NEAR-AUTONOMOUS LARGE EDDY SIMULATIONS OF TURBULENCE BASED ON INTERSCALE ENERGY TRANSFER AMONG RESOLVED SCALES

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ABSTRACT

Spectral eddy viscosity models proposed by Kraichnan (1976) and by Chollet & Lesieur (1981) account explicitly for physical properties of interscale interactions deduced from analytical theories of turbulence. In the present work we show that the main features of the subgrid-scale (SGS) energy transfer can also be obtained directly from the evolving large eddy simulations (LESs), allowing a near autonomous LES where the SGS model is provided by the analysis of the LES fields at each time step in simulations. Specifically, the method computes the SGS energy transfer among resolved scales and its wave number distribution from the evolving LES velocity fields. This information is supplemented by well established asymptotic properties of the energy flux in the inertial range: its locality scaling exponent $4/3$ and the value of the spectral eddy viscosity in the limit $k \to 0$. The resulting SGS energy transfer, when cast in the form of a spectral eddy viscosity, allows self-contained simulations without use of extraneous SGS models. The method is tested in LES of isotropic turbulence at high Reynolds number where the inertial range dynamics is expected and for lower Reynolds number decaying turbulence under conditions of the classical experiments of Comte-Bellot & Corrsin (1971).

INTRODUCTION

Analytical theories of isotropic turbulence as originated by Kraichnan's Direct Interaction Approximation (Kraichnan (1959)) provide closure expressions for the energy transfer term $T(k)$ in the spectral kinetic energy equation in terms of the energy spectrum $E(k)$. Modern, exhaustive review of analytical theories of turbulence and closures has been recently provided by Zhou (2021). Kraichnan (1976) employed such closure expressions to compute the subgrid-scale (SGS) energy transfer $T_{SGS}(k|k_c)$ from a range of resolved scales $k \leq k_c$ caused by nonlinear interactions involving subgrid scales $k > k_c$, where k_c is a cutoff wavenumber of a sharp spectral filter. The SGS energy transfer, when normalized by $2k^2E(k)$, gives a spectral eddy viscosity $\nu_{eddy}(k|k_c)$. Such an eddy viscosity, computed for the infinite inertial range spectrum $E(k) \sim k^{-5/3}$, has a relatively simple form with a constant plateau for wave numbers k less than approximately $0.4k_c$ and rising in a form of a cusp to the maximum value at $k = k_c$ (see Fig. 1). Kraichnan (1976) used a particular analytical theory, the Test Field Model (TFM), while Chollet & Lesieur (1981) used another formulation, the Eddy Damped Quasi-Normal Markovian Approximation (EDQNM), with both approaches leading to similar eddy viscosities. For the EDQNM formulation the authors subsequently provided an analytical fit to the computed eddy viscosity and used it as a SGS model in large eddy simulations of Navier-Stokes equations (see, e.g., Lesieur (1997); Lesieur *et al.* (2005)). In such an approach to SGS modeling the primary physical quantity is the energy transfer across a wave number cutoff k_c between the resolved scales ($k < k_c$) and the subgrid-scales ($k > k_c$) and the eddy viscosity is a derived quantity. This is different from a more common approach to postulate first a functional form of the eddy viscosity and then obtain values of model constants that best match known theoretical and experimental results for a given turbulent flow. The former approach can be advantageous if information about the SGS energy transfer is directly available for a given flow. In previous work by Domaradzki (2021*a*,*b*) it was shown that the subgrid-scale energy transfer among resolved scales in large eddy simulations (LES) as well as its wave number distribution can be obtained directly from the evolving LES velocity fields. This information, supplemented by known asymptotic properties of energy flux in the inertial range, when cast in the form of a spectral eddy viscosity, allows SGS modeling without need for explicit expressions of the analytical theories or

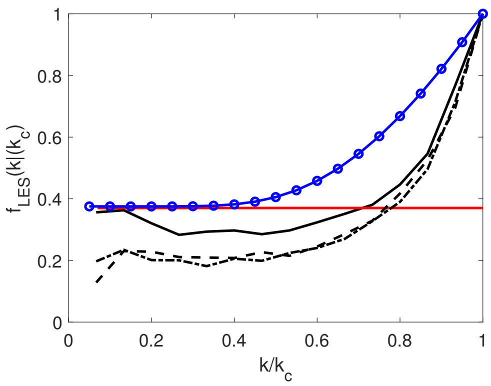

Figure 1. Spectral eddy viscosity shape functions. Solid line with symbols ∘: analytical theory of turbulence (EDQNM); horizontal solid line: asymptotic plateau value from the EDQNM theory; shape functions computed from LES data for cases "ceddy" (solid line), "pconst" (broken line), "pvar" (broken-dotted line).

any other classical SGS models. Effectively, the procedure allows self-contained LES without use of extraneous SGS models, or equivalently, at each time step the model is obtained from a simulated field itself and two asymptotic properties of the energy flux in the inertial range.

DESCRIPTION OF THE METHOD

The spectral LES energy equation for scales $k \leq k_c$ is obtained by defining first energy transfer $T^<(k|k_c)$ among resolved modes, where the notation signifies that only modes satisfying the inequality $k \leq k_c$, i.e. scales that are fully known in LES with the cutoff k_c, are retained in computing $T^<(k|k_c)$. The complete spectral energy equation can then be rewritten for LES scales $k \leq k_c$ as follows

$$\frac{\partial}{\partial t}E^<(k|k_c) = T^<(k|k_c) + T_{SGS}(k|k_c) - 2\nu k^2 E^<(k|k_c),\ k \leq k_c, \tag{1}$$

where the SGS energy transfer term is

$$T_{SGS}(k|k_c) = T(k) - T^<(k|k_c),\ k \leq k_c, \tag{2}$$

where $T(k)$ is the full nonlinear energy transfer computed using all modes, resolved and subgrid scale.

Following Kraichnan (1976), the SGS spectral energy equation can be formally rewritten as

$$\frac{\partial}{\partial t}E^<(k|k_c) = T^<(k|k_c) - 2\nu_{eddy}(k|k_c)k^2E^<(k|k_c) - 2\nu k^2 E^<(k|k_c) \tag{3}$$

where the SGS energy transfer is expressed in the same functional form as the molecular dissipation term by introducing the theoretical, effective eddy viscosity

$$\nu_{eddy}(k|k_c) = -\frac{T_{SGS}(k|k_c)}{2k^2E^<(k|k_c)}. \tag{4}$$

As stressed before, the eddy viscosity is obtained from the primary physical quantity which is the energy transfer across a wave number cutoff k_c between resolved scales ($k < k_c$) and subgrid-scales ($k > k_c$).

It was shown by Domaradzki (2021*a*) that the task of modeling $T_{SGS}(k|k_c)$ can be productively split into finding the total SGS transfer/dissipation, integrated over $0 < k < k_c$ and, separately, its distribution in wave numbers k. The total SGS energy transfer across the cutoff k_c is determined by the formula derived in Domaradzki (2021*a*) using the Germano identity (Germano *et al.* (1991)),

$$T_{SGS}(k_c) = \frac{1}{1-b}T^{res}_{SGS}(\frac{1}{2}k_c), \tag{5}$$

where b is a constant and $T^{res}_{SGS}(\frac{1}{2}k_c)$ is the energy transfer computed for the resolved LES modes ($k < k_c$) and the cutoff $(1/2)k_c$. Using multiple theoretical and DNS results for inertial range turbulence the constant b was determined to be approximately $b \approx 0.40$. The total resolved SGS energy transfer $T^{res}_{SGS}(\frac{1}{2}k_c)$ can be computed by integrating expression (2), written for cutoff $\frac{1}{2}k_c$, over all wave numbers less than this cutoff. However, as shown in Domaradzki (2021*a*) it can also be computed using standard LES formulas for SGS dissipation in the physical space based on the SGS tensor and the resolved rate-of-strain tensor.

A wave number distribution of the resolved SGS energy transfer $T^{res}_{SGS}(k|\frac{1}{2}k_c)$ can be computed from LES data during an actual run and cast in the form of the k-dependent eddy viscosity (4), which is normalized to unity $f^{res}_{LES}(k|\frac{1}{2}k_c) = \nu^{res}_{eddy}(k|\frac{1}{2}k_c)/\nu^{res}_{eddy}(\frac{1}{2}k_c|\frac{1}{2}k_c)$. That last quantity, the eddy viscosity shape function, is rescaled from the test cutoff $(1/2)k_c$ to LES cutoff k_c, using the similarity variable $0 \leq k/k_{cutoff} \leq 1$. Such computed eddy viscosities for several LES cases are shown in Fig. 1. Finally, the values of the eddy viscosity at low k are modified to make them consistent with the asymptotic value provided by the analytical theories for the inertial range at $k/k_c \to 0$. Based on results from the EDQNM theory the plateau asymptotic value p was determined as 0.37 of the peak value at the cusp, i.e., $p = 0.37$ for the eddy viscosity shape function normalized to unity at k_c (horizontal line in Fig. 1). The final shape function $f_{LES}(k|k_c)$ comprise a constant plateau up to an intersection with a cusp of the resolved shape function $f^{res}_{LES}(k|k_c)$, followed by the unmodified cusp part from the intersection point to $k = k_c$.

The complete procedure is implemented in several steps. At each time step in simulations the eddy viscosity is

$$\nu_{eddy}(k|k_c) = C_m f_{LES}(k|k_c), \tag{6}$$

where C_m is a model constant and $f_{LES}(k|k_c)$ is a shape function, determined as described above. The model constant C_m is computed using known total SGS energy transfer as an integral constraint

$$T_{SGS}(k_c) = \int_0^{k_c} dk T_{SGS}(k|k_c) = -\int_0^{k_c} dk\ \nu_{eddy}(k|k_c)2k^2E(k), \tag{7}$$

which gives

$$C_m = \frac{-T_{SGS}(k_c)}{\int_0^{k_c} f_{LES}(k|k_c)2k^2E(k)dk}. \tag{8}$$

In LES runs the eddy viscosity (6) is determined at each time step in simulations and used in the eddy viscosity term added to the Navier-Stokes spectral solver as a SGS modeling term.

In (8) $T_{SGS}(k_c)$ is expressed in terms of SGS transfer among resolved scales $T^{res}_{SGS}(\frac{1}{2}k_c)$, Eq. (5), computed at each time step in LES with the spectral eddy viscosity given by (6). Similarly, the shape function $f_{LES}(k|k_c)$ is computed at each time step from the resolved SGS energy transfer $T^{res}_{SGS}(k|\frac{1}{2}k_c)$, i.e., both factors in the formula (6) are computed from information available in LES. In effect, the SGS model is not prescribed but obtained from the resolved SGS energy transfer $T^{res}_{SGS}(k|\frac{1}{2}k_c)$ in a given LES and two well-established properties of the energy flux for the inertial range in the asymptotic limit $k/k_c \to 0$. Note also that since $T^{res}_{SGS}(k|\frac{1}{2}k_c)$ and $E(k)$ in general are time dependent, both factors in (6) are also functions of time, $C_m(t)$ and $f_{LES}(k,t|k_c)$.

The purpose of this paper is to revisit derivations of parameters b and p and to assess the performance of the method for allowable choices of these parameters. In particular, derivation of constant b using the Germano identity requires assumptions about a form of the shape function for the final spectral eddy viscosity. We show that these assumptions are not necessary because the constant b can be deduced from the scaling properties of the energy flux for $k/k_c \to \infty$, without reference to the Germano identity. Similarly, we show that the plateau value p does not need to be set to a constant value but can be obtained in course of simulations solely from the asymptotic properties of the spectral eddy viscosity for $k/k_c \to 0$.

THE USE OF ASYMPTOTIC PROPERTIES OF ENERGY FLUX

The constant b was computed in Domaradzki (2021*a*) using the Germano identity. However, its value can be obtained using solely asymptotic properties of the energy flux in the ultraviolet limit $k/k' \to \infty$. Kraichnan (1959) introduced a scale locality function $\Pi_{uv}(k'|k)$, $k > k'$ that measures the amount of energy flux across k' caused by interactions involving at least one wave number mode with a wave number greater than k. Analytical theories of turbulence consistent with the Kolmogoroff inertial range (Kraichnan (1971*a*,*b*)) produce the scaling result

$$\Pi_{uv}(k'|k) = K(k'/k)^{4/3},\ k \gg k'. \tag{9}$$

where K is a constant. This result was reviewed and reinforced by theoretical analyses of Navier-Stokes solutions by Eyink (2005) and numerical results of Zhou (1993) and Domaradzki *et al.* (2009). The theoretical analysis predicts the scaling exponent but not the constant K. However, if modes from the forcing band and the band adjacent to the mesh cutoff are removed from the analysis of DNS data one observes that $K \approx 1$ in the entire range of wavenumbers, down to $k'/k = 1$, as long as k' is firmly in the inertial range (Domaradzki *et al.* (2009)). Assuming $K = 1$ and $k' = ak$, $a < 1$, Eq. (9) allows to split the energy flux across k' as follows

$$\Pi(k') = a^{4/3}\Pi(k') + \Pi^{res}(k'), \tag{10}$$

where $\Pi^{res}(k')$ is contribution to the energy flux across k' due to interactions with all modes below wave number k. If k is a cutoff wave number in LES, $k = k_c$, the second term is the energy flux across $k' < k_c$ that is resolved using only LES data and is equal to the resolved SGS energy transfer $T^{res}_{SGS}(k')$. Also, in the inertial range the total flux is independent of the wave number and equal to the total SGS energy transfer, i.e., $\Pi(k') = \Pi(k_c) = T_{SGS}(k_c)$. Using this observation Eq. (10) leads to the relation

$$T_{SGS}(k_c) = \frac{1}{1 - a^{4/3}} T^{res}_{SGS}(ak_c), \tag{11}$$

which is equation (5) with $b = a^{4/3}$. Specifically, for $a = 1/2$ the value of $b \approx 0.4$.

Analytical theories of turbulence predict dependence of a spectral eddy viscosity on a wave number, $\nu_{eddy}(k|k_c)$. The present method, however, uses only the value of the eddy viscosity in the infrared limit $k/k_c \to 0$. In that limit the eddy viscosity has a form

$$\nu_{eddy}(0|k_c) = \frac{1}{15}\int_{k_c}^{\infty} \theta_{0qq}\left[5E(q,t) + q\frac{\partial E(q,t)}{\partial q}\right] dq, \tag{12}$$

where θ_{0qq} is a triad interaction time in that limit, where $q > k_c$ (Kraichnan (1976); Lesieur (1997)). Despite differences in definitions of θ for different analytical theories they all lead to essentially same value of $\nu_{eddy}(0|k_c)$ for the inertial range spectrum $E(q,t) \sim q^{-5/3}$. In Domaradzki (2021*b*) $\nu_{eddy}(0|k_c)$ was used to constrain the plateau of the eddy viscosity computed from LES data to $p = 0.37$ of the peak value at the LES cutoff k_c, consistent with the prediction of the EDQNM theory. This is a pointwise constraint in a sense that it is based on the ratio of the eddy viscosity at two points $k = 0$ and $k = k_c$. Since the cusp value at k_c results from local interactions of modes with wave numbers in the vicinity of k_c the parameter p is not strictly dependent only on the asymptotic properties for $k/k_c \to 0$. To retain a dependence of the plateau level only on asymptotic values at $k/k_c \to 0$ we have explored replacing the pointwise constraint by an integral constraint, based on knowledge of the total SGS energy transfer (11). The total transfer $T_{SGS}(k_c)$ allows to define the average constant eddy viscosity for LES with cutoff k_c, $\bar{\nu}_{eddy}(k_c)$, through the relation

$$T_{SGS}(k_c) = -2\bar{\nu}_{eddy}(k_c)\int_0^{k_c} k^2 E(k)dk. \tag{13}$$

The ratio of asymptotic eddy viscosity from the EDQNM theory and the averaged eddy viscosity with the same energy flux is (Lesieur (1997))

$$\frac{\nu_{eddy}(0|k_c)}{\bar{\nu}_{eddy}(k_c)} = \frac{0.441}{(2/3)} = 0.6615. \tag{14}$$

Note that the averaged eddy viscosity is not dependent on any specific analytical theory so the equation (14) allows to determine the plateau value of the eddy viscosity entirely from the integral relation (13) rather than from the ratio of point values. Parameter p refers to eddy viscosity normalized to unity at $k/k_c = 1$, with the normalization factor being the maximum value of the resolved eddy viscosity at the cusp $\nu^{res}_{max} = \nu^{res}_{eddy}(\frac{1}{2}k_c|\frac{1}{2}k_c)$, giving for p

$$p = f_{LES}(0|k_c) = 0.6615\frac{\bar{\nu}_{eddy}(k_c)}{\nu^{res}_{max}}, \tag{15}$$

which is a time-dependent quantity because both $\bar{\nu}_{eddy}$ and ν^{res}_{max} are functions of time.

RESULTS

To test these concepts and the proposed modification of the method we have performed several forced large eddy simulations initialized with $k^{-5/3}$ energy spectrum. Details of the numerical method and parameters in the simulations are

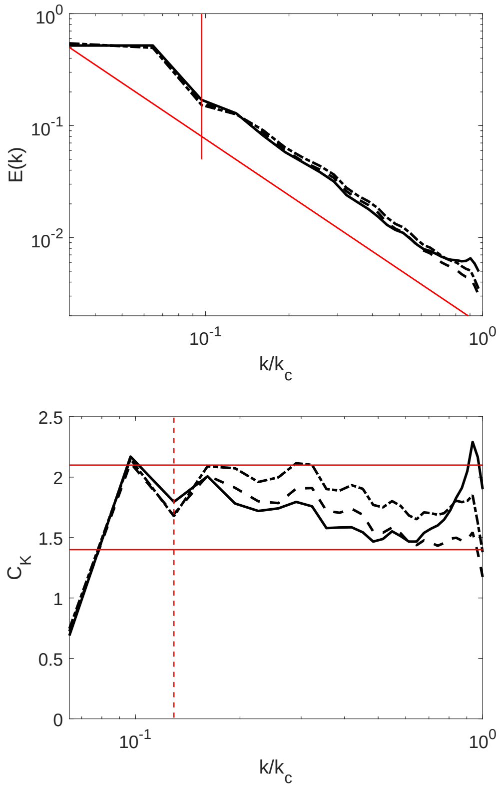

Figure 2. Results for forced LES. Solid line: $k-$independent eddy viscosity, case "ceddy"; broken line: case "pconst" with $p = 0.37$; broken-dotted line: case "pvar" with time dependent p given by Eq. (15). Thin straight lines show, as appropriate, $-5/3$ slope, and a boundary of the forcing band at $k = 3$. For compensated spectra in the bottom figure horizontal lines mark expected range of values for the Kolmogoroff constant.

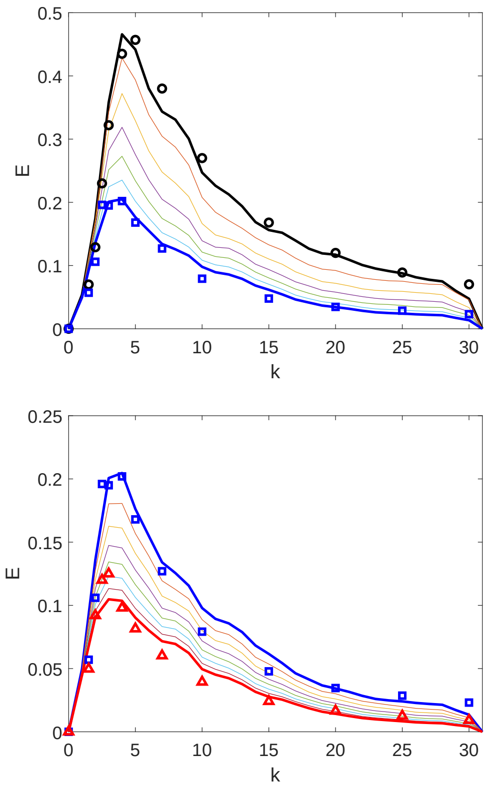

Figure 3. Time evolution of energy spectra in LES for a decaying Comte-Bellot and Corrsin case (symbols show experimental data). Top figure for time interval $U_0t/M = [42, 98]$; run continued in the bottom figure for time interval $U_0t/M = [98, 171]$.

provided in Domaradzki (2021*a*,*b*) for corresponding LES in those papers. Specifically, Reynolds numbers Re_λ exceed 10^4, indicating that the inertial range theory should apply. LESs were run with a resolution of 64^3 modes for 3000 time steps, corresponding to about 15 large eddy turnover times, and results for plotting were averaged over last 1000 time steps. Three implementations of the method were employed. In all cases the parameter $b = 0.4$. Case "ceddy" corresponds to prescribed shape function independent of k, i.e., $f_0(k|k_c) = 1$ (see Domaradzki (2021*a*)). Effectively it is a constant in k eddy viscosity enforcing the integral relation (7). The case "pconst" implements the method with fixed value of parameter $p = 0.37$ (see Domaradzki (2021*b*)). Finally, the case "pvar" implements the method with value of p varying in time according to Eq. (15). One can think of these three cases as a progression in relaxing constraints on the model. Case "ceddy" prescribes probably the simplest form of the spectral eddy viscosity, similar to constant molecular viscosity ν. However, that eddy viscosity is time dependent, with the dependence imposed by enforcing the total SGS energy constraint (7) (or (13)). In cases "pconst" and "pvar" the model shape function f_{LES} is not fully prescribed but partially recovered from the the eddy viscosity obtained from the LES fields. Specifically, the eddy viscosity from LES data in the low wavenumber range is replaced by a constant in k plateau up to point where the plateau intersects the rising cusp in the eddy viscosity curve (Fig. 1). That part of the unmodified cusp is responsible for about 50% of the total SGS transfer. In case "pconst" the plateau value p is constant and is determined by a ratio of pointwise values of theoretical eddy viscosity at $k = 0$ and $k = k_c$. In case "pvar" the plateau value varies in time but depends only on theoretical eddy viscosity at $k = 0$ through formula (15), as a fraction of the averaged, $k-$independent eddy viscosity.

In Fig. 2 we plot energy spectra obtained using all three implementations. In all cases the spectral energy slopes at late times are in an an excellent agreement with $-5/3$ exponent, though the case "ceddy" exhibits slight departure from that form in the vicinity of k_c. The compensated spectra in a form of a k-dependent Kolmogoroff function

$$C_K(k) = \frac{E(k)}{\varepsilon^{2/3} k^{-5/3}}, \tag{16}$$

fall within the expected range $1.4 - 2.1$ outside the forcing wave numbers. However, as the cutoff k_c is approached the case "ceddy" shows a steep increase in C_K. The behaviour of spectra for this case in the vicinity of k_c is consistent with insufficient SGS dissipation in that range. The presence of a cusp at k_c in the eddy viscosity for two other cases (see Fig. 1) increases SGS dissipation in the vicinity of k_c, leading to better agreement with the inertial range form. It is quite clear, however, that all three approaches produce overall similar and acceptable spectral results. This implies that the total SGS transfer constraint (7), being the same for all cases, must play the primary role, while the eddy viscosity wave number distribution plays a secondary role.

In practice, however, enforcing constant value of p (case "pconst") was found to result in most robust LES for several other cases of isotropic turbulence, forced and decaying, at very high as well as at low Reynolds numbers (Domaradzki (2021*b*)). As an example we show in Fig. 3 results of LES with $p = 0.37$ for the classical experimental dataset of Comte-Bellot & Corrsin (1971) (for more details see Domaradzki (2021*b*)). Nevertheless, relaxing extraneous information input by making the parameter p variable through Eq. (15) provides valuable guidance regarding the goal of designing an autonomous LES. We showed that a near autonomous LES procedure is possible, in a sense that beyond actual LES data only two asymptotic results from theory of turbulence are needed: ultraviolet scaling of the energy flux for $k/k_c \to \infty$ and infrared limit of spectral eddy viscosity for $k/k_c \to 0$. It is difficult to anticipate that further limiting this information input could result in acceptable LES methods.

CONCLUSIONS

A previously proposed subgrid-scale modeling procedure of Domaradzki (2021*a*,*b*), based on the interscale energy transfer among resolved scales in LES, has been improved by increasing its reliance on information available directly from known LES fields and minimizing information from theories of turbulence. The original procedure consists of two steps. In the first step, the total unknown SGS transfer across a fixed cutoff wave number k_c is determined using the computed SGS transfer within the resolved range for the cutoff ak_c, $a < 1$, with a set to $\frac{1}{2}$ in this paper. The main parameter in this step is a ratio b of the SGS transfer at test cutoff ak_c due to interactions with scales above the LES cutoff k_c. In the second step a distribution of SGS transfer among resolved wave numbers $k < k_c$ is determined through an eddy viscosity shape function $f(k|k_c)$, normalized to unity at the cutoff k_c. The shape function is obtained directly from a k-dependent eddy viscosity computed using the actual, resolved SGS transfer at the test cutoff ak_c. Such an eddy viscosity is qualitatively similar to the eddy viscosity computed from the analytical theories of turbulence, exhibiting a low wave number plateau and a cusp at ak_c. However, the low wave number plateau level is too small because the resolved SGS transfer is lacking contributions from the nonlocal interactions with modes $k > k_c$. The missing interactions were accounted for by replacing the computed plateau by a k-independent value p, representing a constant asymptotic eddy viscosity acting on large eddies by small eddies in the presence of a spectral gap (here between $(1/2)k_c$ and k_c). For such a hybrid shape function the cusp is attributable primarily to local interactions and its values, greater than the plateau value p, are responsible for about 50% of the total SGS dissipation. This local transfer is not modeled but is a result of the actual interscale interactions operating at a given time step in actual LES. This implementation of the method was very successful in LES of forced, high Reynolds number turbulence, and for decaying turbulence at both high and low Reynolds numbers.

The secondary motivations behind this research was to explore what is minimum information input into LES as compared with DNS for the same physical problem. We postulated a target of fully autonomous LES, defined as a simulation that produces the same quality results within resolved range of scales as DNS, and uses only the same information that is available to DNS. In the previous work we showed that information about the total SGS transfer and the partial dependence of the spectral eddy viscosity on k can be extracted from evolving LES fields, thus moving us in the direction of autonomous LES. The original method, however, requires constants b and p, that are not needed in DNS of the same flows, and thus constitute extraneous information input. The purpose of this paper was to revisit derivations of parameters b and p in order to minimize such extraneous information. In particular, derivation of constant b using the Germano identity requires assumptions about a form of the shape function for the final spectral eddy viscosity. We showed that such assumptions can be entirely avoided because the constant b can be deduced solely from the scaling properties of the energy flux for $k/k_c \to \infty$, without reference to the Germano identity. Similarly, we showed that the plateau value p does not need to be set to a constant value but can be obtained in course of simulations solely from the asymptotic properties of the spectral eddy viscosity in the limit $k/k_c \to 0$. It may be that such asymptotics constitute minimum extraneous information required for well behaved LES of homogeneous, isotropic turbulence, especially for high Reynolds numbers. If that is the case the proposed method can be considered as a near-autonomous LES in a sense that minimizing further extraneous information input is unlikely to be possible.

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