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RESEARCH PAPER

Subgrid-scale contributions to Lagrangian time correlations in isotropic turbulence

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Abstract The application of large-eddy simulation (LES) to particle-laden turbulence raises such a fundamental question as whether the LES with a subgrid scale (SGS) model can correctly predict Lagrangian time correlations (LTCs). Most of the currently existing SGS models are constructed based on the energy budget equations. Therefore, they are able to correctly predict energy spectra, but they may not ensure the correct prediction on the LTCs. Previous researches investigated the effect of the SGS modeling on the Eulerian time correlations. This paper is devoted to study the LTCs in LES. A direct numerical simulation (DNS) and the LES with a spectral eddy viscosity model are performed for isotropic turbulence and the LTCs are calculated using the passive vector method. Both *a priori* and *a posteriori* tests are carried out. It is observed that the subgrid-scale contributions to the LTCs cannot be simply ignored and the LES overpredicts the LTCs than the DNS. It is concluded from the straining hypothesis that an accurate prediction of enstrophy spectra is most critical to the prediction of the LTCs.

Keywords Isotropic turbulence · Large eddy simulation · Lagrangian time correlation · Enstrophy spectra

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1 Introduction

Lagrangian time correlations, or simply LTCs are the correlations of the Lagrangian velocities of particles at different times. They are theoretically and practically important in turbulent dispersion and mixing processes. In the turbulent dispersion process [1], the center displacement and the size increase of contaminants releasing from a localized source can be captured by the LTCs; In the turbulent mixing process [2,3], the LTC provides a time scale for the modeling of turbulent mixing in the probability density function approach. In many other cases such as particle-laden flows [4], the LTC is also a fundamental measurement on the particle motions. The recent progress on the Lagrangian statistics was summarized by Yeung [5].

Recently, there have been increasing applications of large-eddy simulation (LES) to turbulent dispersion, mixing processes and particle-laden flows. The applications raise such a fundamental question: what are the effects of subgrid scale motions on the LTCs. In LES, the large-scale motions of a velocity field are resolved, but its small scale motions are unresolved. The latter need to be modeled by a subgrid-scale (SGS) model. The current existing SGS models are mainly developed based on the energy budget equations. As a result, they are able to correctly predict energy spectra. However, they may not ensure the accurate prediction on time correlations. He et al. [6,7] investigate the effects of SGS modeling on the Eulerian time correlations. Park et al. [8] study the Eulerian time correlation as a second requirement for deterministic LES. However, LTCs are very different from Eulerian velocity correlations [9,10], in the sense that the Eulerian time correlations are mainly determined by the sweeping time and the LTCs determined by the straining time [11–13]. The recent researches [14–19] reveal that the neglect of subgrid scales could yield the errors in the LES prediction on particle motions. In this paper, we will study the subgrid scale contributions to the LTCs and investigate the effects of subgrid scale modeling on the LTCs in isotropic turbulence. A passive vector method will be used in the present study to calculate Lagrangian velocity, which can avoid all explicit interpolation procedure used in the previous study [19].

2 Numerical calculations of LTCs

A Lagrangian velocity, $\boldsymbol{v}(\boldsymbol{x}, t|s)$, is defined as the velocity at time s of a fluid particle that was at the point $\boldsymbol{x}$ at time t. By definition, the Lagrangian velocity of a fluid particle is identical with the local fluid velocity. We define the normalized LTCs of a single particle and two particles, respectively, as follows

$$R(\boldsymbol{x}; t, s) = \frac{\langle u_i(\boldsymbol{x}, t) v_i(\boldsymbol{x}, t|s)\rangle}{\langle u_i(\boldsymbol{x}, t) u_i(\boldsymbol{x}, t)\rangle^{1/2} \langle v_i(\boldsymbol{x}, t|s) v_i(\boldsymbol{x}, t|s)\rangle^{1/2}}, \tag{1}$$

$$C(\boldsymbol{x}, \boldsymbol{x}'; t, s) = \frac{\langle v_i(\boldsymbol{x}', t_0|t) v_i(\boldsymbol{x}, t_0|s)\rangle}{\langle v_i(\boldsymbol{x}', t_0|t) v_i(\boldsymbol{x}', t_0|t)\rangle^{1/2} \langle v_i(\boldsymbol{x}, t_0|s) v_i(\boldsymbol{x}, t_0|s)\rangle^{1/2}}. \tag{2}$$

Here, $\boldsymbol{u}(\boldsymbol{x}, t)$ denotes a Eulerian velocity field and $\langle\cdot\rangle$ an ensemble average over all particle samples. In stationary and isotropically homogeneous turbulence, the LTCs are only dependent on the space and time separations, such as

$$R(\boldsymbol{x}; t, s) = R(t - s), \tag{3}$$

$$C(\boldsymbol{x}, \boldsymbol{x}'; t, s) = C(|\boldsymbol{x} - \boldsymbol{x}'|; t - s). \tag{4}$$

The Eulerian velocity $\boldsymbol{u}(\boldsymbol{x}, t)$ obeys the Navier–Stokes equations for an incompressible fluid of unit density

$$\left(\frac{\partial}{\partial t} + \boldsymbol{u}(\boldsymbol{x}, t) \cdot \nabla\right) \boldsymbol{u}(\boldsymbol{x}, t) = -\nabla p(\boldsymbol{x}, t) + \nu \nabla^2 \boldsymbol{u}(\boldsymbol{x}, t) + \boldsymbol{F}, \tag{5}$$

$$\nabla \cdot \boldsymbol{u}(\boldsymbol{x}, t) = 0. \tag{6}$$

The turbulent flow is forced to be statistically stationary by adding energy to the low-wavenumber modes of the velocity field via a random force $\boldsymbol{F}$. For the velocity field, the large scale statistics are affected by the random force, while the small scale statistics are not appreciably affected [20]. This technique increases the Taylor micro scale Reynolds number and yields a wider inertial range.

The Lagrangian velocity $\boldsymbol{v}(\boldsymbol{x}, t|s)$ satisfies [21]

$$\left(\frac{\partial}{\partial t} + \boldsymbol{u}(\boldsymbol{x}, t) \cdot \nabla\right) \boldsymbol{v}(\boldsymbol{x}, t|s) = 0, \tag{7}$$

$$\boldsymbol{v}(\boldsymbol{x}, s|s) = \boldsymbol{u}(\boldsymbol{x}, s). \tag{8}$$

It is noted in Eq. (7) that the Lagrangian velocity $\boldsymbol{v}(\boldsymbol{x}, t|s)$ is the velocity at time s, of a fluid particle pass through the point x at time t, where t is called the labeling time and s is called the measuring time. Hence, the value of a Lagrangian velocity $\boldsymbol{v}(\boldsymbol{x}, t|s)$ at a fixed time s is unchanged along the fluid particle trajectory. Therefore, the Lagrangian velocity is a passive vector without diffusivity. The passive vector method can avoid all explicit interpolation by transporting the initial velocity as a passive vector, but cannot avoid the errors resulting from the non-diffusive Eulerian transport itself. However, by taking the resolved scales smaller than the dissipation scales, we expect that the error due to the non-diffusivity can be reduced to an acceptable level. The detailed justifications of the passive vector method can be found in [21].

The stationary and homogeneous isotropic turbulence in a cubic box of side 2π is simulated by DNS with the grid size 128^3 and by LES with the grid size 64^3. A standard pseudo-spectral method is used, where spatial differentiation is made by the Fourier spectral method, and time advance is made by an explicit fourth order Runge–Kutta method with same time step for both DNS and LES. In DNS, the Taylor micro-scale Reynolds number is $R_\lambda = 60$. The spatial resolution in the DNS is often monitored by the value of $K_{\max}\eta$, where $\eta = (\nu^3/\varepsilon)^{1/4}$ is the Kolmogorov length scale. This quantity, $K_{\max}\eta$, should be larger than unity for the smallest scales in turbulent flows [6] and approximate to 2 for accuracy of the passive vector method [21]. In the present work, we take this value about 2.08 while the kinematic viscosity ν is taken to 0.01 and $K_{\max}$ to 42. In LES, we use the Chollet–Lesieur standard form for the spectral eddy-viscosity model [22], where the cutoff energy is evaluated from the LES. Figure 1 displays **a** the Eulerian energy spectrum and **b** the Lagrangian energy spectrum which is defined as $E_L(k, t|s) = \int_{\|\boldsymbol{k}\|=k} \langle u_i(\boldsymbol{k}, t) v_i^*(\boldsymbol{k}, t|s)\rangle \mathrm{d}\boldsymbol{k}$. Both of the Eulerian and Lagrangian energy spectrum from the LES is in good agreement with the results from the DNS at low wavenumbers, but the Eulerian energy spectrum from the LES drops off faster and the Lagrangian energy spectrum from the LES exhibits a little overshot at higher wavenumbers.

3 Subgrid-scale contribution to LTCs

A priori test is performed to analyze the subgrid-scale contribution to LTCs. We will compare the LTCs evaluated from the unfiltered velocity fields with those evaluated from the filtered velocity fields. Here, the filtered velocity fields are obtained using a sharp spectral filter, which annihilates all Fourier modes of wavenumber k larger than the cutoff wavenumber k_c without any effect on the lower wavenumber modes.

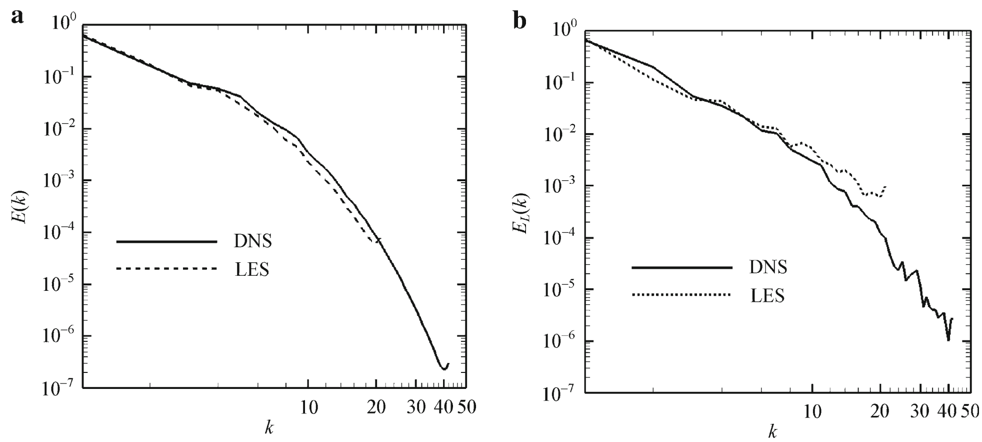

Fig. 1 **a** Eulerian energy spectra; **b** Lagrangian energy spectra

The normalized LTCs of one particle for a unfiltered velocity field can be calculated from the Fourier modes

$$R(t-s) = \frac{\int_0^\infty \langle u_i(\boldsymbol{k},\boldsymbol{t}) v_i^*(\boldsymbol{k},t|s)\rangle \mathrm{d}k}{[\int_0^\infty \langle u_i(\boldsymbol{k},t) u_i(\boldsymbol{k},t)\rangle \mathrm{d}k]^{1/2} [\int_0^\infty \langle v_i(\boldsymbol{k},t|s) v_i(\boldsymbol{k},t|s)\rangle \mathrm{d}k]^{1/2}}, \tag{9}$$

and the analogous quantity for a filtered velocity field can be also calculated from the Fourier modes

$$R(t-s;k_c) = \frac{\int_0^{k_c} \langle u_i(\boldsymbol{k},t) v_i^*(\boldsymbol{k},t|s)\rangle \mathrm{d}k}{[\int_0^{k_c} \langle u_i(\boldsymbol{k},t) u_i(\boldsymbol{k},t)\rangle \mathrm{d}k]^{1/2} [\int_0^{k_c} \langle v_i(\boldsymbol{k},t|s) v_i(\boldsymbol{k},t|s)\rangle \mathrm{d}k]^{1/2}}, \tag{10}$$

where the superscript $*$ is denoted as complex conjugate. The sharp filter with the truncation wavenumber k_c ensures that the large scale motions of the wavenumbers k less than k_c can be truly computed. Therefore, LTC is accurate up to the wavenumber k_c so that the expression (11) can be used to investigate the subgrid scale contribution to the LTCs. This is corresponding to an ideal LES.

Figure 2 plots the one-particle LTCs evaluated from the unfiltered velocity field and the filtered velocity fields with the truncation wavenumber $k_c = 12$, 24 and 42. It can be observed that there are some differences between these curves: the correlations for smaller k_c decay more slowly than those for the larger k_c, and the differences are larger at later time lag rather than at early time lag.

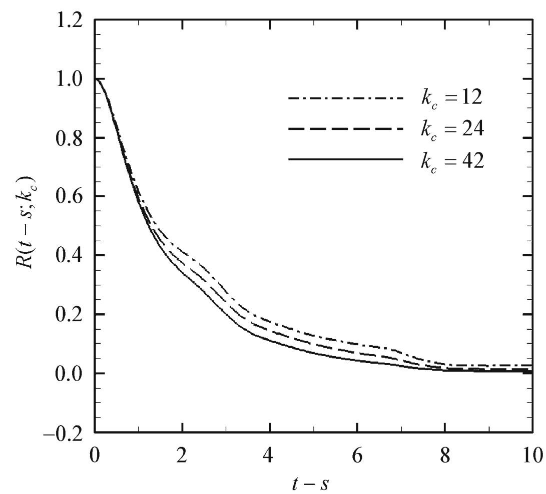

Fig. 2 The one-particle Lagrangian time correlations for different cutoff wavenumbers

4 Effects of subgrid scale modeling on LTCs

A posteriori test will be performed to analyze the effects of subgrid modeling on LTCs. We will compare the LTCs evaluated from the DNS fields and the one evaluated from the LES fields with the spectral eddy viscosity model. The normalized LTCs of Fourier modes are defined as follows

$$Q(t-s,k) = \frac{\langle v_i(\boldsymbol{k},t_0|t) v_i^*(\boldsymbol{k},t_0|s)\rangle}{[\langle v_i(\boldsymbol{k},t_0|t) v_i^*(\boldsymbol{k},t_0|t)\rangle]^{1/2} [\langle v_i(\boldsymbol{k},t_0|s) v_i(\boldsymbol{k},t_0|s)\rangle]^{1/2}}. \tag{11}$$

Here, the Fourier modes are calculated from the DNS and LES fields, respectively.

In Fig. 3a, the normalized LTCs from the DNS and LES fields for wavenumber $k = 6$ and 12 are plotted together. It is evident that the LTCs from the LES fields decays more slowly than those from the DNS fields. In Fig. 3b, the correlations are plotted together, with the time axis rescaled by Lagrangian characteristic time

$$\tau_L(k) = \left[\int_0^k p^2 E(p)\mathrm{d}p\right]^{-1/2}. \tag{12}$$

The collapses of the correlation curves again confirm the validation of the straining hypothesis for isotropic turbulence:

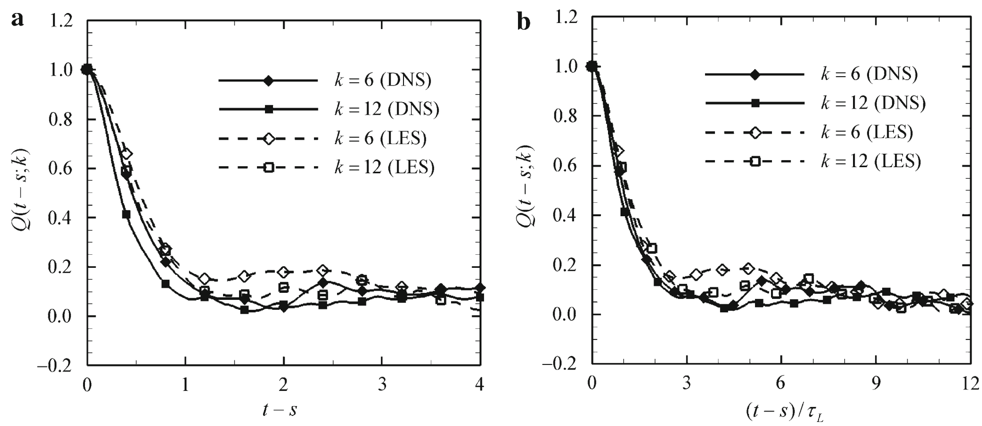

Fig. 3 The Lagrangian time correlation versus **a** time separation and **b** renormalized time separation for the DNS and LES fields, respectively

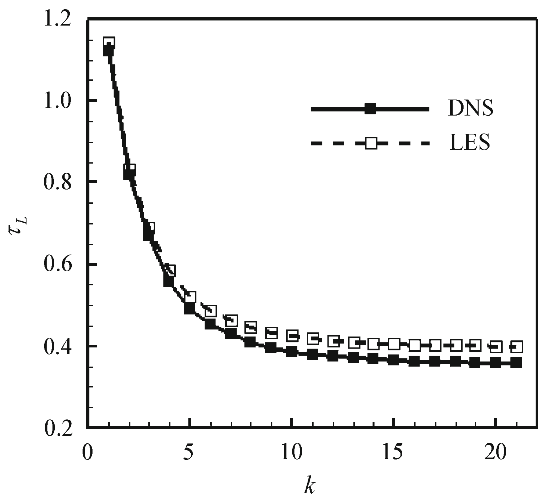

Fig. 4 The Lagrangian characteristic time scales from the DNS and LES fields, respectively

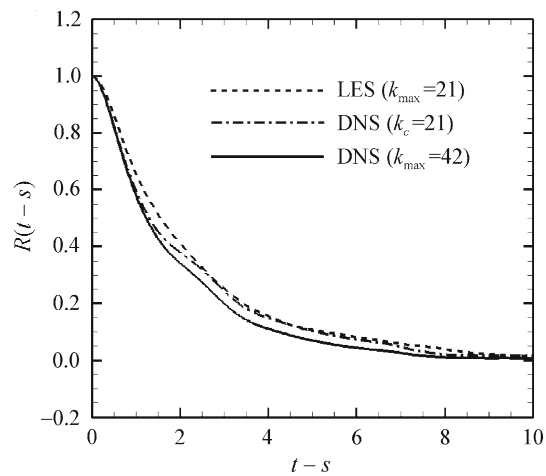

Fig. 5 The one-particle Lagrangian time correlation versus the time separation for the LES, the filtered DNS and the unfiltered DNS fields, respectively

the LTCs are mainly determined by the Lagrangian characteristic time $\tau_L(k)$ [11,21].

$$Q(t, k) \sim \exp[-t^2/\tau_L^2(k)]. \tag{13}$$

Therefore, the accurate prediction of SGS models on the LTCs is mostly dependent on their prediction on the Lagrangian characteristic time. Noting that $\tau_L(k) = [\int_0^k p^2 E(p)\mathrm{d}p]^{-1/2}$ is determined by $p^2 E(p)$, an accurate prediction of LES on the LTCs is dependent on the accurate prediction of LES on the enstrophy spectra.

Figure 4 plots the Lagrangian characteristic time scales for the DNS and LES. It shows that the Lagrangian characteristic scales from the DNS are small than the ones from the LES. In present study, the spectral eddy viscosity model underestimates the energy spectra, especially at larger wavenumbers (seeing Fig. 1a for energy spectra). This leads to an under-prediction on the enstropy spectra. Therefore, the LES with the spectra eddy viscosity model over-predicts the LTCs.

Figure 5 plots the LTCs of a single particle evaluated from the DNS, the filtered DNS and LES velocity fields, where the filtering scale is taken as the minimal resolved scale in LES ($k_c = 21$). The correlation functions from the LES fields still decay more slowly than the ones of the DNS field, while the results from the filtered DNS field is in between.

5 Conclusions

A priori test in the stationary and isotropic turbulence was conducted for the subgrid scale contributions to the LTCs. It is shown that the LTCs evaluated from the filtered velocity fields decay more slowly than the ones evaluated from the unfiltered velocity fields. The errors induced by filtering could be significant, but decrease with increasing the cutoff wavenumber. Therefore, the subgrid scale contributions to the LTCs cannot be ignored. *A posteriori* test on the stationary and isotropic turbulence was also conducted for the effects of subgrid scale modeling on the LTCs. It is observed that, even if it predicts the energy spectra well, the LES field still overpredicts the LTCs than the filtered and unfiltered DNS fields.

The straining hypothesis [11,21] suggests that the Lagrangian characteristic time of the Fourier mode k is dominated by $\int_0^k p^2 E(p) \mathrm{d} p$. Consequently, the Lagrangian characteristic time scales are determined by the enstrophy spectra $p^2 E(p)$. Therefore, an accurate prediction of LES on LTCs is mainly determined by the accurate prediction on enstrophy spectra. The enstrophy spectra represent a new requirement to the applications of LES to particle dispersion, turbulent mixing and particle-laden turbulence, in additional to energy spectra.

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