On the Error Estimate in Sub-Grid Models for Particles in Turbulent Flows

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1 Introduction

The use of Large Eddy Simulation (LES) has emerged in recent years as a powerful simulation technique with the specific goal of achieving a good statistical accuracy while retaining a computational cost lower than Direct Numerical Simulations (DNS) [1]. In LES, only large-scale motions are directly computed (resolved on the computational grid) while small scale motions are not computed explicitly but modeled via Sub-Grid Scale (SGS) models. Due to the complex statistical properties of turbulence, many models and methodologies have been proposed in the past. Although none of the proposed models can be considered a perfect substitute to DNS, their performance can be sometimes considered fairly accurate for what concerns the most common Eulerian turbulent flow statistics. The problem of particle transport in turbulence demands much more to LES than just reproducing low order Eulerian statistics (e.g. spectra, average profiles etc) [2, 3]. Here we propose a way to quantify the effect of (the error due to) sub-grid modeling on particle properties.

2 Description of the numerical methods

Objective of this paper is to provide an accurate quantification of the effect of sub-grid modeling on particle dynamics. To this purpose DNS of both Homogeneous

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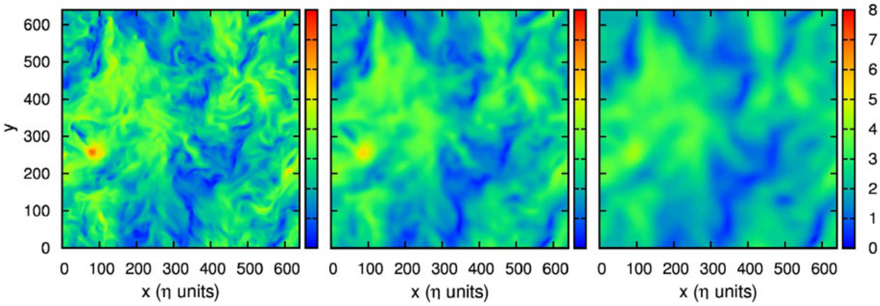

Fig. 1 2D view of the absolute value of the velocity field coarse-grained with larger filter width corresponding to, from left to right, 1η, 5η and 10η respectively.

Isotropic Turbulence (HIT) and Turbulent Channel Flow (TCF) are carried out to generate sets of velocity fields that are subsequently filtered at every time step using a Gaussian filter. This operation allows to smooth out all flow scales smaller than the filter width, Δ. Several filter widths were considered to produce a full temporal evolution of different filtered Eulerian fields, each mimicking a "perfect" LES, i.e. a reduced simulation where the largest scales evolve closely matching DNS ones. Particles dynamics are then determined using a Lagrangian approach: first, the motion of particles initially released as close-by pairs [2] is computed in the (unfiltered) DNS fields; then, a Gaussian filter is applied to generate coarse-grained fields in which the same particles are tracked again. In this way we can generate perfectly comparable LES simulations. For both HIT and TCF, simulations were performed using a pseudo-spectral method. The Eulerian field is governed by the incompressible Navier-Stokes equations discretized on a regular grid of 512^3 grid points for HIT and on an irregular grid of 128^3 grid points stretched in the wall-normal direction for TCF. Governing equations are integrated using a Fourier-Chebyshev representation of field variables and advanced in time with a second-order Adams-Bashforth integrator. For HIT, the solution domain is a cube, subjected to periodic boundary conditions. Turbulence scales are fixed in time by forcing the flow at the small wavenumbers, with constant power, in order to achieve a statistically stationary turbulent flow ($Re_\lambda = 363$). Lagrangian statistics are then extracted tracking large ensembles of particles and of particle pairs with prescribed initial separation, roughly equal to the Kolmogorov length scale, η [2, 3]. For TCF, simulations were performed on a reference domain with periodic boundary conditions in the streamwise and spanwise directions and with no-slip boundary condition enforced at the walls. In this case turbulence is sustained by an imposed pressure gradient along the streamwise direction ($Re_\tau = 150$). Particle pairs are released in wall-parallel planes with three different initial orientations, aligned with each flow direction to investigate also the influence of shear on pair dispersion. In this study we tracked both tracers and particles with inertia. Differently from HIT, the Gaussian filter is employed in TCF only along the two homogeneous directions.

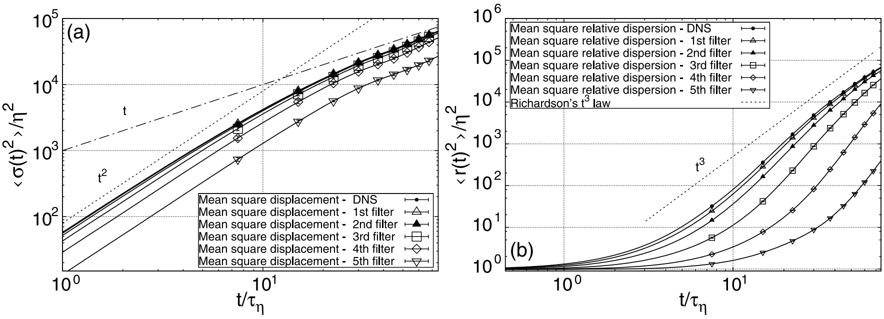

Fig. 2 Mean square displacement (a), and mean square relative dispersion (b) as a function of time t, normalized by Kolmogorov time-scale. Profiles correspond to different degrees of filtering: no filter is applied in DNS, then filter widths of $1.55\eta, 3.1\eta, 6.2\eta, 12.42\eta$ and 24.84η respectively.

3 Results

In Fig. 1 a typical 2D view of homogeneous isotropic turbulence is shown. For increasing filter widths, the field becomes more and more coarse grained. Yet, large scale structures remain unchanged for all filtered evolutions. In isotropic turbulence, mean velocity is zero so the first non-vanishing statistical moment is the variance of particle displacement, σ^2, which measures the displacement of a fluid particle relative to its initial position. In Fig. 2 the variance of particle displacement obtained applying filters of increasing width to the DNS field is shown. For comparison the two asymptotic trends $\langle r(t)^2 \rangle \sim t$ and $\langle r(t)^2 \rangle \sim t^2$ predicted by the theory of G.I. Taylor [4] are also shown. It is observed that particle displacement variance increases with time and exhibits the expected asymptotic scaling behaviors. The results show a good agreement for all cases, yet it can be seen that an increase in filter width leads to lower dispersion. This result allows to conclude that LES under-predicts single particle dispersion. Particle pairs in a turbulent flow will on average move away from each other, leading to mean separations that increase in time. The relative dispersion depends on the properties of the turbulent velocity field and on the initial separation distance. In DNS, the velocity field is fully resolved, and the contributions to relative dispersion are well captured at all scales of motion. However, in our "perfect" LES, the large-scale velocity fields are fully resolved whereas small-scale fluid motions are completely missing. We thus expect a significant effect on the relative dispersion of particle pairs, especially at early dispersion stages. This effect can be measured statistically by looking at relative separations and velocities. An important quantity to measure is particle pair dispersion. For homogeneous isotropic turbulence, two regimes can be identified for relative dispersion: the instantaneous separation of the positions of the two particles $\mathbf{r}(t) = \mathbf{r}^{(1)}(t) - \mathbf{r}^{(2)}(t)$ and the separation magnitude $\mathbf{r} = |\mathbf{r}|$. For short times, the mean square separation between two fluid elements grows either exponentially or quadratically. Furthermore, when the particle separation distance falls in the inertial range, it can be described using a diffusion equation for the probability density function (pdf) of the pair separation

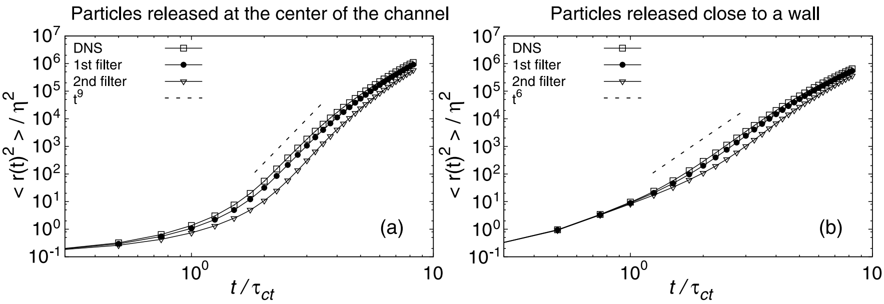

Fig. 3 Particle pair mean square relative dispersion in turbulent channel flow. Time t is normalized by the crossing time τ_{ct}, namely the time taken by the flow to cross the channel in the streamwise direction. Slopes corresponds to different filter widths (□: DNS, •: 1st filter, ▽: 2nd filter).

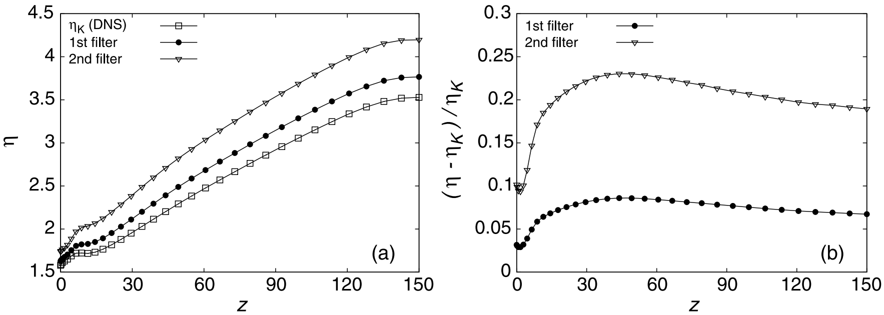

Fig. 4 Left panel: smallest length-scale as a function of wall normal coordinate in turbulent channel flow (wall located at $z = 0$, center of the channel located at $z = 150$). Right panel: the effect of increase of the smallest length-scale by filtering (comparison with η_K obtained with DNS).

$p(r,t)$, following the ideas of Richardson [5]. This gives rise to the celebrated scaling for the second order moment: $\langle r^2 \rangle = g\varepsilon t^3$. Here g is the Richardson constant, and ε is the energy dissipation rate per unit mass. For long times, a diffusion limit exists similar to single-particle dispersion. Regimes depend on the initial particle separation, and only the inertial regime is universal since at long times particles belonging to some pairs become uncorrelated. The t^3 regime is derived theoretically for high Reynolds number flows with a clear inertial range. From Fig. 2 we can see that filters of increasing width shift profiles toward lower values. Based on these results, one can conclude that, similarly to what was observed for single particles, LES under-predicts particle pair dispersion. In this case under-prediction is even higher.

Particle pair dispersion in turbulent channel flow is shown in Fig. 3 for two different locations of release. Although the values of Reynolds number and grid resolution are too small to provide a clear inertial range, we define it as $10\,\overline{\eta_K} < r(t) < h$ (where $\overline{\eta_K}$ is the Kolmogorov length-scale averaged over the all directions and h is the channel half-height) for a comparison with HIT. In inertial range the slope of $\langle r^2 \rangle$ is steeper than in homogeneous isotropic turbulence. This is due to the strong influence of the shear near the channel walls. In this regions the streamwise velocity gradient dominate pair separation. As in HIT LES under-predicts particle pair dispersion. In particular, the degree of under-prediction changes along the wall-normal direction, being stronger for particles released in the center of the channel. Note that initial separation between two particles is always smaller than the Kolmogorov length-scale $\eta_K(z)$. A possible explanation to this behavior is provided in Fig. 4, which shows the wall-normal behavior of the smallest length-scale $\eta(z)$ computed when filters of increasing width are applied to the DNS fields. The smallest length-scale, equal to the Kolmogorov length-scale $\eta_K(z)$ in DNS, increases upon filtering, and the increase is higher in the center of the channel than near the walls, both in absolute and relative terms. This means that filtering removes more "information" in the center of the channel: particles become exposed to a narrower spectrum of structures and under-prediction of pair separation is thus stronger over short times (e.g. $\frac{t}{\tau_{ct}} < 1$).

Particles released in fields with different filtering will have a different evolution because of two effects (see Fig. 5): (i) lack of high frequency oscillations and (ii) error accumulation. Due to the filtered nature of the fields which lack high frequency oscillations, particles will also miss these frequencies from their dynamics. The second effect is the result of particles evolving in the filtered field along a trajectory which differs from the DNS one. This leads particles to experience different values of the velocities (see Fig. 5) and to accumulate an error during their motion. It is of paramount importance to discriminate between these two effects: while the first can be addressed quite easily (e.g. by adding an appropriate stochastic high frequency noise to the particle velocity), the latter poses great modeling challenges. It is hence fundamental to understand in which conditions and for which observables the second effect plays a role. In order to analyze and quantify these two effects, we introduce a new investigation tool. Referring to the velocity field we can calculate its material derivative with respect to the filter width, obtaining

$$\frac{d}{d\Delta}\mathbf{v}_\Delta(\mathbf{x}_\Delta(t),t) = \frac{\partial \mathbf{u}_\Delta}{\partial \Delta} + \frac{\partial \mathbf{x}_\Delta(t)}{\partial \Delta} \cdot \nabla \mathbf{u}_\Delta(\mathbf{x}_\Delta(t),t), \tag{1}$$

where Δ is the filter width. This simple and exact relation is helpful to our purpose, given that we can calculate its two different hand sides and then compare them in order to obtain an error. In our databases, comprehensive of several Eulerian and Lagrangian data, we integrated also the filtered partial derivative and gradients of the evolution of the particles. The left panel of Fig. 5 shows the trend of the error between the two hand sides, defined as their difference divided by their semi-sum.

4 Conclusions

Small turbulent scale effects on the dynamics of individual particles and of particle pairs are analyzed systematically, to validate the use of LES in two-phase flows. To this aim DNS of homogeneous isotropic turbulent flow and of turbulent channel

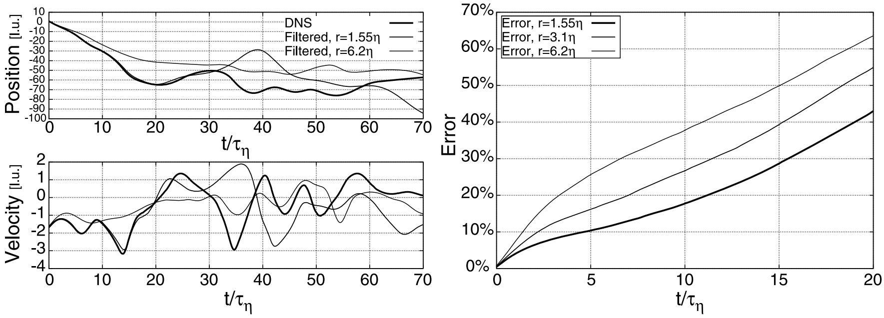

Fig. 5 Left panels: example of the evolution of particles in velocity fields filtered with different filters. Both position and velocity are shown as a function of time. Right panel: error for three different filter widths, averaged over all the particles.

flow are carried out, and the motion of dispersed particles is followed in time. The DNS velocity fields are then filtered with a Gaussian filter of increasing width, to generate a-priori LES fields in which particles are tracked again. In this way it is possible to isolate the effect of the small scales with respect to the real flow field (represented by the DNS one). It is also possible to highlight the behavior of flow field statistics with filter of increasing width. A general under-prediction of particle dispersion is found in both flow configurations. However, while for single particles dispersion under-prediction seems to be small, for particle pairs it becomes more significant. This is due to the stronger influence of the small scales of motion on pair dispersion in the dissipation range. Finally a new analysis tool has been introduced to investigate deviation of particles evolving in the filtered field with respect to "exact" DNS trajectory.

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