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TOWARD THE DE-MYSTIFICATION OF LES

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1. Introduction

Some 35 years have elapsed since large-eddy simulation (LES) was introduced as a computational tool for weather modeling (Lilly, 1966). Because direct numerical simulation (DNS) will remain prohibitively expensive well into the foreseeable future for high-Reynolds-number flow, LES continues to hold great promise for simulating flows of engineering interest. However, despite the attention the method has received over the past decades, and despite important recent developments (e.g., the notions of "explicit" filtering and localized or "dynamic" modeling (Germano *et al.*, 1992)), LES has been slow to mature as a predictive tool. In contrast, parabolized stability equation (PSE) methodology, for example, which originated in the mid 1980's (Bertolotti *et al.*, 1992), matured quickly and is now ready for use by the aerospace industry for transition prediction.

In the author's view, the relatively slow adaptation of LES as a predictive tool arises not from any fundamental flaw in the idea itself but most likely from misconceptions that widely permeate the practice of LES. The current paper addresses three pervasive misconceptions, each of which reveals a lack of clarity regarding the properties of digital filters and the relationship between the grid filter and the subgrid-scale (SGS) model.

2. Misconception 1: Grid Filtering is a Mere Formality

From an otherwise excellent recent text on turbulent flows (Mathieu and Scott, 2000) comes the following quote:

> Note that, if one forgets that the $\hat{U}_i$ is supposed to represent the filtered velocity field, the filter plays *absolutely no role* (emphasis added) in the final LES

equations, which can be understood in terms of adding a subgrid viscosity term to the Navier-Stokes equations, without introducing the notion of filtering.

The mistake here is confuse *formal* invariance under filtering operations with *quantitative* invariance. To be precise, the grid-filtered Navier-Stokes equations are given as follows:

$$\frac{\partial \overline{u}_k}{\partial t} + \frac{\partial(\overline{u}_k \overline{u}_l)}{\partial x_l} = -\frac{\partial \overline{p}}{\partial x_k} + \frac{1}{Re}\frac{\partial^2 \overline{u}_k}{\partial x_l \partial x_l} + \frac{\partial \tau_{kl}}{\partial x_l} \tag{1}$$

$$\tau_{kl} \equiv \overline{u}_k \overline{u}_l - \overline{u_k u_l} \tag{2}$$

Whereas the *form* of Eq. 1 is independent of the filter, the *value* of the residual stress τ_{kl} is not.

To illustrate, suppose that grid filtering is applied at a wavenumber cut-off k_c *greater than* the Kolmogorov wavenumber k_η (Fig. 1). Then, in effect, one conducts fully resolved DNS rather than LES, in which case, for all practical purposes $\tau_{kl} = 0$. As written, Eq. 2 is missing a parameter. In reality, $\tau_{kl} = \tau_{kl}(k_c)$. That is, the exact residual stress depends first and foremost upon the cut-off of the grid filter. What else does it depend upon? Figure 2 compares *exact* residual stresses computed from *a priori* analyses of isotropic turbulence (Pruett and Adams, 2000) by filtering with two different grid filters: one of 2nd-order, the other of 4th-order. The correlation between the *exact* residual stresses, which differ in both distribution and amplitude, is only 0.5! Thus, at minimum, τ_{kl} depends upon both the cut-off and the order of the grid filter. Can the dependence of the residual stress upon the filter be fully characterized?

Yes. A filter is completely characterized in terms of its transfer function $H(\xi)$, which expresses the action of the filter on the Fourier harmonic $\exp(\imath kx)$, where $\xi = k\Delta x$. That is, if the filter is represented by the parameterized (Δ) convolution integral $\bar{u}(x) = \int_{-\infty}^{-\infty} G(x'-x,\Delta)u(x')dx'$, then H is the Fourier transform of the kernel G, and G is its inverse transform. For example, consider the top-hat filter whose kernel is

$$G(x,\Delta) = \begin{cases} 1/\Delta & \text{if } |x| \le \Delta/2 \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

Trapezoidal-rule quadrature over a filter width of $\Delta = 2\Delta x$ results in the discrete 3-point top-hat filter of weights [1/4,1/2,1/4], whose transfer function is

$$H(\xi) = \frac{1+\cos(\xi)}{2} = 1 - \frac{x^2}{2(2!)} + \frac{x^4}{2(4!)} - \ldots \tag{4}$$

Alternately, the action of a filter can be examined by Taylor-series expansion of a filtered field in terms of the un-filtered field and its derivatives.

For example,

$$\bar{u}(x) = u(x) + a_2 u''(x)\Delta x^2 + a_4 u^{(4)}(x)\Delta x^4 + \ldots \tag{5}$$

(Because we have presumed G to be symmetric, the expansion has only even-ordered terms.) For convenience, the factorials in the expansion have been absorbed into the coefficients a_{2m}. A filter is said to be of order $2m$ if a_{2m} $(m > 0)$ is the first non-vanishing coefficient. Equations 4 and 5 carry the same information in different guises, which becomes apparent if Eq. 5 is applied to the function $u(x) = \exp(\iota k x)$, from whence it follows

$$a_{2m} = \frac{(-1)^m H^{(2m)}(0)}{(2m)!} \tag{6}$$

Thus, the coefficients of Eq. 5 are completely determined by derivatives of the filter's transfer function. For the three-point top-hat filter, for example, $a_{2m} = \frac{1}{2(2m)!}$.

Now let G_x and G_y be discrete filters in the x and y dimensions, whose Taylor coefficients are a_{2m} and b_{2m}, respectively. For two-dimensional filtering, suppose $\bar{u} = G_y(G_x((u))$. By two-fold expansion, one obtains the following expression for the *exact* residual stress:

$$\begin{aligned}
-\tau_{kl} &= 2a_2 \frac{\partial u_k}{\partial x}\frac{\partial u_l}{\partial x}\Delta x^2 + 2b_2 \frac{\partial u_k}{\partial y}\frac{\partial u_l}{\partial y}\Delta y^2 \\
&+ \left[4a_4 \frac{\partial u_k}{\partial x}\frac{\partial^3 u_l}{\partial x^3} + (6a_4 - a_2^2)\frac{\partial^2 u_k}{\partial x^2}\frac{\partial^2 u_l}{\partial x^2} + 4a_4 \frac{\partial^3 u_k}{\partial x^3}\frac{\partial u_l}{\partial x}\right]\Delta x^4 \\
&+ \left[\frac{\partial u_k}{\partial x}\frac{\partial^3 u_l}{\partial x \partial y^2} + \frac{\partial u_k}{\partial y}\frac{\partial^3 u_l}{\partial x^2 \partial y} + 2\frac{\partial^2 u_k}{\partial x \partial y}\frac{\partial^2 u_l}{\partial x \partial y} + \frac{\partial^3 u_k}{\partial x \partial y^2}\frac{\partial u_l}{\partial x} + \frac{\partial^3 u_k}{\partial x^2 \partial y}\frac{\partial u_l}{\partial y}\right] \\
&\times 2a_2 b_2 \Delta x^2 \Delta y^2 \\
&+ \left[4b_4 \frac{\partial u_k}{\partial y}\frac{\partial^3 u_l}{\partial y^3} + (6b_4 - b_2^2)\frac{\partial^2 u_k}{\partial y^2}\frac{\partial^2 u_l}{\partial y^2} + 4b_4 \frac{\partial^3 u_k}{\partial y^3}\frac{\partial u_l}{\partial y}\right]\Delta y^4 \\
&+ O(h^6) \quad \text{where } h \in \{\Delta x, \Delta y\}
\end{aligned} \tag{7}$$

Eq. 7 is completely general; it is valid for *any* grid filters G_x and G_y whose coefficients are known, provided the associated Taylor series converge. The issue of convergence is addressed in Vasilyev *et al.* (1998) and Pruett *et al.* (2001). In short, convergence is guaranteed for positive symmetric filters.

We conclude that *the exact SGS-stress tensor is completely determined by the grid filter, as expressed through derivatives of its transfer function.*

3. Misconception 2: Any Model Goes with Any Filter

In the conventional practice of LES, the grid filter and the SGS-model are often selected independently, as observed by Piomelli *et al.* (1988). In contrast, previous discussion reveals the filter, the exact SGS stresses, and the model to be fundamentally interrelated.

To be specific, Fig. 3 compares the transfer functions of filters of selected orders. The order of a filter is related to the flatness (i.e., the number of vanishing derivatives) of its transfer function at $\xi = 0$. Spectral filters, characterized by a sharp cut-off in Fourier space, act with infinite order. From Eq. 7, it follows that the leading term of τ_{kl} is of order h^{2m} if the grid filter itself is of order $2m$ $(m \geq 1)$.

The most common models for LES are of eddy-viscosity type (Mathieu and Scott, 2000), of which the Smagorinsky model ($M1$) is the most familiar. Because $M1$ is scaled by h^2, it is consistent only with filters of (first or) second order. In particular, $M1$ is inconsistent with spectral filters. Even when used in conjunction with second-order filtering, the Smagorinsky model correlates poorly with exact (E) residual stresses, as observed in experiments by Liu *et al.* (1994) and computational studies by Pruett and Adams (2000). Typically $C(E, M1) \leq 0.2$, as suggested in Fig. 4. In contrast, similarity ($M2$) and gradient ($M3$) models perform considerably better in *a priori* analyses. Typically, $C(E, M2) > 0.8$ and $C(E, M3) \approx 0.6$, respectively (Liu *et al.*, 1994; Pruett and Adams, 2000).

The many well-known deficiencies of the Smagorinsky model help to explain, in physical terms, its poor performance. Among these, $M1$ is overly dissipative, which undermines its successful application to laminar-turbulent transition, and it is isotropic, which limits its applicability in the near-wall region. However, from a mathematical perspective, the deficiency of $M1$ is apparent: formally it doesn't match the leading-order terms of Eq. 7. In contrast, $M3$ matches at leading order term and $M2$ matches at leading order and partially matches beyond that. The author is led to concur with Leonard (1997) that the Smagorinsky model has "little justification" beyond some nice properties.

To conclude, further advancement of LES requires that more attention be devoted to filter-model consistency, to models that have greater fidelity to Eq. 7 (for example, similarity models) than does the Smagorinsky model, and/or to promising new mathematical techniques such as deconvolution (Domaradzki and Saiki, 1997; Stolz and Adams, 1999) that avoid explicit modeling.

4. Misconception 3: Fixed-Width Filters are Fine for LES

Whereas the wavenumber k^* and the grid increment Δx^* are dimensional quantities with dimensions $[1/L]$ and $[L]$, respectively, their product $\xi = k^* \Delta x^*$ is dimensionless. (Here, asterisks denote dimensional quantities.) Several problems in LES result from a failure to non-dimensionalize.

To be specific, the maximum wavenumber $k^*_{\max}$ in a simulated flow is determined by *physical* considerations. For fully resolved DNS, $k^*_{\max} \geq k^*_\eta$, where k^*_η, the Kolmogorov wavenumber, depends solely on Reynolds number. For LES, $k^*_{\max} \approx k^*_c$, where k^*_c lies in the inertial range of the energy spectrum (Fig. 1). Either way, physics determines $k^*_{\max}$.

On the other hand, the grid increment Δx^* is mandated by *numerical* considerations, that is, by the resolution necessary to resolve the smallest eddies *for the numerical scheme of choice.* For example, for Fourier and Chebyshev spectral, and fourth- and second-order finite-difference (FD) schemes, respectively,

$$\begin{aligned}
\Delta x^* &= \pi/k^*_{\max} \quad \text{(Fourier spectral)} \\
\Delta x^* &= 2/k^*_{\max} \quad \text{(Chebyshev spectral)} \\
\Delta x^* &= \pi/(6k^*_{\max}) \quad \text{(4th-order FD)} \\
\Delta x^* &= \pi/(16k^*_{\max}) \quad \text{(2nd-order FD)}
\end{aligned} \tag{8}$$

For the spectral schemes, the stated resolution results from application of the Nyquist criterion. For the FD schemes, resolution is based upon the author's computational experience (Pruett *et al.*, 1995).

A fixed-width filter (e.g., the 3-point top-hat filter) has the disadvantage that its cut-off is "hardwired" to the grid increment Δx^*. In contrast, a tunable filter permits the cut-off k^*_c to be adjusted independently of Δx^*. Figure 6 presents the transfer functions of a family of one-parameter second-order filters of Pade type (Lele, 1992), as functions of their dimensionless cut-off $\xi_c = k^*_c \Delta x^*$, where, by definition, $H(\xi_c) = 1/2$. The filter is continuously adjustable over its entire domain of cut-off values $0 < \xi_c \leq \pi$, which represent varying levels of numerical dissipation. In particular, $\xi_c = \pi$ provides no dissipation, and $\xi_c \approx 0$ provides maximum dissipation. The fixed-width top-hat filter corresponds to the particular value $\xi_c = \pi/2$.

What then are the problems with fixed-width filters? First, for FD numerical schemes, allowing the dissipation of the filter to be set by the grid increment virtually guarantees that the unintended truncation error of the numerical scheme will contaminate the intended dissipation of the filter.

Second, suppose we wish to compare LES against the results of *a priori* analysis from fully resolved DNS at, say, twice the grid resolution of the LES. For specificity, presume that both methods exploit Fourier spectral methods. The comparison, of course, should occur at the same physical cut-off in wavenumber space (Fig. 1). Thus $(k^*_c)_{\mathrm{DNS}} = (k^*_c)_{\mathrm{LES}}$. However, because $(\Delta x^*)_{\mathrm{LES}} = 2(\Delta x^*)_{\mathrm{DNS}}$, for the same physical cut-off, the dimensionless cut-offs must have the ratio $(\xi_c)_{\mathrm{DNS}}/(\xi_c)_{\mathrm{LES}} = 1/2$. Without a tunable filter, the comparison cannot be made at the same physical cut-off.

Third, *Ad hoc* attempts at tuning the three-point top-hat filter, for example, can have unintended consequences. By naively extending the filter width Δ^* from $2\Delta x^*$ to $4\Delta x^*$, the transfer function changes from low-pass to U-shaped (Fig. 5). It is therefore highly preferable to begin with a tunable low-pass filter whose behavior is suitable at all values of dissipation (cut-off). The Pade filter shown in Fig. 6, for example, is such a filter.

To summarize, in LES, the dimensional cut-off k_c^* is determined by physical considerations, but the grid resolution Δx^* is mandated by numerical ones. Tunable (one-parameter) filters permit the cut-off and resolution to be specified independently, according to their respective criteria.

Conclusion

Most SGS models for LES have been developed on the basis of physical rather than mathematical considerations. However, it is shown that the *exact* residual stress is completely determined by the *mathematical* properties of the grid filter; that is, by its order, its cut-off wavenumber, and the shape of its transfer function.

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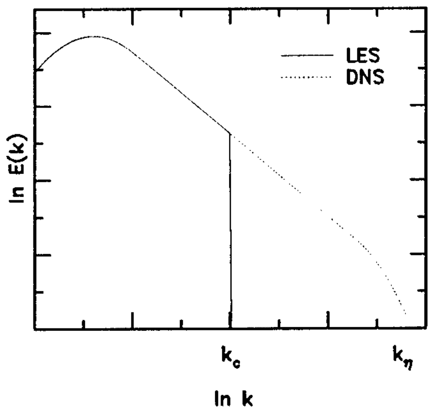

Figure 1. DNS vs. idealized LES.

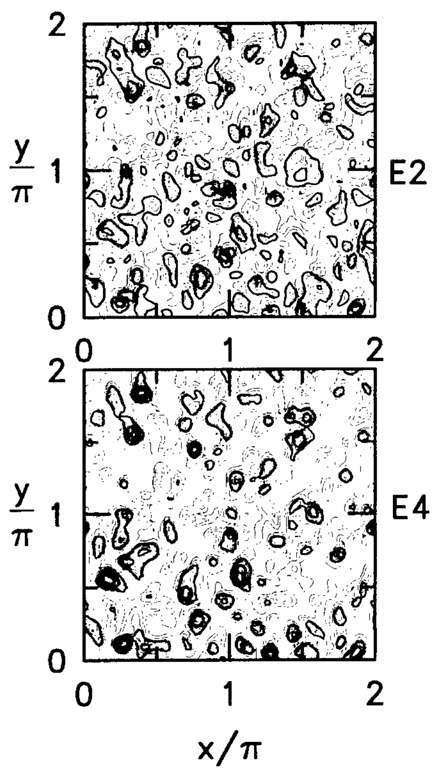

Figure 2. Exact SGS stresses from grid filters of 2nd- ($E2$) and 4th-order ($E4$).

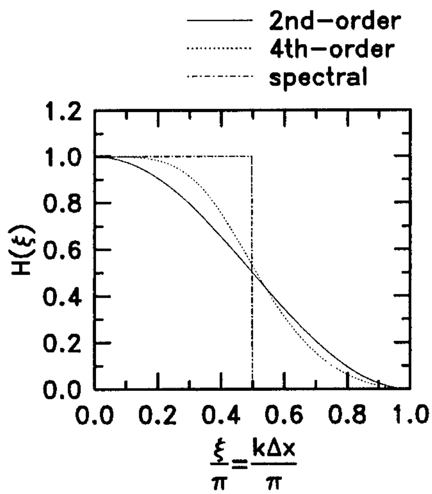

Figure 3. Filters of differing orders.

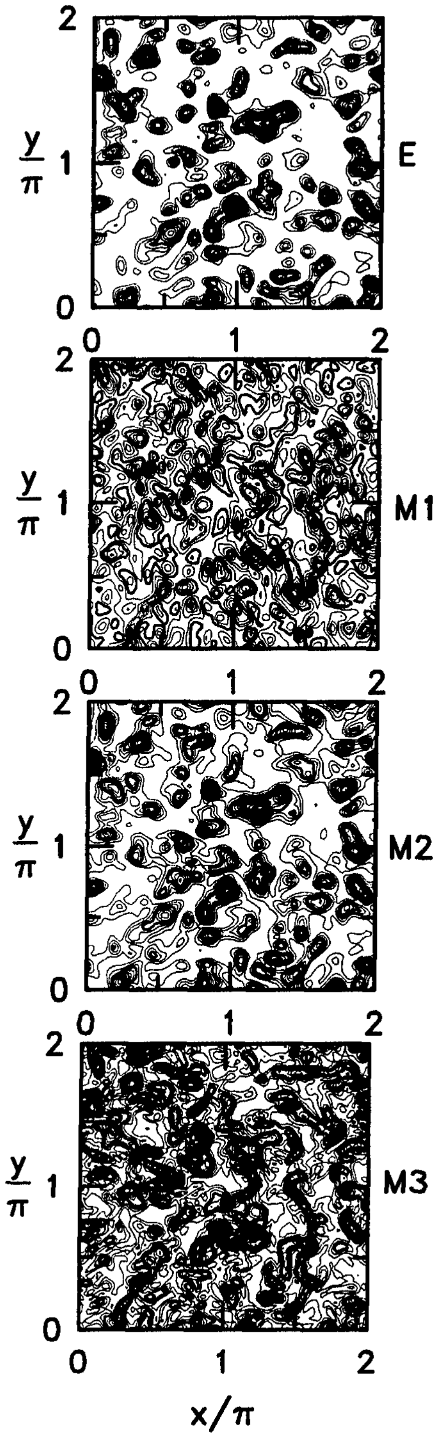

Figure 4. Planar contours of exact (E) and modeled ($M1$-Smagorinsky, $M2$-similarity, $M3$-gradient) SGS stresses (τ_{11} component).

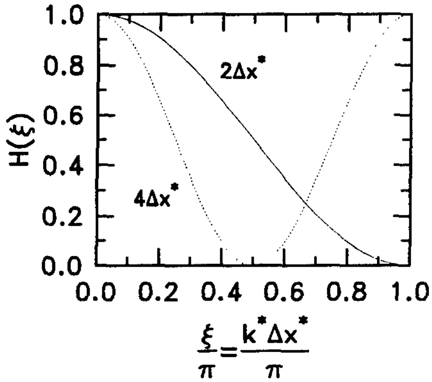

Figure 5. Transfer functions of three-point top-hat filters.

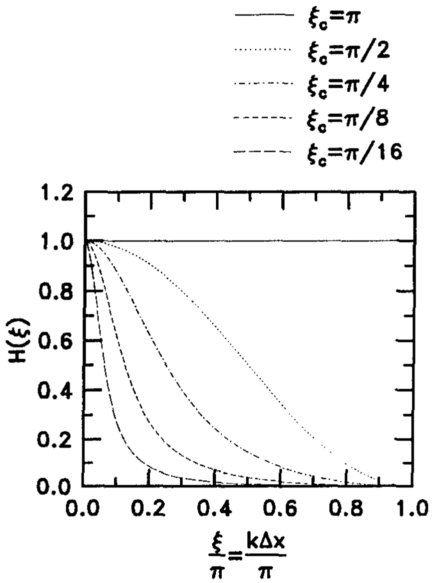

Figure 6. Transfer functions of one-parameter family of Pade filters.