# Near-autonomous large eddy simulations of turbulence based on interscale energy transfer among resolved scales

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A previously developed method for large eddy simulations (LESs), based on spectral eddy viscosity models obtained using analytical theories of turbulence, is reevaluated with a goal of maximizing its dependence on information available directly from actual LES data and minimizing necessary input from theories of turbulence. The method computes the subgrid scale (SGS) energy transfer among resolved scales and its wave number distribution from the evolving LES velocity fields. This information is supplemented by asymptotic properties of the energy flux in the inertial range leading to the form of a spectral eddy viscosity that allows self-contained simulations without use of extraneous SGS models. The method is tested in LESs of isotropic turbulence at high Reynolds number where the inertial range dynamics is expected and is observed in LESs using the proposed method.

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## I. INTRODUCTION

Analytical theories of isotropic turbulence as originated by Kraichnan's direct interaction approximation [1] provide closure expressions for the energy transfer term $T(k)$ in the spectral kinetic energy equation in terms of the energy spectrum $E(k)$. A modern, exhaustive review of analytical theories of turbulence and closures has been recently provided by Zhou [2]. Kraichnan [3] employed such closure expressions to compute the subgrid-scale (SGS) energy transfer $T_{\mathrm{SGS}}(k|k_c)$ from a range of resolved scales $k \leqslant k_c$ caused by nonlinear interactions involving SGSs $k > k_c$, where $k_c$ is a cutoff wave number of a sharp spectral filter. The SGS energy transfer, when normalized by $2k^2E(k)$, gives a spectral eddy viscosity $\nu_{\mathrm{eddy}}(k|k_c)$. 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 [3] used a particular analytical theory, the test field model, while Chollet and Lesieur [4] used another formulation, the eddy damped quasinormal Markovian (EDQNM) approximation, 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 (LESs) of Navier-Stokes equations (see Refs. [5,6]). 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 SGSs ($k > k_c$), and the eddy viscosity is a derived quantity. This is different from a more common approach to first postulate 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

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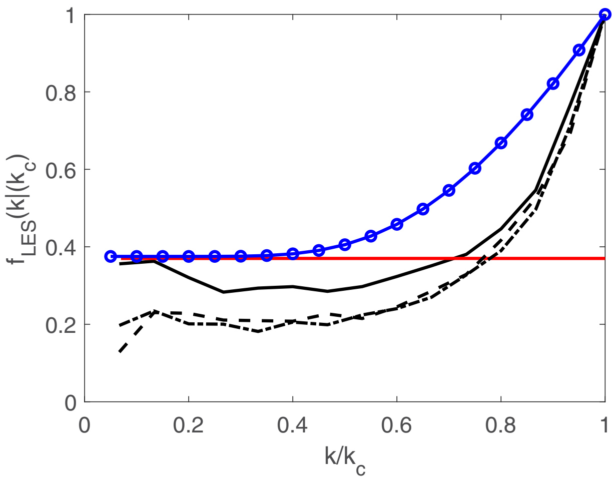



FIG. 1. Spectral eddy viscosity shape functions. Solid line with symbols ○: Analytical theory of turbulence (EDQNM); horizontal solid line: Asymptotic plateau value from the EDQNM theory; shape functions computed from LES data for cases ceddy (solid line), pconst (broken line), pvar1 (broken-dotted line).

directly available for a given flow. A method to compute the SGS energy transfer as well as its wave number distribution from direct numerical simulations (DNSs) of isotropic turbulence fields has been introduced by Domaradzki *et al.* [7]. Subsequently, the method was extended and used in numerous investigations as a diagnostic tool to elucidate and understand physics of nonlinear interactions acting in isotropic and wall bounded turbulent flows, simulated using DNS and LES methods. Attempts were made to explore the potential of the method beyond its diagnostic capability as a modeling tool for actual LESs in recent work by Domaradzki [8,9]. In those papers, it was shown how the detailed SGS energy transfer among resolved scales obtained directly from the evolving LESs velocity fields can be used as a self-contained SGS model. Specifically, the SGS energy transfer among resolved scales and its wave number distribution is computed from LES fields at each time step and cast in the form of a spectral eddy viscosity. Such a computed eddy viscosity is then modified to make it consistent with two known asymptotic properties of energy flux in the inertial range and used in the eddy viscosity term added to the Navier-Stokes spectral solver as a SGS modeling term. Note that in this approach, SGS modeling is accomplished without need for explicit expressions of the analytical theories or any other classical SGS models. Effectively, the procedure allows self-contained LESs without use of extraneous SGS models or, equivalently, at each time step the model is obtained from a simulated field itself and asymptotic properties of the energy flux in the inertial range.

In Ref. [9] we also introduced a concept of fully autonomous LES, defined as a simulation that produces the same quality statistical results as DNS within resolved range of scales, and uses only the same information that is available to DNS. We showed in Ref. [9] that information about the total SGS transfer and the partial dependence of the spectral eddy viscosity on $k$ can be extracted from evolving LESs fields, thus moving us in the direction of autonomous LESs. Specifically, the method formulated in Ref. [9] requires values of two constants ($b$ and $p$, defined in the next section). Their values are determined from the asymptotics of the inertial range dynamics and while required in LESs, they are not needed in DNS of the same flows. In this paper we explore how reliance of the model on information already encoded in the resolved LES fields can be further increased or, equivalently, if extraneous information input can be further limited. Specifically, we demonstrate that information about scaling of the energy flux in the ultraviolet limit $k/k_c \to \infty$ provides value of the constant $b$ and is sufficient to design the method for accurate LESs of inertial range dynamics. We argue that this constitutes the minimum extraneous, quantitative information required for such a purpose, resulting in the near-autonomous LES method in a sense that further reduction of extraneous information input is unlikely to be possible.

## II. DESCRIPTION OF THE METHOD

Details of the method and of the numerical code are described in Refs. [8,9]. In this section we summarize main features of the method for the purpose of self-contained exposition of the procedure.

The spectral LES energy equation for scales $k \leqslant k_c$ is obtained by first defining energy transfer $T^<(k|k_c)$ among resolved modes, where the notation signifies that only modes satisfying the inequality $k \leqslant k_c$, 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 $k \leqslant k_c$ as follows:

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

where the SGS energy transfer term is

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

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

Following Ref. [3], the SGS spectral energy equation can be formally rewritten as

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

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

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

Frequently, the eddy viscosity is nondimensionalized using values of the energy spectrum at the cutoff:

$$\nu^+_{\mathrm{eddy}}(k|k_c) = \frac{\nu_{\mathrm{eddy}}(k|k_c)}{\sqrt{E(k_c)/k_c}}. \tag{5}$$

Assuming infinite inertial range spectrum $k^{-5/3}$, theoretical formulas for $T_{\mathrm{SGS}}(k|k_c)$ can be computed numerically [3–5] and the normalized eddy viscosity Eq. (5) is well fitted by the expression given by Chollet [10],

$$\nu^+_{\mathrm{eddy}}(k|k_c) = C_K{}^{-3/2}(0.441 + 15.2e^{-3.03k_c/k}) \equiv C_K{}^{-3/2} f_1(k|k_c), \tag{6}$$

where $C_K$ is the Kolmogorov constant, taken usually as 1.4, and $f_1$ is a spectral model shape function dependent only on $k/k_c$. As stressed previously, 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 SGSs ($k > k_c$).

It must be recognized that deriving the deceptively simple analytical formula Eq. (6) required immense theoretical effort spanning several decades. It started with development of analytical theories of turbulence by Kraichnan [1], Orszag [11], and many others quoted in the monograph by Lesieur [5]. These theoretical developments occurred largely before the advent of large-scale numerical simulations but were later employed to propose SGS models appropriate for LESs by Kraichnan [3], culminating in the analytical formula Eq. (6) derived by Lesieur and Chollet [4,10]. Analytical theories of turbulence predict dependence of the spectral eddy viscosity $\nu_{\mathrm{eddy}}(k|k_c)$ on all scales, $0 < k < k_c$. However, in the present paper, only the value of the eddy viscosity in the infrared limit $k/k_c \to 0$, corresponding to the horizontal line in Fig. 1 will be needed. Its form is

$$\nu_{\text{eddy}}(0|k_c) = \frac{1}{15}\int_{k_c}^{\infty} \theta_{0qq}\left[5E(q,t) + q\frac{\partial E(q,t)}{\partial q}\right]dq, \tag{7}$$

where $\theta_{0qq}$ is a triad interaction time in that limit, where $q > k_c$ ([3,5]). For example, the EDQNM approximation gives

$$\theta_{0qq} = \frac{1 - \exp(-[\mu_{0qq} + 2\nu q^2]t)}{\mu_{0qq} + 2\nu q^2}, \tag{8}$$

where

$$\mu_{0qq} = 2a_1\left[\int_0^q p^2 E(p,t)dp\right]^{1/2} \tag{9}$$

is the eddy damping rate in that limit. The expression Eq. (9) was proposed by Pouquet *et al.* [12] and the constant $a_1$ was related to the Kolmogoroff constant, $a_1 = 0.218C_K^{3/2}$, by André and Lesieur [13].

It was shown by Domaradzki [8] that the task of modeling $T_{\text{SGS}}(k|k_c)$ can be approached differently, with limited reliance on the analytical theories. That approach splits the task of modeling $T_{\text{SGS}}(k|k_c)$ 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 Ref. [8] using the Germano identity [14], which is a relation between transfers at two different cutoffs, here $k_c$ and $\frac{1}{2}k_c$:

$$T_{\text{SGS}}\left(\frac{1}{2}k_c\right) - \int_0^{\frac{1}{2}k_c} dk T_{\text{SGS}}(k|k_c) = T_{\text{SGS}}^{\text{res}}\left(\frac{1}{2}k_c\right). \tag{10}$$

$T_{\text{SGS}}^{\text{res}}(\frac{1}{2}k_c)$ is the total SGS transfer across $(1/2)k_c$ computed using resolved LES scales $k < k_c$. For the infinite inertial range, energy flux across the spectrum is constant, allowing us to replace the first term in Eq. (10) by $T_{\text{SGS}}(k_c)$, but the second term requires knowledge of the SGS transfer distribution in wave number $k$. In modeling practice, this information is obtained by postulating a SGS model and then using formula Eq. (10) as a constraint to compute model constants. It is also possible to obtain this information from analyses of DNS data, though only for a limited range of Reynolds numbers. As shown in Refs. [8,9], these approaches allow us to express the second term as a fraction of the total transfer $T_{\text{SGS}}(k_c)$, i.e., $bT_{\text{SGS}}(k_c)$, where $b$ could vary between zero and 0.4, depending on the distribution of SGS transfer in $k$, leading to the relation

$$T_{\text{SGS}}(k_c) = \frac{1}{1-b}T_{\text{SGS}}^{\text{res}}\left(\frac{1}{2}k_c\right). \tag{11}$$

A wave-number distribution of the resolved SGS energy transfer $T_{\text{SGS}}^{\text{res}}(k|\frac{1}{2}k_c)$ can be computed from LES data during an actual run and cast in the form of the $k$-dependent eddy viscosity Eq. (4), which is normalized to unity:

$$f_{\text{LES}}^{\text{res}}\left(k\middle|\frac{1}{2}k_c\right) = \frac{\nu_{\text{eddy}}^{\text{res}}\left(k\middle|\frac{1}{2}k_c\right)}{\nu_{\text{eddy}}^{\text{res}}\left(\frac{1}{2}k_c\middle|\frac{1}{2}k_c\right)}. \tag{12}$$

Subsequentl, 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 $0 \leqslant k/k_{\text{cutoff}} \leqslant 1$. 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 $f_{\text{LES}}(k|k_c)$ comprises a constant plateau up to an intersection with a cusp of the resolved shape function $f^{\text{res}}_{\text{LES}}(k|k_c)$, followed by the unmodified cusp section 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 computed from instantaneous LES data and has a form

$$\nu_{\text{eddy}}(k|k_c) = C_m f_{\text{LES}}(k|k_c), \tag{13}$$

where $C_m$ is a model constant and $f_{\text{LES}}(k|k_c)$ 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

$$T_{\text{SGS}}(k_c) = \int_0^{k_c} dk T_{\text{SGS}}(k|k_c) = -\int_0^{k_c} dk\ \nu_{\text{eddy}}(k|k_c) 2k^2 E(k), \tag{14}$$

which gives

$$C_m = \frac{-T_{\text{SGS}}(k_c)}{\int_0^{k_c} f_{\text{LES}}(k|k_c) 2k^2 E(k) dk}. \tag{15}$$

In LES runs, the eddy viscosity Eq, (13) 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 Eq. (15), $T_{\text{SGS}}(k_c)$ is expressed in terms of SGS transfer among resolved scales $T^{\text{res}}_{\text{SGS}}(\frac{1}{2}k_c)$, Eq. (11), computed at each time step in LES with the spectral eddy viscosity given by Eq. (13). Similarly, the shape function $f_{\text{LES}}(k|k_c)$ is computed at each time step from the resolved SGS energy transfer $T^{\text{res}}_{\text{SGS}}(k|\frac{1}{2}k_c)$, i.e., both factors in the formula Eq. (13) are computed from information available in LES. In effect, the SGS model is not prescribed but obtained from the resolved SGS energy transfer $T^{\text{res}}_{\text{SGS}}(k|\frac{1}{2}k_c)$ in a given LES and well-established properties of the energy flux for the inertial range in the asymptotic limits. Note also that since $T^{\text{res}}_{\text{SGS}}(k|\frac{1}{2}k_c)$ and $E(k)$, in general, are time dependent, both factors in Eq. (13) are also functions of time, $C_m(t)$ and $f_{\text{LES}}(k, t|k_c)$.

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 $k/k_c \to 0$ or the mean value of the resolved eddy viscosity.

## III. THE USE OF ASYMPTOTIC PROPERTIES OF ENERGY FLUX

The constant $b$ was computed in Ref. [8] using the Germano identity Eq. (10). It must be noted that the Germano identity does not provide information about physics of the SGS energy transfer but only a relation between transfers at two different cutoffs, here $k_c$ and $\frac{1}{2}k_c$. In particular, the second term in Eq. (10) requires knowledge of the SGS transfer distribution in wave number $k$, which requires postulating a SGS model. However, we show below that the value of $b$ for the infinite inertial range can be obtained without postulating a specific SGS model, using solely asymptotic properties of the energy flux in the ultraviolet limit $k/k' \to \infty$.

Kraichnan [1] introduced an ultraviolet 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 produce the scaling result [15,16]

$$\Pi_{uv}(k'|k) = K(k'/k)^{4/3}\Pi(k'),\ \ k \gg k', \tag{16}$$

where $\Pi(k')$ is the total energy flux across $k'$ and $K$ is a constant. This result was reviewed and reinforced by theoretical analyses of Navier-Stokes solutions by Eyink [17] and numerical results of

Zhou [18] and Domaradzki *et al.* [19]. 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 wave numbers, down to $k'/k = 1$, as long as $k'$ is firmly in the inertial range (see Ref. [19]). Assuming $K = 1$ and $k' = ak,\ a < 1$, Eq. (16) allows us to split the energy flux across $k'$ as follows:

$$\Pi(k') = \Pi_{uv}(k'|k) + \Pi^{\text{res}}(k') = a^{4/3}\Pi(k') + \Pi^{\text{res}}(k'), \tag{17}$$

where $\Pi^{\text{res}}(k')$ 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 $T^{\text{res}}_{\text{SGS}}(k')$. Also, in the inertial range the total flux is independent of the wave number and equal to the total SGS energy transfer, i.e., $\Pi(k') = \Pi(k_c) = T_{\text{SGS}}(k_c)$. Using this observation, Eq. (17) leads to the relation

$$T_{\text{SGS}}(k_c) = \frac{1}{1 - a^{4/3}} T^{\text{res}}_{\text{SGS}}(ak_c), \tag{18}$$

which is Eq. (11) with $b = a^{4/3}$. Specifically, for $a = 1/2$ the value of $b \approx 0.4$.

As discussed previously, the analytical theories of turbulence predict dependence of the spectral eddy viscosity on a wave number, $\nu_{\text{eddy}}(k|k_c)$, but the method discussed here requires 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 given by Eq. (7). Despite differences in definitions of $\theta$ for different analytical theories, they all lead to essentially the same value of $\nu_{\text{eddy}}(0|k_c)$ for the inertial range spectrum $E(q,t) \sim q^{-5/3}$. In Ref. [9], $\nu_{\text{eddy}}(0|k_c)$ 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 dependent solely on the asymptotic properties for $k/k_c \to 0$. To restrict the dependence of the plateau level only on asymptotic values at $k/k_c \to 0$, we will explore replacing the pointwise constraint by an integral constraint, based on knowledge of the total SGS energy transfer Eq. (18). The total transfer $T_{\text{SGS}}(k_c)$ allows us to define the average constant eddy viscosity for LES through the relation

$$T_{\text{SGS}}(k_c) = -2\bar{\nu}_{\text{eddy}} \int_0^{k_c} k^2 E(k)dk. \tag{19}$$

The ratio of asymptotic eddy viscosity from the EDQNM theory and the averaged eddy viscosity with the same energy flux is [5]

$$\frac{\nu_{\text{eddy}}(0|k_c)}{\bar{\nu}_{\text{eddy}}} = \frac{0.441}{(2/3)} = 0.6615. \tag{20}$$

Note that the averaged eddy viscosity is not dependent on any specific analytical theory, so Eq. (20) allows us to determine the plateau value of the eddy viscosity entirely from the integral relation Eq. (19) rather than from the ratio of point values. Using Eq. (18),

$$\bar{\nu}_{\text{eddy}} = \frac{1}{1 - a^{4/3}} \bar{\nu}^{\text{res}}_{\text{eddy}}, \tag{21}$$

where $\bar{\nu}^{\text{res}}_{\text{eddy}}$ refers to the resolved average eddy viscosity:

$$\bar{\nu}^{\text{res}}_{\text{eddy}} = C_m \bar{f}^{\text{res}}_{\text{LES}} = C_m \frac{\int_0^{k_c} f^{\text{res}}_{\text{LES}}(k|k_c) k^2 E(k)dk}{\int_0^{k_c} k^2 E(k)dk}. \tag{22}$$

Using these formulas, the plateau value $p$ is set to

$$p = f_{\mathrm{LES}}(0|k_c) = 0.6615 \frac{1}{1 - a^{4/3}} \bar{f}_{\mathrm{LES}}^{\mathrm{res}}. \tag{23}$$

Note that $p$ is a time-dependent quantity because $\bar{f}_{\mathrm{LES}}^{\mathrm{res}}$ is a function of time.

Finally, we will also consider the value of $p$ that does not depend on the asymptotic value of the eddy viscosity Eq. (7) at all. Such a possibility is suggested by results discussed in Ref. [8]. In that paper, LESs were performed with the fixed value of $b = 0.4$ and a prescribed analytical shape function $f_2$ that approximates the theoretical shape function $f_1$ of Chollet and Lesieur [4]:

$$f_1(k|k_c) \approx C_2(D_2 + (k/k_c)^4) \equiv C_2 f_2(k|k_c), \text{ where } C_2 = 0.8 \text{ and } D_2 = 0.55. \tag{24}$$

The plateau level for $D_2 = 0.55$ is $p = 0.35$, close to the value $p = 0.37$ of Chollet and Lesieur [4]. To investigate dependence of the predictions on the plateau level, the constant $D_2$ was increased and then decreased by a factor of 2, resulting in values of $p = 0.52$ and $p = 0.22$, respectively. Spectral results for all three cases were close to each other though some deterioration was observed for $p = 0.22$ in the vicinity of $k_c$. However, the agreement between cases $p = 0.52$ and the benchmark case with the theoretical shape function was excellent, even with minor improvements in the vicinity of $k_c$ (see Fig. 4 in Ref. [8]). We concluded that spectral predictions are not very sensitive to the exact plateau level (within a factor of 2 of the theoretical value) as long as the total SGS transfer is enforced through the appropriate value of constant $b$. Such mild dependence of the simulations on the plateau level suggests that rather than using condition Eq. (23), derived from the asymptotics of transfer in the limit $k/k_c \to 0$, one may try using a simpler expression, namely, the average value of the resolved shape function given in Eq. (22) :

$$p = f_{\mathrm{LES}}(0|k_c) = \bar{f}_{\mathrm{LES}}^{\mathrm{res}}. \tag{25}$$

Note that for $a = 1/2$ the prefactor multiplying $\bar{f}_{\mathrm{LES}}^{\mathrm{res}}$ on the right-hand side of Eq. (23) is equal to 1.10, i.e., in that case, expressions Eqs. (23) and (25) are quite similar. The main advantage of Eq. (25) is that the plateau level is determined entirely by the average value of the resolved shape function without a reference to the asymptotic value required in Eq. (20) and thus without any reference to quantitative results of the analytical theories.

## IV. RESULTS

To test these concepts and the proposed modification of the method, we have performed several forced LESs initialized with the $k^{-5/3}$ energy spectrum as well as a pulse type initial condition where $E(k) = 0$ for $k > 4$. Details of the numerical method and parameters in the simulations are provided in Refs. [8,9] for corresponding LESs in those papers. The flow is assumed to be contained in a cube of side $L = 2\pi$ and periodic boundary conditions in all three spatial directions are imposed on the independent variables. The domain is discretized in physical space using $N$ uniformly spaced grid points in each direction resulting in a mesh size $\Delta x = L/N$ and a total of $N^3$ grid points. The independent variables are transformed between physical and spectral space using the discrete Fourier transform

$$\mathbf{u}(\mathbf{k}) = \frac{1}{N^3} \sum_{\mathbf{x}} \mathbf{u}(\mathbf{x}) \exp(-i\mathbf{k} \cdot \mathbf{x}) \tag{26}$$

and the inverse transform

$$\mathbf{u}(\mathbf{x}) = \sum_{\mathbf{k}} \mathbf{u}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x}), \tag{27}$$

where $\mathbf{x}$ are the mesh points in physical space and $\mathbf{k}$ are the discrete wave numbers with components $k_i = \pm n_i \Delta k,\ n_i = 0,\ 1,\ 2,\ \ldots\ N/2,\ i = 1,\ 2,\ 3,$ and $\Delta k = 2\pi/L = 1$. The LES equations are solved using a pseudospectral numerical method of Rogallo [20] in the implementation of Yeung and Pope [21]. We use the forcing scheme of Sullivan *et al.* [22] in which the sum of squared amplitudes of velocity modes in a sphere of prescribed radius $K_f = 3$ is kept constant in time. This is accomplished by multiplying all modes in the forced sphere by the same constant factor at the end of each time step to restore the energy in the sphere to the value at the beginning of the time step.

Note that the test cases were selected to be consistent with the physics of the inertial range. Specifically, Reynolds numbers $\mathrm{Re}_\lambda$ exceed $10^4$, indicating that the inertial range theory should apply. Because of that, model assumptions are satisfied and LESs should recover assumed features of the inertial range dynamics if the modeling procedure is correct. In what follows, we show that, indeed, the method maintains (or develops) the inertial range spectrum with a correct value of the Kolmogoroff constant outside the forcing wave number band.

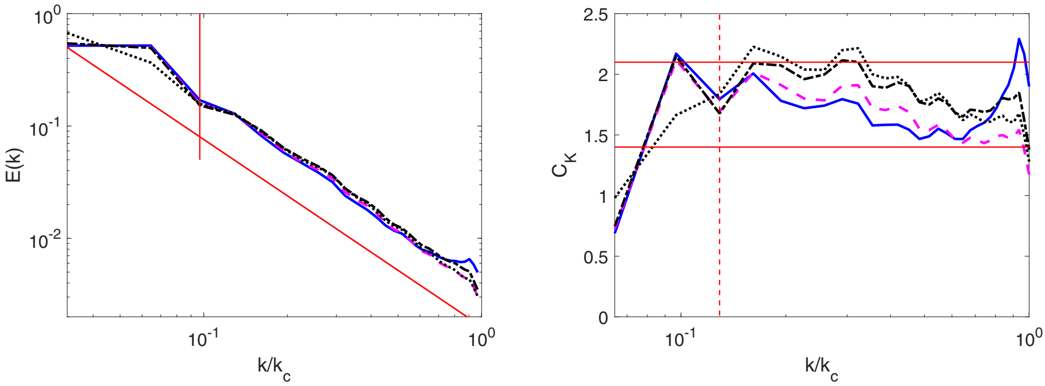
LESs were run with a resolution of $64^3$ modes for 3000 time steps, corresponding to about 15 large eddy turnover times, and results for plotting were averaged over the last 1000 time steps. In the majority of cases, the test cutoff was $(1/2)k_c$ and the corresponding value of parameter $b = 0.4$. To demonstrate generality of the relation Eq. (18), we also considered an additional case corresponding to the test cutoff $(1/4)k_c$ with $b = (1/4)^{4/3} \approx 0.16$. Four implementations of the method were employed. Case ceddy corresponds to the prescribed shape function independent of $k$, i.e., $f_0(k|k_c) = 1$ (see Ref. [8]). Effectively, it is a constant in $k$ eddy viscosity enforcing the integral relation Eq. (14), i.e., the averaged eddy viscosity $\bar{\nu}_{\mathrm{eddy}}$ in Eq. (19) for $T_{\mathrm{SGS}}(k_c)$ given by Eq. (11). The case pconst implements the method with a fixed value of parameter $p = 0.37$ (see Ref. [9]). Finally, the cases pvar1 and pvar2 implement the method with value of $p$ varying in time according to Eq. (23) or (25), respectively. One can think of these four 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 $\nu$; however, that eddy viscosity is time dependent, with the dependence imposed by enforcing the total SGS energy constraint Eq. (14) (or (19)). In cases pconst, pvar1, and pvar2, the model shape function $f_{\mathrm{LES}}$ is not fully prescribed but partially recovered from the eddy viscosity obtained from the LES fields. Specifically, the eddy viscosity from LES data in the low wave-number range is replaced by a constant in $k$ plateau up to the 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 the case of pconst, the plateau value $p$ is constant in $k$ and is determined by a ratio of pointwise values of theoretical eddy viscosity at $k = 0$ and $k = k_c$. In case, pvar1, the plateau value varies in time but depends only on theoretical eddy viscosity at $k = 0$ through formula Eq. (23), as a fraction of the averaged, $k-$independent eddy viscosity. Finally, in case pvar2, dependence on the eddy viscosity limit at $k = 0$ is relaxed by setting the plateau value to the averaged eddy viscosity Eq. (19).

In Fig. 2, we plot energy spectra obtained using all four implementations and initialized with the $k^{-5/3}$ function with no prefactors. Note that cases ceddy and pconst were already considered and discussed in previous papers [8,9]. In all cases, the spectral energy slopes at late times are in an excellent agreement with the $-5/3$ 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

$$C_K(k) = \frac{E(k)}{\varepsilon^{2/3} k^{-5/3}} \tag{28}$$

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 behavior 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 the other cases increases SGS dissipation in the vicinity of $k_c$, leading to better agreement with the inertial range form (see Fig. 1).

Simulations were repeated with a pulse initial condition, i.e., setting $E(k) = 0$ for $k > 4$. In Fig. 3, we plot the energy spectra and the compensated spectra only for LESs performed for modeling approaches pvar1 and pvar2 (results for cases ceddy and pconst are available in Ref. [8],

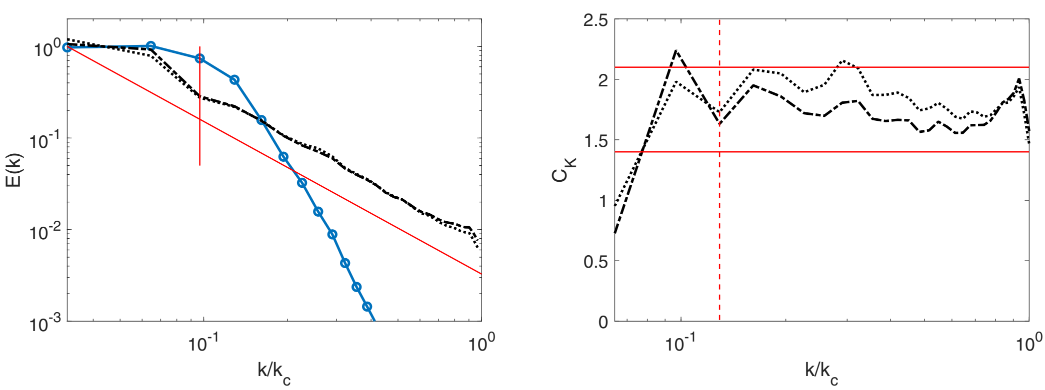



(a) Energy spectra (b) Compensated energy spectra

FIG. 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 pvar1 with time dependent $p$ given by Eq. (23); dotted line: Case pvar2 with time dependent $p$ given by Eq. (25). Thin straight lines show, as appropriate, $-5/3$ slope, and a boundary of the forcing band at $k = 3$. For compensated spectra, the horizontal lines mark expected range of values for the Kolmogoroff constant. (a) Energy spectra. (b) Compensated energy spectra.

Fig. 8, and in Ref. [9], Fig. 2, respectively). The evolution of the energy spectrum from the pulse initial condition towards the inertial range $k^{-5/3}$ form is completed within few large eddy turnover times as shown in Fig. 4 for case pvar1.

In all cases above, the test cutoff $(1/2)k_c$ was used and the corresponding value of the parameter $b = 0.4$. In principle, any test cutoff $ak_c$ with $a < 1$ could be chosen in relation Eq. (18). However, there are practical limitations on choices of $a$ imposed by numerics. For instance, discrete numerical mesh size $\Delta x$ and maximum wave number $k_c$ in spectral codes, most often given as an integer power of 2, make successive doubling of mesh size, or halving $k_c$, the most convenient choice, implying values of $a = 1/2,\ 1/4,\ 1/8, ....$ The finite numerical resolution also prevents very small values of $a$ because it would limit number of modes contributing to resolved energy transfer $T^{\rm res}_{\rm SGS}(k|ak_c)$




(a) Energy spectra (b) Compensated energy spectra

FIG. 3. Results for forced LES with the pulse initial condition. Solid line with symbols: The energy spectrum evolved for 50 time steps corresponding to 0.3 of the large eddy turnover time; broken-dotted line: Case pvar1 with time dependent $p$ given by Eq. (23); dotted line: Case pvar2 with time dependent $p$ given by Eq. (25). Various straight lines are described in the caption to Fig. 2. (a) Energy spectra. (b) Compensated energy spectra.

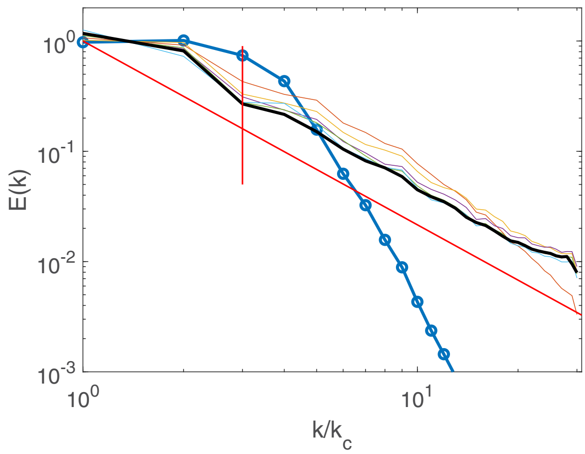
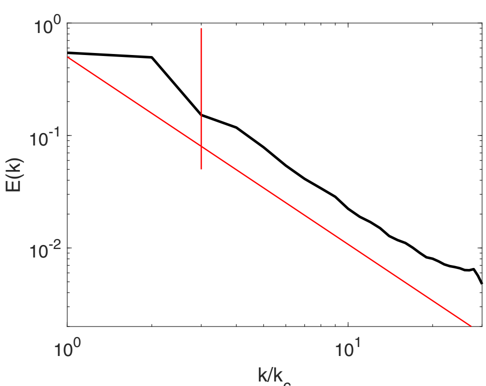
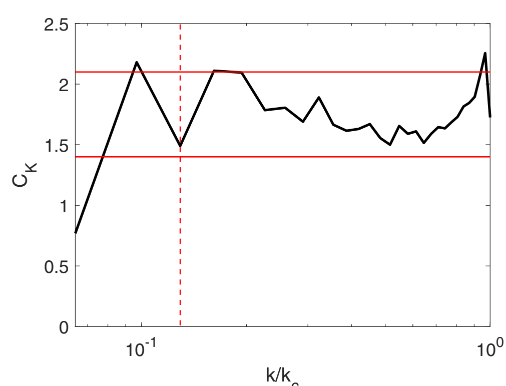



FIG. 4. Time evolution of the energy spectrum from the pulse type initial condition for 1000 time steps (about six large turnover times). Solid line with symbols: The energy spectrum evolved after 50 time steps, corresponding to 0.3 of the large eddy turnover time; thin solid lines plotted at time intervals equal about 1.25 the large eddy turnover time; solid black line: The energy spectrum averaged over the last three data sets.

and/or would put the test cutoff $ak_c$ too close to the forcing band. For a specific spectral code and the numerical resolution of $64^3$ modes used in this paper, these numerical restrictions come into play already for $a = 1/8$ because the test cutoff $(1/8)k_c = 4$ is just outside the forcing band boundary $K_f = 3$. Because of that the only reasonable choices available in the current work are $a = 1/2$ and $a = 1/4$. In Fig. 5, we show results of LES performed using the modeling procedure for the test cutoff $(1/4)k_c = 8$ and corresponding value of $b = 0.16$. The plateau value of the eddy viscosity is computed using formula Eq. (25), i.e., as an average value of the resolved shape function without any reference to the analytical theories results. The spectral results are in a good agreement with LES results obtained for the test cutoff $(1/2)k_c$, except for the immediate vicinity of $k_c$ where the method appears slightly under dissipative for the test cutoff $(1/4)k_c$. More detailed comparison of eddy viscosities in these two cases revealed that contributions to the energy flux from the forcing




(a) Energy spectrum




(b) Compensated energy spectrum

FIG. 5. Results for forced LES case pvar2 with time dependent $p$ given by Eq. (25) and test cutoff $(1/4)k_c$ with $b = 0.16$. Various straight lines are described in the caption to Fig. 2. (a) Energy spectra. (b) Compensated energy spectra.

band across the test cutoff are larger for the $(1/4)k_c$ case. This is expected because the wave number $(1/4)k_c = 8$ is much closer to the forcing band boundary $K_f = 3$ than the wave number $(1/2)k_c = 16$. Because of that, the plateau level computed using averaging Eq. (25), also involving the forcing band wave numbers, is somewhat larger than for the $(1/2)k_c$ case, reducing the relative importance of the cusp in the eddy viscosity at $k_c$. We thus attribute differences in spectral predictions for these two cases to a larger influence of the forcing band on the $(1/4)k_c$ case. Another way of looking at this is to note that the results for the $(1/4)k_c$ case tend toward results for the case with a constant in $k$ eddy viscosity in Fig. 2, i.e., the elevated plateau level with respect to the cusp enhances contribution of the plateau to the SGS energy transfer but diminishes contribution of the cusp, leading to decreased SGS dissipation near $k_c$.

It is quite clear that all distinct approaches discussed above produce overall similar and acceptable spectral results for two different initial conditions considered. This suggests that the total SGS transfer constraint Eq. (14), 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 ([9]). Nevertheless, the purpose of the present investigation was not to find the best overall method but to assess the feasibility of an autonomous LES where the SGS model is recovered from LES data in course of simulations. While the fully autonomous LES appears unlikely, relaxing extraneous information input by making the parameter $p$ variable through Eqs. (23) and (25) brings us close to that goal. 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 in case pvar1: Ultraviolet scaling of the energy flux for $k/k_c \to \infty$ and infrared limit of spectral eddy viscosity for $k/k_c \to 0$. The latter condition is further relaxed in case pvar2, leaving the energy flux scaling as a sole quantitative condition required for modeling. It is difficult to anticipate that further limiting this information input could be possible.

## V. CONCLUSIONS

A previously proposed SGS modeling procedure of Domaradzki [8,9], based on the interscale energy transfer among resolved scales in LES, has been modified 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 $\frac{1}{2}$ and $\frac{1}{4}$ in this paper. The main parameter in this step is a ratio $b$ of the SGS transfer at the test cutoff $ak_c$ due to nonlinear interactions with at least one wave number above $k_c$. In the second step, a distribution of SGS transfer among resolved wave numbers $k < k_c$ is determined through an eddy viscosity shape function $f_{\mathrm{LES}}(k|k_c)$, 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 $ak_c$ 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 [9].

The main motivation behind the current 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 a 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 $p$ 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 in time value but can be obtained in course of simulations solely from the asymptotic properties of the spectral eddy viscosity in the limit $k/k_c \to 0$ or from the mean value of the resolved eddy viscosity. It may be that such assumptions constitute minimum, quantitative extraneous information required for well-behaved LESs of homogeneous, isotropic turbulence, especially for high Reynolds numbers. If that is the case, the proposed method can be considered a near-autonomous LES in a sense that minimizing further extraneous information input is unlikely to be possible.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