing moments, as pointed out by Vasilyev et al.[1] One example is the one-parameter family (33) introduced by Van der Ven.[11] Another is the correlation function of the Daubechies scaling function used for constructing orthonormal wavelet bases. Vasilyev et al. also show how to construct discrete versions of such filters on numerical grids.

D. Grid and Test Filters, Self-Similarity, and So Forth

In the classical Smagorinsky model

$$\tau_{ij} - \tfrac{1}{3}\tau_{kk}\delta_{ij} = -2C\Delta^2|\bar{S}|\bar{S}_{ij} \tag{36}$$

with a constant C, though the concept of a filter is required, one does not need to know how exactly it is defined because one does not need to use the filtering operation explicitly in solving the basic equations (4), (5), and (36).

The situation is different in various types of mixed models.[12,13] Here one decomposes τ_{ij} as follows:

$$\tau_{ij} = L_{ij} + C_{ij} + R_{ij} \tag{37}$$

where $L_{ij} = \overline{\bar{u}_i\bar{u}_j} - \bar{u}_i\bar{u}_j$, $C_{ij} = \overline{\bar{u}_i u'_j} + \overline{\bar{u}_j u'_i}$, and $R_{ij} = \overline{u'_i u'_j}$. One then argues that it is only the parts C_{ij} and R_{ij} that need to be modeled because L_{ij} is known in terms of the LES field $\bar{u}_i$. Therefore, the Smagorinsky model is applied only to the traceless part of $C_{ij} + R_{ij}$, and L_{ij} is computed explicitly. In this formulation one does need to know explicitly what the filter is because it is needed in the formulation.

Another class of models where knowledge of the filter is required, at least indirectly, is the dynamic model.[14–17] In the dynamic model one formally applies a second filter $\hat{}$ with filter width $\hat{\Delta} > \Delta$ to Eqs. (4) and (5) to generate a set of equations identical to Eqs. (4) and (5) but with the operation $\hat{}$ replacing the $\bar{}$ and $T_{ij} = \widehat{\overline{u_i u_j}} - \hat{\bar{u}}_i\hat{\bar{u}}_j$ replacing τ_{ij}. One then argues that these equations are essentially identical to the LES equations (4) and (5) except for the length scale Δ. Therefore, one may use the same subgrid model for T_{ij} as for τ_{ij} but simply use $\hat{\Delta}$ as the relevant length scale instead of Δ. There exists a relation between T_{ij} and τ_{ij}, as noted by Germano et al.[14]:

$$L_{ij} = T_{ij} - \hat{\tau}_{ij} \tag{38}$$

Taking the traceless part of this identity and substituting the Smagorinsky model in it, using the self-similarity assumption for T_{ij}, we obtain

$$L_{ij} - \tfrac{1}{3}L_{ii}\delta_{ij} = -2C\Delta^2|\hat{\bar{S}}|\hat{\bar{S}}_{ij} + 2\hat{\Delta}^2\widehat{C|\bar{S}|\bar{S}_{ij}} \tag{39}$$

This is an equation for C that can be used in various ways to determine C, as is well known (see the references at the beginning of this paragraph). This was first recognized by Germano et al.,[14] who showed great ingenuity in figuring out a way to exploit the identity to extract the unknown coefficient C, a task that at first sight would seem impossible.

One of the assumptions in the preceding argument is that the filters $\bar{}$ and $\hat{}$ are self-similar, that is, the kernels are identical except for a scale factor. Although this is certainly true for the Gaussian filter as well as the Fourier cutoff filter, it is not true in general. In practical implementations of the dynamic model, the so-called top-hat filter [$G(x) = 1$ if $|x| < \Delta/2$ and 0 otherwise] is often used. However, the convolution of two top-hat filters is not another top-hat filter, as one can easily verify. This apparent inconsistency was pointed out by Carati and Vandeneijnden,[18] who also proposed an ingenious solution to the dilemma reminiscent of renormalization group ideas. They considered filters constructed by infinite iteration of base filters or generators $\mathcal{G}_\Delta$:

$$G_\Delta \equiv \mathcal{G}_\Delta * \mathcal{G}_{\Delta/2} * \mathcal{G}_{\Delta/4} * \mathcal{G}_{\Delta/8} * \cdots \tag{40}$$

where $*$ denotes the convolution operator and $\mathcal{G}_\Delta$ is the kernel of the generator with the filter width parameter equal to Δ. Thus, if $\hat{\Delta} = 2\Delta$, the test filter $\hat{G}_{\hat{\Delta}} = \mathcal{G}_{2\Delta} * G_\Delta$ is by construction self-similar to the grid filter. In practical implementations of the dynamic model, one only uses the filter $\hat{}$, that is, $\mathcal{G}$, explicitly. According to Eq. (40), once the test filter $\mathcal{G}$ is chosen, the grid filter is determined uniquely from the requirement of self-similarity. In particular, as mentioned before, the Fourier cutoff filter and Gaussian filter fall within the class of filters defined by Eq. (40). The top-hat filter does not. However, the top-hat filter may be used as the generator to generate self-similar filters according to the prescription (40).

III. Constraints on Subgrid Models

As discussed in the Introduction, as of this date there exists no systematic method for deriving a closure for the subgrid stress; i.e., there exists no satisfactory theory of turbulence. Under the circumstances, subgrid modeling is essentially the art of making an educated guess. Therefore, it is a wise strategy to reduce the possible choices somewhat by restricting the guesses to those that satisfy properties of the subgrid stress that can be proven to be true. These restrictions belong to two classes: the symmetry requirements and the realizability requirements, the subject of the remainder of this section.

A. Symmetry Requirements

The concept of symmetry is fundamental in physics. It means, e.g., that nature does not distinguish between different points and directions in space so that the equations describing physical phenomenon should have the same form in reference frames translated or rotated with respect to each other. The NS equations themselves show many symmetries such as invariance under translation and rotation of the coordinate system, mirror reflections, Galilean transformations, and scale invariance. One must not, however, jump to the conclusion that the LES equations, therefore, do or should exhibit the same symmetries. The point is, in performing the coarse graining by means of the filtering operation to go from NS to the LES equations, one may break one or more of these symmetries. For example, if one chooses different filter widths for different points of space the symmetry under translational invariance of the NS is broken. This is not something that is wrong or must be avoided, but it is merely a consequence of our choosing not to treat all points of space as equivalent but deliberately choosing different resolutions in different regions for good reason. Of course, the subgrid model must reflect the same symmetries as the exact LES equations, but in deciding which symmetries the subgrid model needs to satisfy, one must be careful in recognizing which symmetries are inherited by the LES equations from the NS and which symmetries are broken.

1. *Translation Symmetry*

If the origin of the coordinate system is shifted by an amount $\boldsymbol{a}$, a given point has coordinates $\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{a}$ in the new reference frame. Clearly, the velocities are unaffected, so that $\boldsymbol{u}'(\boldsymbol{x}') = \boldsymbol{u}(\boldsymbol{x})$. Now the question is, Does the filtered field $\bar{\boldsymbol{u}}$ satisfy the same symmetry, that is, is $\bar{\boldsymbol{u}}'(\boldsymbol{x}') = \bar{\boldsymbol{u}}(\boldsymbol{x})$? By elementary transformation of variables it follows that

$$\bar{\boldsymbol{u}}'(\boldsymbol{x}') = \int G(\boldsymbol{x}', \boldsymbol{y}')\boldsymbol{u}'(\boldsymbol{y}')\,\mathrm{d}\boldsymbol{y}' = \int G(\boldsymbol{x} - \boldsymbol{a},\ \boldsymbol{y} - \boldsymbol{a})\boldsymbol{u}(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \quad (41)$$

and this equals $\bar{\boldsymbol{u}}(\boldsymbol{x})$ if and only if $G(\boldsymbol{x} - \boldsymbol{a},\ \boldsymbol{y} - \boldsymbol{a}) = G(\boldsymbol{x}, \boldsymbol{y})$, that is, if G is a function of $\boldsymbol{x} - \boldsymbol{y}$ only.

In inhomogeneous flows one often uses filters such as Eqs. (9) and (29), which do not have the form of Eq. (41), and translational symmetry is, therefore, broken in the LES equations. As an example let us consider the problem of a wall-bounded flow. If one uses a subgrid model $\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk} = -2\nu_t\bar{S}_{ij}$, where the eddy viscosity is defined as $\nu_t \propto y^3$ when y is less than some length L and constant otherwise, the subgrid model would not be invariant under translations in the y direction. This, however, is perfectly legitimate because invariance under translations in the y direction is a broken symmetry for the LES equations derived with a y-dependent filter. Any attempt to enforce this nonexistent symmetry in the subgrid model would result in incorrect behavior of the equations.

2. *Rotational Symmetry*

Arbitrary rotations of the coordinate system with the origin fixed are described by $x_i' = A_{ij}x_j$, where A_{ij} is a unitary matrix. It is well known that u_i transforms as a vector $u_i' = A_{ij}u_j$. The question that we should ask in whether $\bar{u}_i$ has the same transformation rule as u_i, that is, whether the filter $^-$ is a scalar operator. It is easy to convince oneself that this is not in general true, because

$$\bar{u}_i'(\boldsymbol{x}') = \int G(\boldsymbol{x}', \boldsymbol{y}')u_i'(\boldsymbol{y}')\,\mathrm{d}\boldsymbol{y}' = \int G(A\boldsymbol{x}, A\boldsymbol{y})A_{ij}u_j(\boldsymbol{y})|\det A|\,\mathrm{d}\boldsymbol{y} \quad (42)$$

and the right-hand side equals $A_{ij}\bar{u}_j(\boldsymbol{x})$ if and only if (note that $|\det A| = 1$ for rotations)

$$G(A\boldsymbol{x}, A\boldsymbol{y}) = G(\boldsymbol{x}, \boldsymbol{y}) \quad (43)$$

that is, if G depends only on $|\boldsymbol{x} - \boldsymbol{y}|$ the invariant under arbitrary rotations.

A consequence of this is that, for filters that are not spherically symmetric, the filtered fields do not necessarily inherit the vector or tensor properties of the underlying field. In particular, the subgrid stress τ_{ij} is not a tensor, that is, $\tau_{ij}' \neq A_{im}A_{jn}\tau_{mn}$ unless the filter is spherically symmetric. However, if the Reynolds number is sufficiently high so that the effective filtering zone characterized by the length δ still contains a very large number of subgrid eddies, the filtered field is expected to be almost independent of the shape of the kernel G. This expectation is the consequence of the general observation that averages become insensitive to the nature of the sampling as the sample size becomes large, e.g., the macroscopic properties of a gas that are given by averages over molecular distributions do not depend on the shape of the vessel containing the gas as long as this vessel is of macroscopic size. Similarly, the specific heat of a solid does not depend on the shape of the sample so long as it is much larger than molecular dimensions. Thus, the departure of τ_{ij} from the tensor transformation rule would be negligible for robust turbulence away from walls or other sources of anisotropy on a scale comparable to the filter size. Therefore, invariance under rotations is always preserved for spherically symmetric filters and also preserved to a very good approximation for other filters provided the filtering zone contains a sufficiently large sample of subgrid scales.

All subgrid models known to the author are designed so that the modeled subgrid stress has the tensorial property in situations where the filtering can be regarded as a scalar operation.

3. *Parity Invariance*

Reflections or parity transformations (replacing a right-handed system by a left-handed one) is described by the coordinate transformation rule $x_i' = A_{ij}x_j$, where $\det A = -1$. The NS equations (and all of classical physics) are known to be invariant under such mirror reflections. The transformation rule for the velocity in this case is

$$\bar{u}_i'(\boldsymbol{x}') = \int G(\boldsymbol{x}', \boldsymbol{y}')u_i'(\boldsymbol{y}')\,\mathrm{d}\boldsymbol{y}' = \int G(A\boldsymbol{x}, A\boldsymbol{y})A_{ij}u_j(\boldsymbol{y})|\det A|\,\mathrm{d}\boldsymbol{y} \quad (44)$$

and the right-hand side equals $A_{ij}\bar{u}_j(\boldsymbol{x})$ if and only if (note that $|\det A| = 1$ for reflections)

$$G(A\boldsymbol{x}, A\boldsymbol{y}) = G(\boldsymbol{x}, \boldsymbol{y}) \quad (45)$$

that is, if G remains unchanged when one passes from right-handed to left-handed systems.

A consequence of this is that asymmetric filters such as Eq. (9) may cause the reflection invariance of the NS equations to be broken in the LES equations.

The subgrid models known to the author satisfy this symmetry requirement when the filter is chosen so that the LES equations inherit this symmetry.

4. *Galilean Invariance*

The NS equations and all of the basic laws of physics are Galilean invariant; i.e., all reference frames translating uniformly with respect to each other are equivalent. Because the filter kernel of LES $G(\boldsymbol{x}, \boldsymbol{y})$ is time independent, Galilean invariance is satisfied whenever translational invariance is an inherited symmetry. Thus, for filters of the type $G(\boldsymbol{x} - \boldsymbol{y})$ the LES equations preserve the symmetry under arbitrary Galilean transformations. In situations where one direction, for example, the y direction, is inhomogeneous (requiring y-dependent filter widths) Galilean invariance is true only for the homogeneous directions.

All subgrid models known to the author satisfy the requirements of Galilean invariance with the exception of the so-called mixed models discussed earlier. It is easily seen that each of the component terms L_{ij}, C_{ij}, and R_{ij} change on transforming to a frame uniformly translating with respect to the given one. However, the extra terms cancel on adding the components together so that τ_{ij} is invariant. This precise cancellation no longer happens when $C_{ij} + R_{ij}$ are replaced by a model that does not necessarily produce the additional term needed for the cancellation on transforming to the moving frame. The problem has been known for some time and prescriptions for curing it have been proposed.[19]

The requirement of Galilean invariance can be extended to the more general concept of frame invariance provided one is willing to augment the NS equations with the appropriate inertial forces. The requirements on the filtering kernel for the LES to inherit this symmetry together with discussions on the degree to which various commonly used subgrid models satisfy this symmetry requirement have been provided by Speziale,[20] Fureby,[21] and Fureby and Tabor.[7]

5. Scale Invariance

Scale invariance is simply a statement that our basic units of measuring space and time are arbitrarily chosen so that the equations describing physical phenomenon should have the same form no matter what units are adopted. Dimensional analysis used extensively in fluid dynamics is simply a statement of this scale invariance symmetry. Because the filter G is always written in terms of dimensionless variables

$$G(\boldsymbol{x}, \boldsymbol{y}) = (1/\Delta^3) G_0[(\boldsymbol{x}/\Delta), (\boldsymbol{y}/\Delta)] \tag{46}$$

(G_0 is dimensionless) for the filtered fields to have the correct dimensions, the scale invariance symmetry must always be inherited by the LES equations.

All subgrid models (unless they are dimensionally incorrect) satisfy the scale invariance symmetry.

B. Realizability Requirements

The requirements of realizability of subgrid models were first pointed out by Schumann[22] in the context of RANS. They have been discussed in the context of LES by Fureby and Tabor[7] and by Vreman et al.,[23] who also analyze commonly used subgrid models for compliance with these requirements and present tests of such compliance using numerical simulation data. The realizability condition implies in particular that the turbulent kinetic energy $k = \frac{1}{2}\langle u_i' u_i' \rangle$ is nonnegative, where $\langle\,\rangle$ denotes ensemble average, space average, or time average. A more general statement of the realizability condition is that all three eigenvalues, λ_1, λ_2, and λ_3, of the stress tensor τ_{ij} must be nonnegative. This follows immediately on choosing a coordinate system in which τ_{ij} has the diagonal form (this is always possible because τ_{ij} is symmetric). Then we have

$$\lambda_1 = \tau_{11} = \tfrac{1}{2}\langle u_1' u_1' \rangle \geq 0 \tag{47}$$

$$\lambda_2 = \tau_{22} = \tfrac{1}{2}\langle u_2' u_2' \rangle \geq 0 \tag{48}$$

$$\lambda_3 = \tau_{33} = \tfrac{1}{2}\langle u_3' u_3' \rangle \geq 0 \tag{49}$$

Equations (47–49) can be written in several equivalent forms.[22] Some of these are as follows:

1) The quadratic form

$$Q = x_i \tau_{ij} x_j \tag{50}$$

is positive semidefinite ($Q \geq 0$).

2) The three principal invariants of τ_{ij} are nonnegative:

$$I_1 = \sum_i \tau_{ij} \geq 0 \tag{51}$$

$$I_2 = \sum_{i \neq j} \left[\tau_{ii}\tau_{jj} - \tau_{ij}^2\right] \geq 0 \tag{52}$$

$$I_3 = \det[\tau_{ij}] \geq 0 \tag{53}$$

(no summation over repeated indices, $i, j \to 1$–3.)

3) The following chain of inequalities are true (they are not independent):

$$\tau_{ij} \geq 0 \qquad \text{if } i = j \tag{54}$$

$$\tau_{ij}^2 \leq \tau_{ii}\tau_{jj} \qquad \text{if } i \neq j \tag{55}$$

$$\det[\tau_{ij}] \geq 0 \tag{56}$$

(no summation over repeated indices).

4) The following conditions are true:

$$\tau_{11} \geq 0 \tag{57}$$

$$\tau_{11}\tau_{22} - \tau_{12}^2 \geq 0 \tag{58}$$

$$\det[\tau_{ij}] \geq 0 \tag{59}$$

LES differs from the RANS approach in that the ensemble average $\langle\,\rangle$ must now be replaced by the filtering operation $\bar{}$. The proof of the realizability requirements rests on the following properties of the averaging operator: 1) $\langle a \rangle = a$, 2) $\langle af \rangle = a\langle f \rangle$, 3) $\langle f + g \rangle = \langle f \rangle + \langle g \rangle$, 4) $\langle f^2 \rangle \geq 0$, and 5) $\langle f \rangle$ is a constant, where f and g are any two dynamic fields and a and b are constants. It is easy to see that the linearity properties 1–3 also hold for the filtering operation. However, property 4 is true only for nonnegative filters. Property 5 is not valid; the filtered field is slowly varying compared to the unfiltered field, but it is not a constant. However, the realizability conditions can be shown to be true in LES for nonnegative filters provided one adopts the standard LES definition of the subgrid stress, $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$. In situations where the filtering can be considered a scalar operator (see earlier discussion), we can write the definition of the subgrid stress in the coordinate frame in which the stress tensor has the diagonal form. Thus,

$$\lambda_1 = \tau_{11} = \overline{u_1^2} - \bar{u}_1^2 \tag{60}$$

$$\lambda_2 = \tau_{22} = \overline{u_2^2} - \bar{u}_2^2 \tag{61}$$

$$\lambda_3 = \tau_{33} = \overline{u_3^2} - \bar{u}_3^2 \tag{62}$$

The right-hand sides of each of these expressions are nonnegative if the filter G is nonnegative. This can be proved in the following way. Let us assume that $G \geq 0$, and without loss of generality, we choose to work with filters that are normalized to unity, $\int G(x)\,dx = 1$. If we represent continuous integrals in terms of discrete sums, then

$$\overline{f^2} - \bar{f}^2 = \lim\left[\sum_i w_i f_i^2 - \left(\sum_i w_i f_i\right)^2\right] \tag{63}$$

where w_i are a set of weights such that $w_i \geq 0$ and

$$\sum_i w_i = 1$$

and lim denotes the usual operation of passing to the limit of an infinite number of infinitesimal subdivisions. We now note the following inequality obtained on substitution of the n-dimensional vectors $a_i = \sqrt{w_i}$ and $b_i = \sqrt{(w_i)} f_i$ (note w_i must be nonnegative) in the Cauchy–Schwarz inequality $|\boldsymbol{a} \cdot \boldsymbol{b}| \leq \|\boldsymbol{a}\|\,\|\boldsymbol{b}\|$ with respect to the Euclidean metric:

$$\left(\sum_i w_i f_i\right)^2 \leq \left(\sum_i w_i\right)\left(\sum_i w_i f_i^2\right) \tag{64}$$

On using this inequality on the right-hand side of Eq. (63), it follows that all three eigenvalues λ_1, λ_2, and λ_3 in Eq. (62) are nonnegative. Thus, the realizability conditions (47–49) and their various equivalent forms are rigorously true in LES provided only nonnegative filters are employed. The restriction to nonnegative filters may be undesirable because the commuting filters discussed earlier and several commonly used filters (such as Fourier cutoff) do not have this property. However, if the Reynolds number of the turbulence is sufficiently high so that the effective filtering volume contains a statistically significant range of eddies, it is expected that the result of the filtering would be independent of the precise form of the filtering kernel. Thus, in practice, the realizability conditions (47–49) can be assumed to be valid for LES even though strict validity can only be demonstrated in the case of nonnegative filters. Numerical simulation databases for a mixing layer do show some regions of flow where strict positivity of the subgrid kinetic energy is violated,[23] though both the magnitude of the negative energy as well as the volume of the region where this occurs are both quite small.

In the standard algebraic closures of the incompressible version of the LES equations, only the traceless part of the subgrid stress is modeled; the isotropic part is absorbed into the pressure term to give the effective pressure $p + \frac{2}{3}k$ (where k is the subgrid kinetic energy), which is determined from the continuity equation. Because k is never known separately, there is no way to check in these models whether or not the realizability conditions are satisfied. In one-equation versions of the model[16] one solves an additional transport equation for k so that k is known. The usual subgrid closure in this case is

$$\tau_{ij} = \tfrac{2}{3}k\delta_{ij} - 2C\Delta\sqrt{k}\bar{S}_{ij} \tag{65}$$

If $(s_\alpha, s_\beta, s_\gamma)$ denote the principal strains ordered such that $s_\alpha \geq s_\beta \geq s_\gamma$ (note that $s_\alpha + s_\beta + s_\gamma = 0$ for incompressible turbulence so that $s_\alpha \geq 0$ and $s_\gamma \leq 0$), the realizability conditions may be written as

$$-\frac{\sqrt{k}}{3\Delta|s_\gamma|} \leq C \leq \frac{\sqrt{k}}{3\Delta s_\alpha} \tag{66}$$

It is difficult to supply a proof that any given one-equation closure satisfies Eq. (66). One is usually restricted to a numerical proof, where statistics are collected at each grid point and the inequality (66) is checked to see if realizability is violated at only a small fraction of the computational volume. Sometimes the C value is "clipped" if it falls outside the theoretically allowed range (66), but this is not a satisfactory method for obvious reasons. The condition $k \geq 0$, which is necessary but not sufficient for realizability, can usually be theoretically guaranteed for one-equation models.[16]

IV. Analysis of Discretization Errors

The discussion so far was restricted to issues related to the derivation of the equations for the filtered fields from the NS equations. Once the basic equations are written down, the next step is to discretize them in time and space and solve them numerically to complete the LES procedure. For LES to have any credibility, the sources of errors in the numerical procedure must be understood, quantified, and controlled. In the author's view, rigorous error analysis of this kind needs to complement performance tests where certain physical quantities are computed and compared with experiments in a full-scale simulation.

Careful error analysis in LES, and indeed in DNS as well, involves some special difficulties. The problem is that turbulence cannot be characterized by a single space and timescale that can be normalized to unity. Consider, for example, the one-dimensional wave equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \tag{67}$$

If the space variable is discretized and the x derivative evaluated with a second-order central difference scheme, it is well known that the resulting truncation error $\sim u'''\Delta^2/6$. In simple problems, such as the propagation of a wave packet, one can reasonably define unique characteristic length and timescale so that u''' is of order unity if the equations are nondimensionalized with these characteristic scales. Thus, one may reasonably conclude that for the central difference scheme the truncation error $\sim\Delta^2$. This is no longer true in turbulence or in other nonlinear problems characterized by a broad spectrum of scales. In LES or DNS one could write the preceding error estimate in Fourier space as $k^3\Delta^2\hat{\boldsymbol{u}}(\boldsymbol{k})/6$; however, the magnitude of this error depends on which Fourier modes one looks at and the magnitude of $\hat{\boldsymbol{u}}(\boldsymbol{k})$, which depends on the turbulence spectrum. Therefore, it is difficult to judge without a more precise analysis what the true magnitude of the errors are.

A method for more carefully quantifying numerical errors in such nonlinear broadband-spectrum-type problems may be developed along the following lines.[24] To be specific we consider a hypothetical numerical simulation using a finite difference scheme of isotropic turbulence in a box with periodic boundary conditions. We consider only the numerical error due to the spatial discretization at a given point in time. The subject of time-discretization errors and numerical stability is rather large and is not discussed here. The effect of time discretization on turbulence with a realistic energy spectrum has recently been studied by Fabignon et al.[25] using a generalization of the Von Neumann analysis.

The essential idea in the analysis of space discretization errors in turbulence[24] is to write the finite difference implementation of a numerical scheme in spectral space by using the modified wave number to represent the differencing scheme. The numerical error for a wave of given wave number $\boldsymbol{k}$ can be written as the sum of three terms: 1) the subgrid modeling error, 2) the truncation error, and 3) the aliasing error. The origin of error 1 is clear; it appears because the subgrid model does not exactly equal the true subgrid stress τ_{ij}. Because we do not know what the true subgrid stress is, any theoretical treatment is difficult. The problem either needs to be studied by a priori testing, where the subgrid stresses are extracted from a well-resolved DNS field and compared to the model,[26,27] or by a posteriori testing, where a full simulation is run (see the review paper by Lesieur and Metais[5] and references therein) and various statistics from the simulation are compared to DNS or experiments. Both of these approaches are prevalent in the LES literature and will not be discussed here. Instead, we will assume that τ_{ij} is exactly known so that any numerical errors incurred in computing the model will also be neglected. The truncation error in differentiating τ_{ij} on the right-hand side of the momentum equation is, however, included.

The truncation error arises because numerical differentiation cannot find the exact derivative of a Fourier mode. Thus, if we apply a finite differencing operator D to a wave $A\exp(ikx)$, then the result is $ik'A\exp(ikx)$, where k' is a function of k and the grid spacing h and k' is called the modified wave number of the finite difference operator D.

The aliasing error arises when nonlinear terms are evaluated by multiplying together variables defined on a discrete grid, generating higher harmonics. The wavelengths of some of these waves are so short that they cannot be resolved on the grid. They get misinterpreted as a wave of much larger wavelength (they acquire an alias or duplicate identity). This description can be presented in a more formal way[24]; in the literature on spectral methods the origin of aliasing errors is well-known[9] and so is their potential to inflict serious damage on simulations.[4] The aliasing error depends on how the nonlinear term is written. For example, $\mathrm{d}/\mathrm{d}x(u^2)$ is not the same as $2u(\mathrm{d}u/\mathrm{d}x)$ on discretization.

Once these error terms are written down, they would contain quadratic terms in the velocities, such as $u_i u_j$, due to the quadratic nonlinearity inherent in the NS equations. A useful thing to know about these errors is their power spectra. These, too, can be written down in a formal way, but they now contain terms that are quartic in the velocities. One now uses the quasinormal hypothesis that works quite well at the kinematic level (though the long-term effect of the deviations from quasinormality has prevented its successful exploitation as a closure scheme) to express fourth-order velocity moments by second-order ones. Further, for isotropic turbulence, these second-order moments can be reexpressed in terms of the energy spectrum. A similar strategy was used by Bachelor[28] to deduce the pressure spectrum of isotropic turbulence from the energy spectrum. The end result is a set of analytical formulas for the error spectra. These will not be written down here, but the reader may find them in the original reference.[24]

Figure 1 shows the power spectrum of the truncation error for central differences schemes of second, fourth, sixth, and eighth order for a turbulence spectrum modeled with the Von Kármán spectrum $[E(k) \sim k^4$ as $k \to 0$ and $E(k) \sim k^{-5/3}$ as $k \to \infty]$ at a Reynolds number considered essentially infinite. The normalization is chosen so that the energy spectrum has its maximum value of unity at $k = 1$. The symbols represent upper and lower bounds for the true subgrid force computed using similar quasinormal analysis. It is clear that, even for the high-order schemes, truncation errors are unacceptably large. The physical reason for this is the modified wave number has the largest deviation from the true wave number near the cutoff. However, in LES, the energy spectrum does not fall off sharply near the cutoff due to a dissipation range as it does in DNS. In the standard

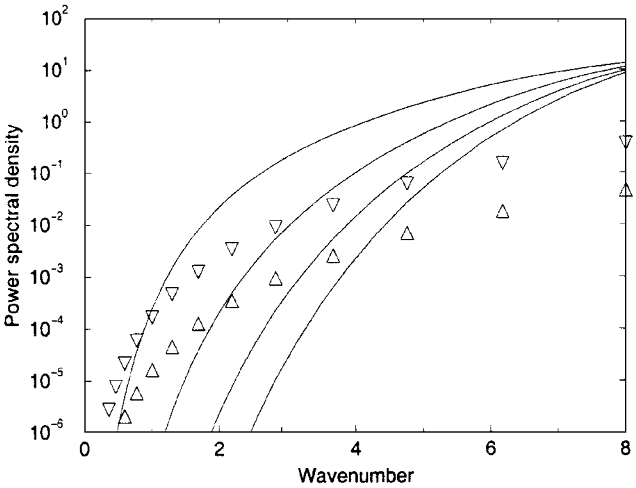

Fig. 1 Power spectra of the truncation error for (top to bottom) second-, fourth-, sixth-, and eighth-order central difference schemes (——) compared to upper and lower bounds of subgrid force (▽△).

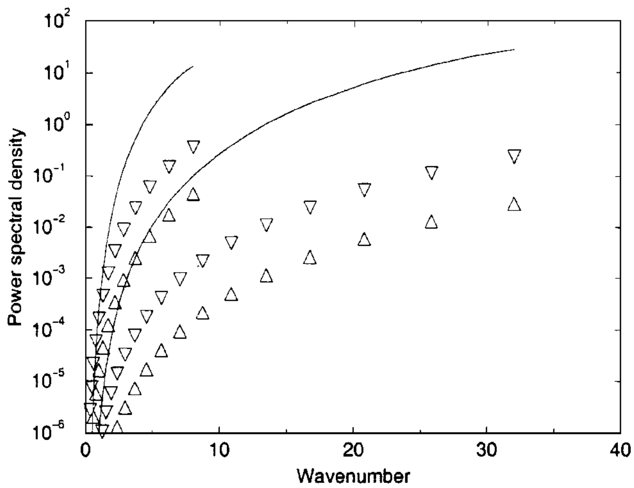

Fig. 2 Power spectra of the truncation error for a second-order central difference scheme for two different grid resolutions (——) compared to upper and lower bounds of subgrid force (▽△).

implementation of LES the grid size is usually considered equal to the filter size. As a result, increasing the resolution essentially changes the problem by bringing in new modes. Both the subgrid term and the truncation error changes without changing the fact that the truncation error dominates the subgrid force. This relation could only change when the LES converges to a DNS and all scales of motion are resolved. There is no concept of grid independence in the standard implementation of LES.

Figure 2 shows how the truncation error spectrum for the second-order central difference scheme changes when the grid size is reduced by a factor of 4. Also shown for comparison are the power spectra (upper and lower bounds) for the subgrid force at the two different resolutions. The results support the statements made at the end of the last paragraph. Both the truncation error and the subgrid force are altered by the increased resolution, but the truncation error continues to dominate the subgrid force.

Figure 3 shows the aliasing error spectra for central difference schemes of second and fourth order as well as that of a (undealiased) pseudospectral scheme that has no truncation errors. The aliasing error is once again seen to dominate the subgrid force. The schemes with the larger truncation errors have somewhat reduced aliasing errors. This effect is well known[4] and is because the modified wave number of the approximate differencing schemes goes to zero near the grid cutoff.

One possible method of controlling these errors is shown in Fig. 4. Here the filter width is taken as twice the grid spacing (the filter being assumed to be of the Fourier cutoff type), and the truncation error

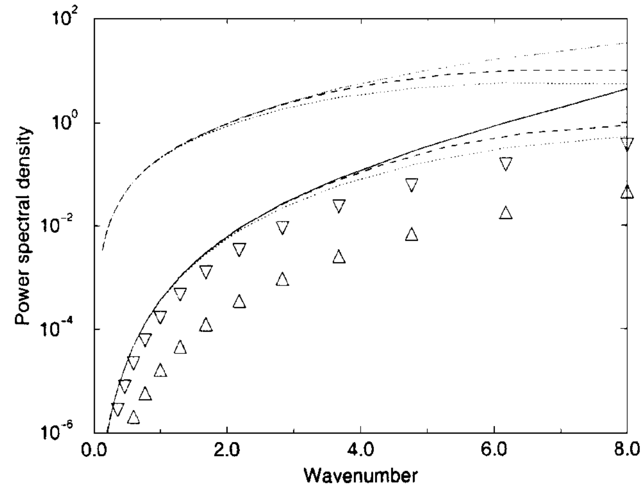

Fig. 3 Power spectra of the aliasing error for an undealiased pseudospectral scheme (——), fourth-order central difference scheme (- - -), and second-order central difference scheme (· · · ·) compared to upper and lower bounds of subgrid force (▽△).

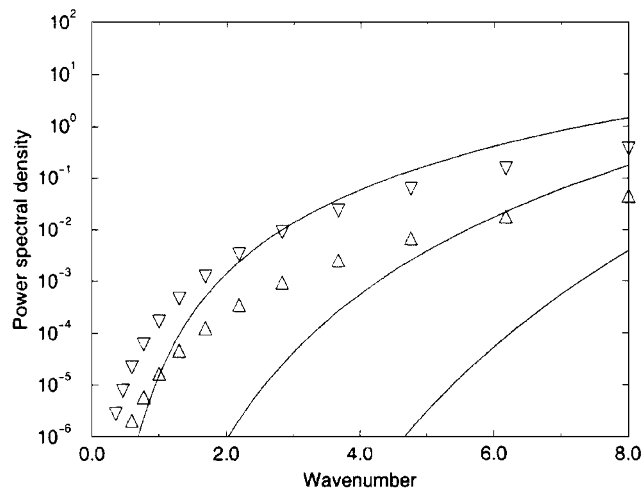

Fig. 4 Power spectra of the truncation error for (top to bottom) second-, fourth-, and eighth-order central difference schemes (——) compared to upper and lower bounds of subgrid force (▽△) when the filter width is taken as twice the grid spacing.

spectrum is plotted for the second-, fourth-, and eighth-order central differencing scheme. In this case, the truncation error is reduced several orders of magnitude below the subgrid force for the eight-order scheme. Further, for the Fourier cutoff filter, the aliasing error is reduced exactly to zero (a manifestation of the familiar $\frac{3}{2}$ dealiasing rule). A filter to grid ratio of 2, however, implies an eightfold increase of grid points and a further increase in computational time if the maximum time step is limited by the Courant–Friedrichs–Lewy condition.

The preceding analysis of errors is essentially kinematic in nature. It quantifies the magnitude of the error but gives no information about the long-term dynamic effect of these errors on the computation. Such information, however, is critical for the success of the numerical method. A systematic study of this issue in the context of LES has recently been undertaken by Kravchenko and Moin.[29] These authors used a channel flow code that used a high-order B-spline method in the wall normal direction and a pseudospectral method in the remaining two homogeneous directions. The effect of using finite difference implementations in the homogeneous directions could be studied by replacing the wave numbers by modified wave numbers in the spectral evaluation of derivatives in the code. The effect of aliasing errors could be simulated by simply omitting the dealiasing procedure. Further, by introducing appropriate phase shifts in the Fourier modes, the code could be made to mimic computations on a staggered mesh.

As a result of a series of systematic numerical experiments, the authors[29] concluded that both aliasing and truncation errors of low-order schemes do seriously degrade LES computations, as conjectured earlier based on a theoretical analysis.[24] (Note that a similar problem was observed and reported earlier[26,30,31] in the context of mixing layer calculations.) Of these, the aliasing error was found to be the source of the most serious problems because it interfered with the energy conserving nature of the scheme and could lead to unstable calculations. The magnitude of the aliasing error depended on the form in which the nonlinear term was written. The skew-symmetric form had the lowest aliasing error due to some cancellations between the partial contributions. This dependance of the aliasing error on the form of the nonlinear term has also been studied earlier by Blaisdell et al.[32] These studies have motivated a move toward high-order finite difference schemes for LES calculations that retain, at the discrete level, the energy, momentum, and mass conserving properties of the basic LES equations.[33]

V. Conclusions

The numerical simulation of turbulence is an extremely computationally intensive enterprise and quickly saturates even the impressive gains in computer speeds that marks every new development in computer technology. This fact, coupled with the extraordinary theoretical difficulties involved in developing any statistical closure theory of turbulence, propels LES as the most versatile tool for engineering calculations. The potential of LES for visualization of the essential structures in the flow, as well as for reliable quantitative predictions, has been demonstrated, at least in relatively simple geometries. One of the challenges ahead would be to demonstrate unambiguously that LES is able to predict quantitatively statistical measures of interest in the domain of truly complex engineering flows.

This transition naturally raises questions such as the following:

1) Can the theoretical framework of LES originally envisaged for uniform grids be extended to include nonuniform grid distributions?

2) Are finite difference methods, which are the most convenient to implement in complex geometry, adequate for LES?

3) What is the best way to restrict the class of subgrid models so that they have as many of the properties of the true subgrid stress built into them?

An attempt has been made in this review to summarize recent research on questions of this kind.

Acknowledgment

The author would like to thank Thomas Lund for his helpful comments.

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