Multi-scale modeling of subgrid-scale stresses in the large-eddy simulation

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This paper presents a multi-scale approach to the modeling of subgrid-scale (SGS) stresses in turbulent flows. An expression is derived that couples the SGS fluctuations to the resolved field with a dynamically-determined constant. From this expression the SGS stress may be computed. The approach is investigated in detail for isotropic decaying turbulence. A numerical *a priori* comparison of the method in predicting the eddy viscosity exhibits good agreement with direct numerical simulations. In particular, the method appears to perform well even when the energy-containing eddies are in the SGS part of the spectrum.

1. Motivation and objectives

The purpose of this work is to assess how well one may treat a SGS turbulent field as a *heterogeneous medium*, and to derive the Large-Eddy Simulation (LES) equations based on averaging methods (see, e.g., Bensoussan *et al.* 1978). Such methods are successful for flows in porous media (see, e.g., Farmer 2002), where the heterogeneous medium (e.g., sand) does not change in time. The objectives of LES modeling and upscaling in porous media are the same: we seek an approximation to the original equations of fluid motion that can be solved with fewer computing resources. Both approaches obtain their respective approximations by filtering out small scales. The key distinction between these approaches is in the modeling. In porous media theories the structure of the small scales is modeled, and the corresponding effect of the modeled scales on the larger scales is deduced using a multi-scale analysis. In contrast, in turbulence modeling for LES it is often the case that it is the *effect* of the small scales on the larger scales that is modeled via the SGS stress, and the structure of the subgrid scale field is usually not considered.

Modeling of the subgrid stress in LES is often based on the universality assumption about the inertial range of turbulent flows (Kolmogorov 1941). This assumption requires the restriction that the subgrid scales cannot be too large, i.e., that the energy containing eddies should not be filtered out. Multi-scale methods do not need to make this restriction. Their use in deriving less computationally expensive models of turbulence is not new, but they have not received much attention. Debussche *et al.* (1993) used a Fourier decomposition to derive approximate equations for motion below a dynamically-determined large-scale/small-scale cutoff wavenumber in their non-linear Galerkin method. In a variational multi-scale method (Hughes *et al.* 2000) two-scale formulation is developed where eddy-viscosity type modeling is confined to the equation of smaller-scale evolution only. A coherent vortex simulation method (Farge *et al.* 1999) and a stochastic coherent adaptive large eddy simulation method (Goldstein and Vasilyev 2004) use wavelet decomposition. Periodic averaging for scale-separated flows was performed in Frisch (1995); Sivashinsky (1985); Sivashinsky and Frenkel (1992); Sivashinsky and Yakhot (1985); among others. A

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multi-scale derivation of the k-epsilon model can be found in Mohammadi and Pironneau (1994).

A multi-scale formulation LES was proposed, and its effectiveness was verified, in a previous report (Novikov and Bodony 2005). The method is based on multi-scale asymptotics (Novikov and Papanicolaou 2001), which was rigorously verified for two-dimensional flows (Novikov 2003, 2004). This formulation, however, relied on the assumption that the SGS flow be given *a priori*. Thus, the relevance of the proposed approach to turbulence modeling is dependent on its ability to replicate the behavior of the unresolved stress on the resolved LES field without prescribing the subgrid field. As a first step in this direction, we develop here an LES model based on a multi-scale asymptotic analysis, which requires as input only the second-order statistics, i.e., the energy spectrum, of the SGS field.

The numerical experiments in this work utilize three ingredients: DNS data, another set subgrid velocity fields obtained by phase-randomization of the DNS data, and a modification of the multi-scale algorithm from Novikov and Bodony (2005), all of which are described below. Following an outline of the multi-scale algorithm, predictions of the eddy viscosity are compared with the corresponding values from the dynamic Smagorinsky model (Germano *et al.* 1991) and from the Eddy-Damped Quasi-Normal Markovian (EDQNM) model (Chollet and Lesieur 1991).

2. Background and notation

2.1. *DNS field*

For the *a priori* tests and in evaluating the model, we use a numerical database of isotropic turbulence. The turbulent velocity $v(x,t)$, $v, x \in \mathbb{R}^3$ was obtained from direct numerical simulations (DNS) of decaying isotropic turbulence on a periodic cube $\Omega = [0, 2\pi]^3$. The DNS code used a (dealiased) Fourier-spectral representation in space and a second-order accurate Runge-Kutta method in time. Viscous effects were implemented as an integrating factor and the non-linear terms were computed in the physical domain. The simulations were run by specifying an initial three-dimensional energy spectrum and arranging the individual velocity Fourier coefficients to be divergence free and of random phase. This initial condition was then forced with a space-time random forcing at low wavenumber until a steady state was reached. The forcing was then removed and the turbulence allowed to decay.

2.2. *Phase randomization*

Given a realization $v(x,t)$ corresponding to decaying isotropic turbulence, a phase randomized realization at fixed t is constructed as follows. A *randomized DNS field* v' is constructed from v by setting

$$|\widehat{v'_k}| = |\widehat{v_k}|, \; k = (k_1, k_2, k_3), \tag{2.1}$$

and choosing the direction of $\widehat{v'_k}$ at random with the constraint that v' is incompressible, i.e., $\widehat{v'_k} \cdot k = 0$. Note that v' will have the same second-order statistics as v, but is devoid of the spatial structure of v.

2.3. *Scale decomposition*

Consider the turbulent velocity $u(x,t)$ of an incompressible fluid and decompose it into a large-scale part U associated with the resolved portion of an LES field, and the subgrid, small-scale part v

$$u = U + v. \tag{2.2}$$

This decomposition is affected by applying a sharp spectral filter at the wavenumber k_0. That is, if G is such a sharp spectral filter, then

$$U = \langle u \rangle = \int_\Omega G(x - y) u(y)\, \mathrm{d}y \tag{2.3}$$

and $v = u - U$.

2.4. *Standard LES modeling*

The main question of LES modeling stems from the stresses due to large-scale–small-scale interactions and from the dependence of these stresses on the resolved field. The LES velocity $U(x,t)$ satisfies

$$\frac{\partial}{\partial t} U + U \cdot \nabla U + \nabla \cdot \tau = \frac{1}{Re} \Delta U - \nabla P, \tag{2.4}$$

where the subgrid stress τ is

$$\tau_{ij} = \langle U_j v_i + v_j U_i + v_j v_i \rangle, \tag{2.5}$$

and the brackets $\langle \cdot \rangle$ denote averaging, via the sharp spectral filter, of the subgrid scales. The subgrid stress cannot be determined by U, and, therefore, it must be modeled.

The standard Smagorinsky model (Smagorinsky 1963) and its dynamic variation (Germano *et al.* 1991) model τ_{ij} as

$$\tau_{ij} = -2\nu_T S_{ij},\ S_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right),\ |S| = \sqrt{2 S_{ij} S_{ij}}, \tag{2.6}$$

where in the dynamic Smagorinsky model the constant ν_T can be found from the DNS data u (2.2) via

$$\nu_T = \frac{1}{2} \frac{\int_\Omega L_{ij} M_{ij} dx}{\int_\Omega M_{ij} M_{ij} dx},\ M_{ij} = |S| S_{ij},\ L_{ij} = \langle u_i u_j \rangle - \langle U_i U_j \rangle. \tag{2.7}$$

For a given wavenumber n, the ratio of the subgrid stresses relative to viscous stresses is

$$\nu_{dns}(n) = \frac{1}{n} \frac{\sum_{|k|=n} \sqrt{\hat{L}_{ij}(k) \hat{L}_{ij}(k)}}{\sum_{|k|=n} \sqrt{\hat{S}_{ij}(k) \hat{S}_{ij}(k)}}. \tag{2.8}$$

The normalizing constant $1/n$ in the previous formula provides eddy-viscosity scaling of the relative stress: if $\nabla \cdot \tau_{ij}$ is proportional to $\nabla \cdot S_{ij}$, then $\nu_s(n)$ is a constant. For the dynamic Smagorinksy model, the relative stress may be expressed as

$$\nu_s(n) = \frac{\nu_T}{n} \frac{\sum_{|k|=n} \sqrt{\hat{M}_{ij}(k) \hat{M}_{ij}(k)}}{\sum_{|k|=n} \sqrt{\hat{S}_{ij}(k) \hat{S}_{ij}(k)}}. \tag{2.9}$$

For the EDQNM model (Chollet and Lesieur 1991), one may compute the relative stress as

$$\nu_{cl}(n) = C\left(0.441 + 15.2 \exp(-3.03 k_0/n)\right), \tag{2.10}$$

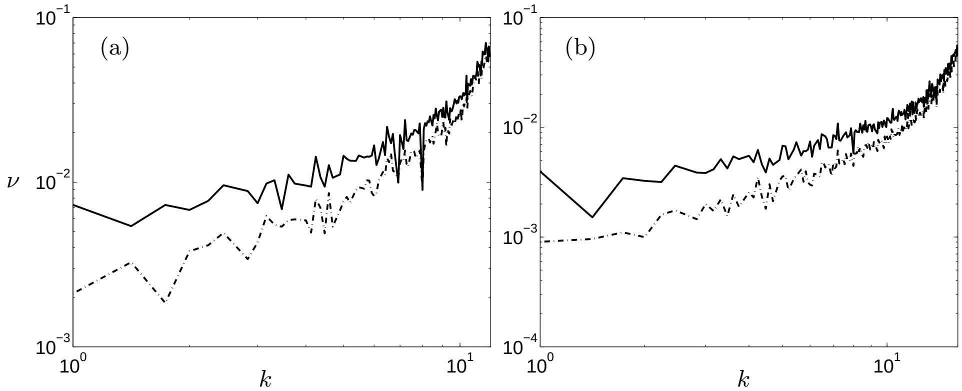

FIGURE 1. Randomized DNS field underestimates subgrid stresses (a) $k_0 = 12$, (b) $k_0 = 16$. Legend: ——, $\nu_{\rm dns}$, −−, $\nu'_{\rm dns}$.

where k_0 is the subgrid cutoff and the normalizing constant C, is computed dynamically (as in Eq. (2.7)) so that the following equality holds

$$\frac{1}{2\pi}\sum_{n\leq k_0}\left(\nu_{cl}(n)n^2\sum_{|k|=n}\hat{S}_{ij}(k)\hat{S}_{ij}(k)\right)=\int_\Omega L_{ij}S_{ij}dx.$$

2.5. *Eddy viscosity dependence on the structure of turbulence*

A natural question here is how significantly the subgrid scales depend on the cutoff wavenumber k_0, which defines the large and small scales. Let us compare the relative stresses ν_{dns} and ν'_{dns} computed directly using Eq. (2.8) for DNS and randomized DNS velocity fields, respectively. In Fig. 1 we plot ν_{dns} and ν'_{dns} for two cutoff numbers $k_0 = 12$, $k_0 = 16$ and the DNS velocity with maximum of the energy at $k = 2$. When randomized DNS velocity field is used, it significantly under-predicts the stresses at small wavenumbers, implying that the underlying structure of the turbulence is important.

3. The multi-scale algorithm

The main observation of the multi-scale algorithm (Novikov and Bodony 2005) is that if v is the subgrid scale field, then its effect on the LES-scale field U is the same as the effect of another subgrid scale field

$$u' = Re\,\Delta^{-1}\mathbb{P}\left(U\cdot\nabla v + v\cdot\nabla U\right), \tag{3.1}$$

where $\mathbb{P}$ is the projection onto a divergence free vector field (see Constantin and Foias (1988)) defined as

$$\mathbb{P}(v) = v - \nabla\cdot\Delta^{-1}(\nabla v),$$

Δ^{-1} is the inverse of the Laplace operator, and Re is the Reynolds number.

The derivation of Eq. (3.1) is based on the assumption that the effective properties of U in the presence of the subgrid scales v can be determined by investigation of the equation for a perturbation of U. Further assumption that the subgrid flow can be accurately found from a quasi-static approximation (Debussche *et al.* 1993) leads to (3.1).

The motivation for the computation of the subgrid stress in Novikov and Bodony (2005) came from the assumption of separation of scales (see, e.g., Frisch (1995); Novikov and

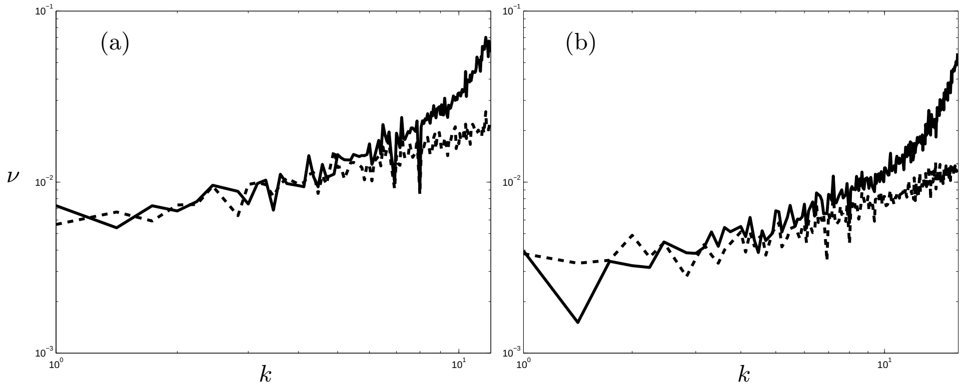

FIGURE 2. Multi-scale method (Novikov and Bodony 2005) performance for two different cutoff wavenumbers. (a) $k_0 = 12$, (b) $k_0 = 16$. Legend: ——, $\nu_{\rm dns}$; – –, ν computed using the multi-scale algorithm.

Papanicolaou (2001); Sivashinsky (1985); Sivashinsky and Frenkel (1992); Sivashinsky and Yakhot (1985)). The scale separation implies that the cross stresses may be neglected

$$\langle U_i v_j + U_j v_i \rangle \sim 0, \tag{3.2}$$

and that the full subgrid stresses may be approximated by the SGS Reynolds stress

$$\langle u_i u_j \rangle - \langle U_i U_j \rangle \sim \langle v_i v_j \rangle \sim \langle u'_j v_i + v_j u'_i \rangle.$$

Since the analysis was based on separation of scales, the subgrid stresses computed by the multi-scale method are in good agreement with DNS data for small wavenumbers, where the scale separation assumption holds, while exhibiting poor performance at higher wavenumbers (Fig. 2).

In previous work (Novikov and Bodony 2005) we used the assumption of scale separation to conclude that the cross stress was negligible (see Eq. (3.2)). If there is no scale separation, this is not accurate. As a consequence, the SGS stresses were underestimated near the cutoff wavenumber, as shown in Figure 2. The results in Figs. 1 and 2 suggest that the multi-scale method performs well at small wavenumbers, whereas the direct use of second-order statistics performs well at large wavenumbers. A combination of the two should perform well for the whole spectrum. Therefore, our first modification of the algorithm of Novikov and Bodony (2005) is to model the cross stress as

$$\langle U_i v_j + U_j v_i \rangle = \langle U_i v'_j + U_j v'_i \rangle, \tag{3.3}$$

where v' is a randomized subgrid velocity (see Eq. (2.1)).

Equation (3.1) does not make the development of an LES model simpler, yet, because, in order to compute u' we need to know the subgrid scale flow v. The expression of u' is, however, similar to expressions that arise in the general method of upscaling: u' depends on the large-scale U and microstructure v. Hence, our second modification of the method (c.f. Novikov and Bodony (2005)) is

$$u' = C\Delta^{-1}\mathbb{P}\left(U \cdot \nabla v' + v' \cdot \nabla U\right), \tag{3.4}$$

where v' is a randomized subgrid velocity, and the constant C is computed dynamically

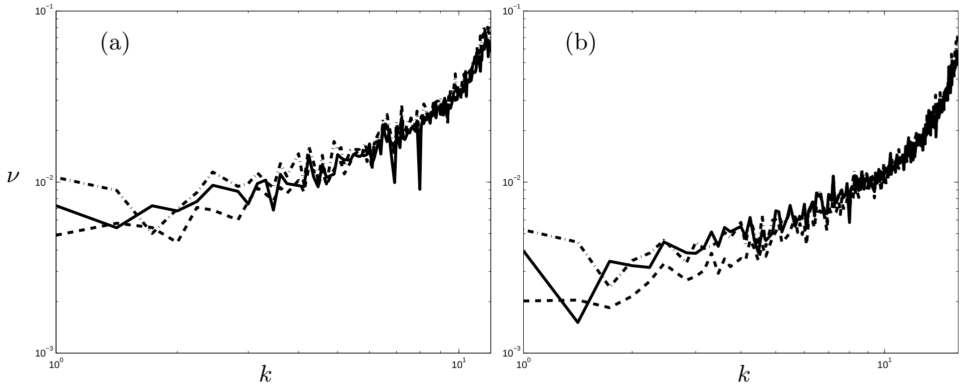

FIGURE 3. Two different methods of computing τ_{ij} using the multi-scale method. Legend: ——, DNS; $- \cdot -$, non-linear; $--$ linear (a) $k_0 = 12$, (b) $k_0 = 16$.

so that

$$\int_\Omega (u')^2 dx = \int_\Omega (v')^2 dx.$$

Then the SGS Reynolds stress is approximated as

$$\langle v_i v_j \rangle = 1/2 \langle u'_j v'_i + v'_j u'_i \rangle. \tag{3.5}$$

In summary, we modify the multi-scale algorithm of Novikov and Bodony (2005) in two ways. The new algorithm does not use DNS subgrid field, only its second-order statistics; and the cross stress is not neglected. We model the subgrid velocity v as two different velocities: either randomized DNS velocity v' or by u' as given by Eq. (3.4). The subgrid stresses are then not modeled, in contrast to the classical LES models, but computed. We use Eq. (3.5) to model the Reynolds stress as in Novikov and Bodony (2005) and propose a new expression (3.3) to model the cross stress. We mention here that the cross stresses and Reynolds stresses can also be computed as

$$\langle U_i v_j + U_j v_i \rangle = \langle U_i u'_j + U_j u'_i \rangle, \ \langle v_i v_j \rangle = \langle u'_j u'_i \rangle, \tag{3.6}$$

respectively. Numerical simulations show that both methods have similar performance (see Fig. 3), but Eqs. (3.3) and (3.5) are linear in U and are therefore easier to analyze and implement numerically.

4. Numerical investigations of simulated decaying turbulence

We now examine the multi-scale model using DNS data from decaying isotropic turbulence. Phase randomized subgrid velocity was synthesized as described in Section 2.2. A Fourier spectral method is used to invert the Laplacian in the Poisson equation (3.4). All the non-linear terms are computed in the real space, and all the derivatives are computed in the Fourier space. The Reynolds stress is found by computing Eq. (3.5), and the cross stress is found by computing Eq. (3.3). The cutoff number k_0 was variable. All the stresses are measured and plotted using spectrally resolved subgrid stresses relative to viscous stresses (2.8). For comparison, we also used the dynamic Smagorinsky model (2.9) and EDQNM (2.10).

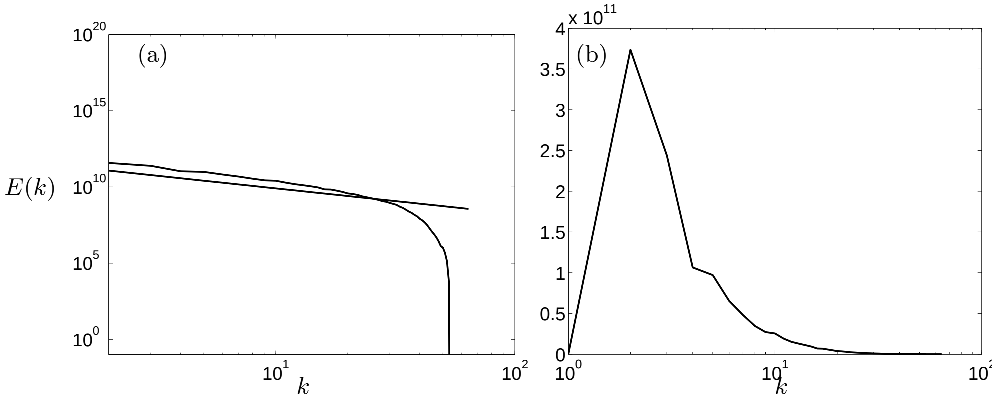

FIGURE 4. Energy spectrum of first set of DNS data (a) log-log scale, (b) log-linear scale.

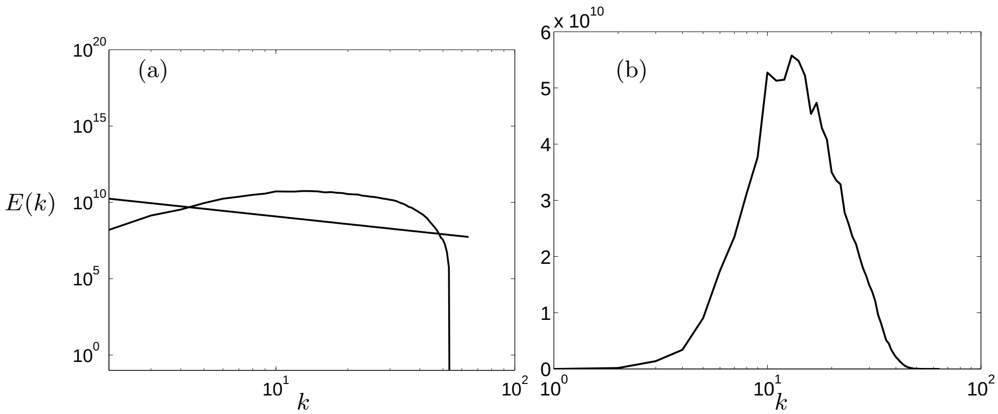

FIGURE 5. Energy spectrum of second set of DNS data (a) log-log scale, (b) log-linear scale.

4.1. *Cutoff in the inertial region*

For decaying isotropic turbulence with spectrum in Fig. 4, the algorithm's performance is shown in Fig. 6. Here the cutoff occurs in the inertial region ($k_0 = 12$ or $k_0 = 16$). As a result both Smagorinsky and EDQNM models show reasonable agreement with DNS. Note that at high wavenumbers the multi-scale algorithm performs well.

4.2. *Cutoff in energy-containing region*

A wavelet-based analysis of homogeneous isotropic turbulence was conducted by Meneveau (1991) wherein the importance of backscatter was highlighted. For the second set of DNS data, which has an energy spectrum that peaks near $k \sim 10$ (see Fig. 5), backscatter is expected. With this data the Smagorinsky and the EDQNM models do not perform as well as our model, though we have admittedly pushed the models beyond their normal usage.

4.3. *Further characterization in decaying isotropic turbulence*

Our final set of experiments was made with a synthesized subgrid field. The synthesized velocity field v' was constructed using the Kolmogorov spectrum for the spectrally

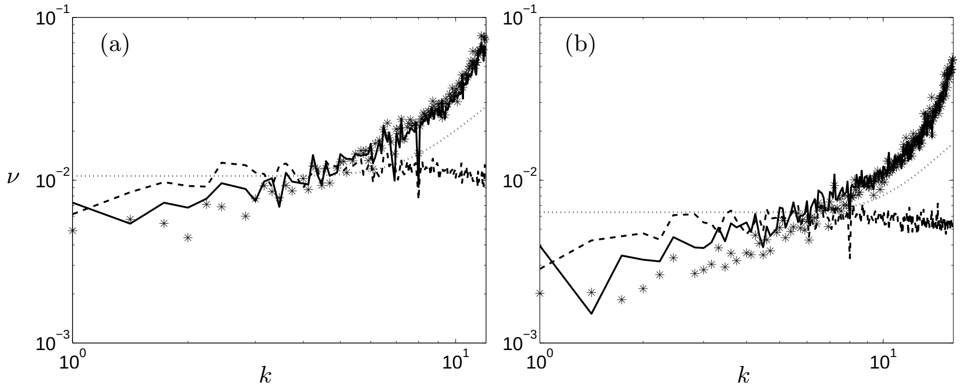

FIGURE 6. Model predictions of the eddy viscosity using the first set of DNS data. Legend: —— DNS; −−, Smagorinsky model, $\cdots$, EDQNM; $*$ our model (a) $k_0 = 12$, (b) $k_0 = 16$.

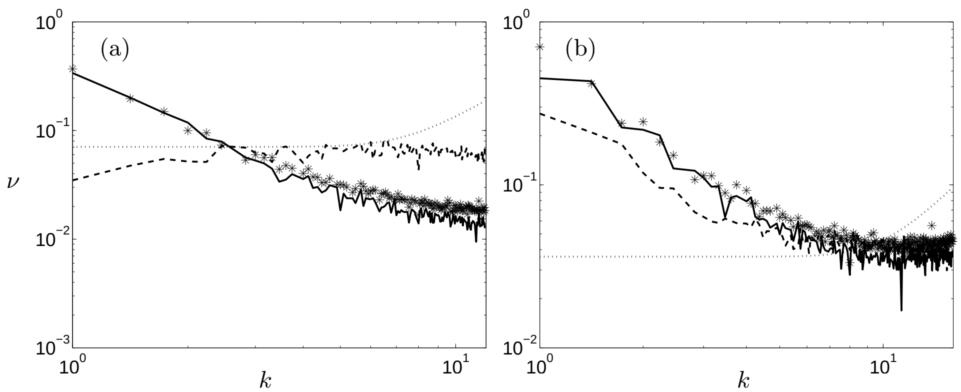

FIGURE 7. Model predictions of eddy viscosity using second set of DNS data. Legend: ——, DNS; −−, Smagorinsky model; $\cdots$, EDQNM; $*$ current model. (a) $k_0 = 12$, (b) $k_0 = 16$.

resolved energy

$$E(k) = C/k^{5/3}, \text{ with amplitudes } |\hat{v}'(n_1)| = |\hat{v}'(n_2)|, \text{ if } |n_1| = |n_2|, \tag{4.1}$$

and random uniform distribution of phases. In other words, v' is a random incompressible velocity field such that its spectrally resolved energy has the Kolmogorov spectrum. The results are presented in Fig. 8. We observe that the model's performance using the synthesized data is similar to the case using randomized DNS data.

5. Conclusions and future work

A model for the SGS stresses has been developed by formulating the large-lddy approach in a multi-scale asymptotic framework. In contrast to previous approaches, the current model first presumes a form for the *structure* for the subgrid scale field, and then deduces the resulting subgrid scale stresses. In doing so we find that the model is able to predict the eddy viscosity of decaying, isotropic turbulence in an *a priori* manner. When the separation between "resolved" and "unresolved" scales is made in the inertial range of wavenumbers, as is assumed in typical LES models, the current model's prediction of the

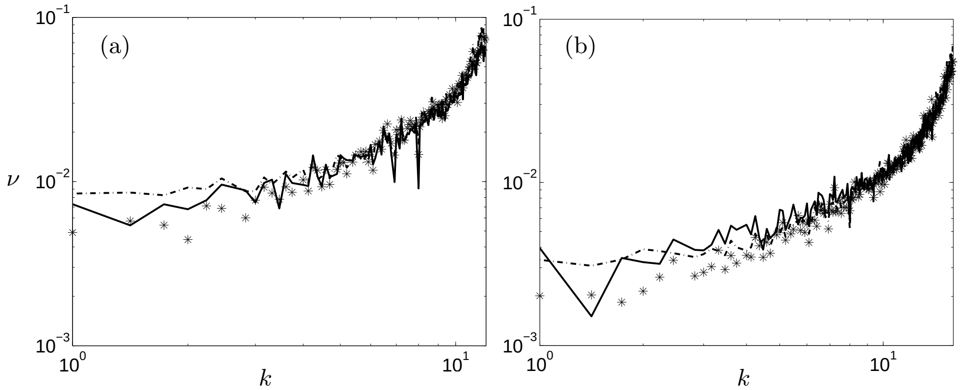

FIGURE 8. Model predictions of the eddy viscosity using the first set of DNS data and synthesized data for the model. Legend: —— DNS; $*$, current model with randomized DNS data; $- \cdot -$, current model with synthesized data from Kolmogorov spectrum. (a) $k_0 = 12$, (b) $k_0 = 16$.

eddy viscosity is similar to Smagorinsky and EDQNM predictions. However, the current model appears to perform better than either pre-existing model at higher wavenumbers. For a separation wavenumber that is within the energy containing range, the multi-scale formulation is superior over a broad range of wavenumbers.

Based on the present results we are preparing the model for future work, including *a posteriori* evaluation on decaying isotropic turbulence and for more realistic, anisotropic (e.g., wall bounded) flows.

Further improvement of our model may also be obtained if other methods for representing the subgrid scales are used. For example, we may follow Pullin and Saffman (1994), who proposed to use Lundgren stretched vortices (see Lundgren (1982)) to model subgrid scale velocity.

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