AUTONOMOUS LARGE EDDY SIMULATIONS OF TURBULENCE USING EDDY VISCOSITY DERIVED FROM THE SUBGRID SCALE SIMILARITY STRESS TENSOR

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ABSTRACT

A method for large eddy simulations (LES), inspired by spectral eddy viscosity models, is developed and implemented in the physical space representation. The method estimates the subgrid scale (SGS) energy transfer using a similarity-type model expression for the SGS tensor obtained using Gaussian filtering. Following steps for the spectral space representation, the SGS transfer in the physical space is used to obtain a spatially varying eddy viscosity at each time step in LES. The method is autonomous in a sense that the functional form of the eddy viscosity is not postulated but is extracted at each time step from the LES data without any adjustable constants. The method is tested in LES of isotropic turbulence at high Reynolds numbers where the inertial range dynamics is expected and for lower Reynolds number decaying turbulence under conditions of the classical Comte-Bellot and Corrsin experiments. In both cases the agreement with reference data is very good and the SGS transfer computed for the proposed eddy viscosity model is highly correlated with the transfer computed for the similarity-type stress tensor.

INTRODUCTION

Traditional SGS models fall into three general categories: eddy viscosity models, similarity models and so-called mixed models which combine eddy viscosity and similarity expressions. Eddy viscosity models originated in work of Smagorinsky (1963) and similarity models in work of Bardina *et al.* (1983). Initially, the Bardina model attracted a lot of interest because of the simplicity of the expression for the SGS stress tensor and its behavior in *a priori* tests. Bardina *et al.* (1983) demonstrated that the similarity model predictions were highly correlated with the actual SGS quantities, with correlation coefficients significantly larger than for the Smagorinsky model, and that it was able to predict the reverse energy transfer, the so-called backscatter, which is common in turbulence. However, Bardina *et al.* (1983), as well as many others later, observed that the model in its proposed form was not sufficiently dissipative in *a posteriori* tests. This usually leads to similarity-type models failing in actual LES, especially when the viscous dissipation is small.

The purpose of this work is to show that while the similarity-type models are not suitable for use directly in LES, they contain sufficient information for designing an autonomous, dissipative, eddy viscosity model. The eddy viscosity developed here is autonomous in a sense that its functional form is not postulated but is obtained from a simulated LES fields itself at each time step in simulations. Additionally, because the eddy viscosity is derived from the similarity model expression, the respective SGS dissipations are highly correlated.

The proposed procedure is guided by the recent work that developed an autonomous eddy viscosity model in spectral space based on the physics of interscale energy transfer among resolved scales (Domaradzki (2021*a*,*b*, 2022)). The general idea has been originated by Kraichnan (1976) who used analytical theories of turbulence for SGS modeling. A good overview of analytical theories of turbulence and their use in modeling can be found in Lesieur (1997); Lesieur *et al.* (2005), and in Zhou (2021). Compared with traditional SGS models that are based on more-or-less phenomenological arguments to develop functional forms of the modeling expressions, the distinguishing feature of the spectral SGS models is that the primary quantity used in modeling is the subgrid-scale energy transfer $T_{SGS}(k|k_c)$. The notation $T_{SGS}(k|k_c)$ indicates the energy transfer 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 unknown SGS term in LES equations for the cutoff k_c is modeled through an eddy viscosity expression $-\nu_{eddy}(k|k_c)k^2 u_n(\mathbf{k})$, linear in the velocity $u_n(\mathbf{k})$ in the spectral representation. The form of the eddy viscosity itself is derived from the computed SGS energy transfer for the range of resolved wave numbers $k < k_c$ as

$$\nu_{eddy}(k|k_c) = -\frac{T_{SGS}(k|k_c)}{2k^2 E(k)} \tag{1}$$

where $E(k)$ is the energy spectrum. Thus the main advantage of such an approach to SGS modeling is that, if the SGS energy transfer $T_{SGS}(k|k_c)$ is known, there is no need to postulate the functional form of the eddy viscosity because it can be obtained directly from Eq. (1). In the original approach of Kraichnan (1976) $T_{SGS}(k|k_c)$ is computed from the underlying turbulence theory. In Domaradzki (2021*a*,*b*, 2022) the SGS energy transfer $T_{SGS}(k|k_c)$ is computed from LES fields and two known asymptotic properties of energy flux in the inertial range. 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 asymptotic properties of the energy flux in the inertial range. The method has been tested in LES of isotropic turbulence at high Reynolds numbers and at lower Reynolds numbers decaying turbulence under conditions of the classical Comte-Bellot & Corrsin (1971) experiments. In both cases the agreement with reference data was excellent, providing numerical justification for the proposed approach.

THE GOVERNING EQUATIONS

The main goal of this work is to extend the methodology to the physical space representation which is most widely used in LES practice where various finite difference/volume codes are used. The procedure seeks an expression for the eddy viscosity in the physical space $\nu_{eddy}(\mathbf{x},t)$ that is appropriate for advancing in time the LES velocity field $\mathbf{u}(\mathbf{x},t)$. In our notation $\mathbf{u}(\mathbf{x},t)$ is the complete velocity field projected on the LES mesh (or, in spectral space, truncated to wavenumbers $k < k_c$), while $\overline{\mathbf{u}}(\mathbf{x})$ denotes the complete velocity first filtered using a graded filter and then projected on the LES mesh. Note that sometimes an explicit notation for projection (or spectral truncation), may be useful, e.g., $\mathbf{u}^<(\mathbf{x},t) \equiv \mathbf{u}(\mathbf{x},t)$, $\overline{\mathbf{u}}^<(\mathbf{x}) \equiv \overline{\mathbf{u}}(\mathbf{x})$. In particular, LES equations for spectrally truncated LES velocity are

$$\frac{\partial}{\partial t}u_i + \frac{\partial}{\partial x_j}u_i\,u_j = -\frac{\partial}{\partial x_i}p + \nu\frac{\partial^2}{\partial x_j \partial x_j}u_i - \frac{\partial}{\partial x_j}\tau_{ij} \qquad (2)$$

where $u_i = (u_1,u_2,u_3) = (u,v,w)$, p, and ν are the velocity, pressure, and the kinematic viscosity, respectively, and τ_{ij} is the SGS stress tensor which is based on the complete velocity, i.e., $\mathbf{u}^{com}(\mathbf{x},t) = \mathbf{u}^<(\mathbf{x},t) + \mathbf{u}^>(\mathbf{x},t)$, where $\mathbf{u}^>(\mathbf{x},t)$ is an explicit notation for subgrid scales. With such an explicit notation

$$\tau_{ij} = \left(u_i^{com}u_j^{com}\right)^< - \left(u_i^< u_j^<\right)^< \qquad (3)$$

When a spatial filtering procedure is used, e.g., Gaussian or top-hat filters, indicated by the overbar, the LES equations for filtered and truncated fields $\overline{\mathbf{u}}^<(\mathbf{x}) \equiv \overline{\mathbf{u}}(\mathbf{x})$ are

$$\frac{\partial}{\partial t}\overline{u}_i + \frac{\partial}{\partial x_j}\overline{u}_i\,\overline{u}_j = -\frac{\partial}{\partial x_i}\overline{p} + \nu\frac{\partial^2}{\partial x_j \partial x_j}\overline{u}_i - \frac{\partial}{\partial x_j}\tau_{ij}^{full} \qquad (4)$$

where the full SGS stress is written explicitly as

$$\tau_{ij}^{full} = (\overline{u_i^{com}u_j^{com}})^< - (\overline{u}_i^< \,\overline{u}_j^<)^< \qquad (5)$$

The full SGS stress tensor can be split into two components, $\tau_{ij}^{full} = \tau_{ij}^{res} + \tau_{ij}^{phy}$ (see, e.g., Domaradzki *et al.* (2002)). The resolved SGS stress tensor

$$\tau_{ij}^{res} = (\overline{u_i^< u_j^<})^< - (\overline{u}_i^< \,\overline{u}_j^<)^< = \overline{u_i u_j} - \overline{u}_i\,\overline{u}_j \qquad (6)$$

is a SGS similarity-like stress, computed using only the velocity projected on the LES mesh $\mathbf{u}(\mathbf{x})^<$. The second equality in (6) indicates that the superscripts $<$ may be ignored in the notation if only LES resolution is considered. The remaining term τ_{ij}^{phy} has a form

$$\tau_{ij}^{phy} = (\overline{u_i^< u_j^>})^< + (\overline{u_i^> u_j^<})^< + (\overline{u_i^> u_j^>})^< \qquad (7)$$

which accounts for the physics of the nonlinear interactions that involve unknown subgrid scales $\mathbf{u}(\mathbf{x})^>$. Note that the above decomposition clarifies approximations involved in the similarity modeling. Indeed, the similarity modeling for filtered LES equations (4) is equivalent to approximating the full SGS stress (5) by the resolved SGS stress (6) and entirely ignoring the component (7) that involves true subgrid scales $\mathbf{u}(\mathbf{x})^>$, not resolved on the LES mesh. To be more precise, the original SGS similarity stress in Bardina *et al.* (1983) is written as

$$\tau_{ij}^{sim} = \overline{\overline{u}_i\overline{u}_j} - \overline{\overline{u}}_i\,\overline{\overline{u}}_j \qquad (8)$$

and the form (6) is used in the deconvolution models where the velocity $\mathbf{u}^<(\mathbf{x}) \equiv \mathbf{u}(\mathbf{x})$ is obtained by an inversion (exact, or approximate) of the spatial filtering operation in definition of $\overline{\mathbf{u}}^<(\mathbf{x}) \equiv \overline{\mathbf{u}}(\mathbf{x})$ (see Domaradzki *et al.* (2002)).

The SGS energy transfer associated with the full SGS stress tensor (5) in filtered LES equations (4) is

$$\varepsilon_{SGS}(\mathbf{x}) = \tau_{ij}^{full}(\mathbf{x})\overline{S}_{ij}(\mathbf{x}) \qquad (9)$$

where $\overline{S}_{ij}$ is the resolved rate-of-strain tensor for filtered velocity $\overline{\mathbf{u}}^<(\mathbf{x})$

$$\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) \qquad (10)$$

The contribution to the total SGS dissipation provided by the resolved SGS stress in the physical space representation is

$$\varepsilon_{SGS}^{res}(\mathbf{x}) = \tau_{ij}^{res}(\mathbf{x})\overline{S}_{ij}(\mathbf{x}). \qquad (11)$$

Note that if LES are performed with only resolved SGS stress retained in (4), in general they will fail because they lack information contained in τ_{ij}^{phy} about dynamically important actual subgrid scales for modes with $k > k_c$. This deficiency leads to insufficient SGS dissipation in actual LES performed with such pure similarity/deconvolution models.

THE MODELING PROCEDURE

The procedure seeks an expression for the eddy viscosity in the physical space $\nu_{eddy}(\mathbf{x},t)$ that is appropriate for advancing in time the unknown LES velocity field $\mathbf{u}^<(\mathbf{x},t)$ using LES Eqs. (2). Note that the equations and the unknown velocity in the procedure are the same for the spectral and the physical space method. The eddy viscosity model for the SGS stress tensor in Eq. (2) is

$$\tau_{ij} = -2\nu_{eddy}(\mathbf{x})S_{ij}(\mathbf{x}) \tag{12}$$

where S_{ij} is the rate of strain tensor for unfiltered LES velocity $\mathbf{u}(\mathbf{x})^<$. Note that (12) ignores the usual term with the trace of the SGS stress because the procedure uses only energy equations where that term does not contribute.

The corresponding eddy viscosity closure model for the resolved SGS stress tensor (6) for Eq. (4) is

$$\tau_{ij}^{mod} = -2\nu_{eddy}^{mod}(\mathbf{x})\overline{S}_{ij}(\mathbf{x}) \tag{13}$$

where $\overline{S}_{ij}$ is the resolved rate-of-strain tensor given by Eq. (10). Eq. (13) implies a formal relation for $\nu_{eddy}(\mathbf{x})$ that involves computed resolved SGS transfer

$$\varepsilon_{SGS}^{res}(\mathbf{x}) = \tau_{ij}^{mod}(\mathbf{x})\overline{S}_{ij}(\mathbf{x}) = -2\nu_{eddy}^{mod}(\mathbf{x})\overline{S}_{ij}(\mathbf{x})\overline{S}_{ij}(\mathbf{x}) \tag{14}$$

It is well known that a naive application of this formula on a pointwise basis

$$\nu_{eddy}^{mod}(\mathbf{x}) = -\frac{\varepsilon_{SGS}^{res}(\mathbf{x})}{2\left(\overline{S}_{ij}(\mathbf{x})\right)^2} \tag{15}$$

will cause numerical instabilities when implemented in actual LES. This is because the SGS dissipation $\varepsilon_{SGS}^{res}(\mathbf{x})$, Eq. (11), contains negative and positive regions and the computed eddy viscosity will contain negative values that may become a source of instabilities. The key observation from the spectral procedure is that in computing the eddy viscosity the SGS transfer averaged over shells is used. While different types of averaging in the physical space can be considered, a simple filtering, the same as applied to derive Eq. (4), was found to be sufficient, and the eddy viscosity is rewritten as

$$\nu_{eddy}(\mathbf{x}) = -\frac{\overline{\varepsilon}_{SGS}^{res}(\mathbf{x})}{2\overline{S}_{ij}^2(\mathbf{x})}. \tag{16}$$

Formally, the above eddy viscosity expression is appropriate for the LES equations for filtered velocity $\overline{\mathbf{u}}^<(\mathbf{x})$ with the SGS stress tensor (5) approximated by the resolved SGS stress (6). An important observation from the spectral procedure was that the eddy viscosity is computed first for the spectrally filtered field, e.g., $k < \frac{1}{2}k_c$, and subsequently, it is rescaled and applied in simulations to the full LES field, $k < k_c$. We follow this sequence of steps in the physical space as well. The eddy viscosity is computed first for the filtered field, signified by the resolved rate of strain in the denominator in (16), but the eddy viscosity computed through (16) is then applied in LES to the full, unfiltered LES field u_i, i.e., the SGS stress tensor is modeled through Eq. (12) and used to solve LES equations (2). A simple, physical interpretation is that for two similar fields, here $\overline{u}_i$ and u_i, the eddy viscosities should be similar, here assumed to be the same.

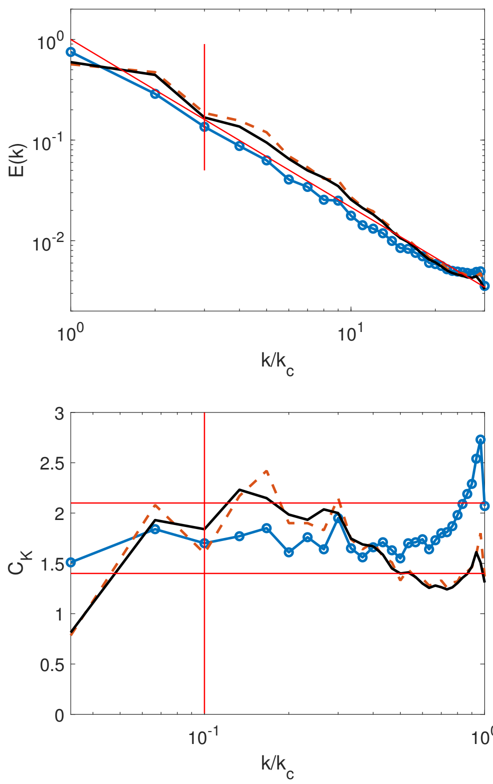

Figure 1. Results for forced LESs initialized with the inertial range spectral form. Lines with symbols ∘: initial conditions; broken line: spectrum after $N_t = 2000$ time steps (around 10 large eddy turnover times); solid line: spectrum averaged over last 1000 steps. In this and all subsequent figures thin straight lines show, as appropriate, $-5/3$ slope, and a boundary of the forcing band at $k = 3$. For compensated spectra (lower panel) horizontal lines mark expected range of values for the Kolmogoroff constant.

RESULTS

The proposed SGS model for LES in the physical space representation requires specification of a graded filter, indicated by an overbar in the previous sections. In this work the filtering operation in Cartesian coordinates for an arbitrary function $f(x,y,z)$ is given by the formula

$$\overline{f}(x,y,z) = \int G(x,x')G(y,y')G(z,z')f(x',y',z')dx'dy'dz' \tag{17}$$

which is a tensor product of 1-D Gaussian filters. The 1-D filter kernel G has an explicit form (see Pope (2000))

$$G(x,x') = \sqrt{\frac{6}{\pi\Delta^2}}\exp\left(-\frac{6|x-x'|^2}{\Delta^2}\right) \tag{18}$$

where the filter width was set to $\Delta = 2\Delta x$, where Δx is a mesh size, the same in each Cartesian direction.

To test the proposed implementation of the method in the physical space we have repeated LES for several forced and decaying isotropic turbulence cases simulated previously using the spectral implementation of the method (Domaradzki, 2021*a*,*b*, 2022) with the resolution of 64^3 mesh points. Steady

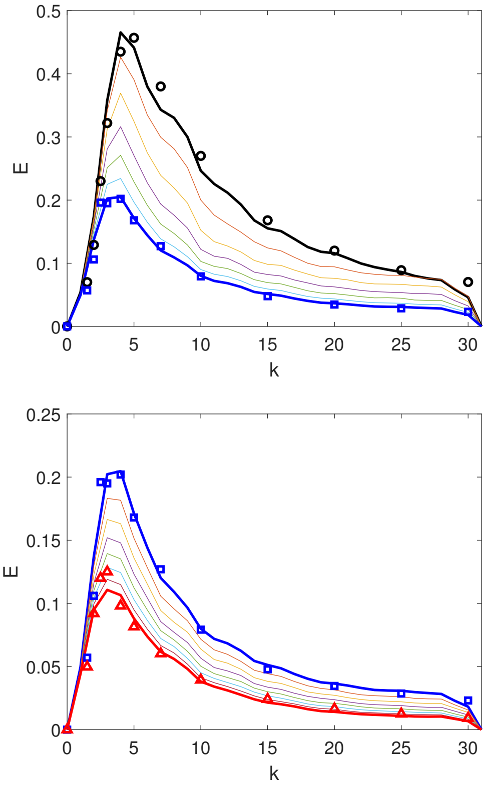

Figure 2. Time evolution of energy spectra in an autonomous LES run. Upper panel: for time interval $U_0t/M = [42,98]$; lower panel: run continued for time interval $U_0t/M = [98,171]$. Experimental results: circles, $U_0t/M = 42$; squares, $U_0t/M = 98$; triangles, $U_0t/M = 171$.

state test cases were selected to be consistent with the physics of the inertial range. Specifically, Reynolds numbers Re_λ exceed 10^4, indicating that the inertial range theory should apply. Because of that, if the modeling procedure is correct, LES should recover known features of the inertial range dynamics. In Fig. 1 we plot energy spectra obtained in simulations initialized with the $k^{-5/3}$ function with no prefactors. The spectral energy slopes at late times are in a good agreement with the $-5/3$ exponent, with minor departures in the vicinity of the LES cutoff k_c. Also, the compensated spectra in a form of a k-dependent Kolmogoroff function

$$C_K(k) = \frac{E(k)}{\varepsilon^{2/3}k^{-5/3}}, \tag{19}$$

fall within the expected range $1.4-2.1$ outside the forcing wave numbers. For testing the spectral method at lower Reynolds number in Domaradzki (2021*b*), decaying turbulence results of the classical experiments of Comte-Bellot & Corrsin (1971) were used. We repeated LES for the same test case using the current physical space method. Time evolution of the energy spectra in LES obtained using the physical space procedure is shown in Fig. 2 and can be compared with corresponding results for the spectral procedure (shown in Fig. 7 in Domaradzki (2021*b*)). Time evolution of the energy spectrum is predicted quite well for both time intervals $U_0t/M = [42,98]$ and $U_0t/M = [98,171]$.

As has been noted the fundamental quantity in the method development in the physical space is the resolved SGS dissipation $\varepsilon^{res}_{SGS}(\mathbf{x})$ (Eq. (11)). The resolved SGS stress tensor τ^{res}_{ij}, Eq. (6), can be considered as a generalized similarity model in a sense that it is computed using the velocity $\mathbf{u}(\mathbf{x})^<$ with the same spectral support as used for LES equations, i.e., no true subgrid scales with $k > k_c$ enter into its computation. Alternatively, it can be considered as a deconvolution model, in a sense that the velocity $\mathbf{u}(\mathbf{x})^<$ can be recovered from the filtered velocity $\overline{\mathbf{u}}(\mathbf{x})^<$ by inversion of the filtering operation, which for a Gaussian filter can be performed exactly. The SGS stress tensor for similarity or deconvolution models is known to be highly correlated with the exact SGS stress computed from full velocity data containing subgrid scales $k > k_c$ (Liu *et al.*, 1994; Meneveau & Katz, 2000). Despite that, similarity and exact deconvolution models fail in actual LES because they cannot maintain adequate SGS energy dissipation as simulation time progresses. On the other hand, eddy viscosity based models show very low correlations with exact SGS quantities but perform well in actual LES because of their good dissipative properties. Contrary to such common observations, for the method proposed here we find very high correlations between the eddy viscosity results and the results obtained with the similarity model. Specifically, in Fig. 3 we plot SGS energy transfer for both models. Note that forward transfer is signified by negative values, i.e., acting as an energy sink in the LES dynamics, and backscatter is signified by positive values, i.e., acting as an energy source in the dynamics. Visual inspection of color plots indicates that the energy transfer for both cases appears quite correlated. The computed correlation coefficient for these planar data is 0.81. We have also computed a correlation coefficient for the full 3-D data, getting values also in excess of 0.8. Note these are much higher values than the value around 0.4 found for the standard Smagorinsky model. High correlations are not surprising because the eddy viscosity is derived from the SGS dissipation of the similarity model. Yet the presence of backscatter for the SGS dissipation of the eddy viscosity model is surprising, as it is commonly believed that it would lead to unstable simulations. Despite that, none of the cases simulated with this approach showed any hints of instability. The analysis of the computed fields showed that the total forward energy transfer was at least an order magnitude greater than the backscatter. We suspect that its overall dominance in the total energy transfer may explain why relatively small negative values of eddy viscosity, fluctuating in space and time, do not lead to catastrophic instabilities. It must be noted that above conclusions were reached for graded filters, here specifically for the Gaussian filter. Correlations between the actual SGS stresses and similarity-type stresses computed using sharp spectral filters are known to be significantly smaller (Liu *et al.*, 1994). Also, for sharp spectral filtering the forward and inverse SGS transfers are of the same order of magnitude, with the magnitude of the net forward transfer being much smaller than each individual forward/inverse component as shown in, e.g., Piomelli *et al.* (1991) and Domaradzki *et al.* (1993).

CONCLUSIONS

A previously proposed subgrid-scale modeling procedure based on the interscale energy transfer among resolved scales in LES, described for the spectral space implementation in Domaradzki (2021*a*,*b*, 2022), has been extended to the physical space representation. As the fundamental quantity the method employs the SGS energy transfer computed using a similarity-type model expression for the SGS tensor obtained using filtered velocity fields advanced in the simulations. The computed eddy viscosity is then employed to model the SGS stress

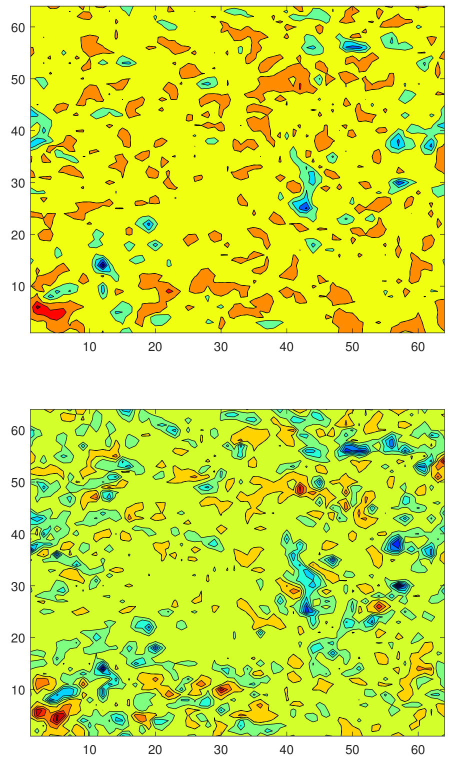

Figure 3. SGS energy transfer in a cross-sectional plane. Upper panel: for the similarity model (Eqs. (6) and (11)); lower panel: for the eddy viscosity model (Eqs. (12) and(16)). Positive values are signified by red and orange colors, and negative values by yellow, green, and blue.

tensor in the familiar Boussinesq form for use in LES. The method is autonomous in a sense that the form of the eddy viscosity (16) is not postulated but is extracted from the LES data without any adjustable constants. However, the method is unlikely to be universal because it is expected that it must depend on the filter type and the filter width. This should be contrasted with the spectral method utilizing the sharp spectral filter where all model constants can be determined uniquely from the LES data and the analytical theories of turbulence (Domaradzki, 2021*a*,*b*, 2022). In this work a graded filter was chosen as a tensor product of 1-D Gaussian filters applied in each Cartesian direction. The method was tested in LES of isotropic turbulence at high Reynolds numbers where the inertial range dynamics is expected and for lower Reynolds number decaying turbulence under conditions of the classical Comte-Bellot and Corrsin experiments. For both flows the agreement with reference data is very good and the SGS transfer computed for the proposed eddy viscosity model is highly correlated with the transfer computed for the similarity stress tensor.

In summary, the current procedure, based on the SGS energy transfer of the similarity model, can produce the eddy viscosity expressions in the physical space representation that are not only as globally dissipative as standard eddy viscosity models, but also that they predict modeled SGS dissipation which approximates the SGS dissipation of the similarity model well and is highly correlated with it.

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