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# MIXED MODEL FOR HEAVY PARTICLES IN LARGE EDDY SIMULATION OF TURBULENT FLOW

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*Abstract*
In the present contribution, we propose a subgrid-scale (SGS) model for dispersed phase in two-phase Eulerian-Lagrangian Large-Eddy Simulation (LES) with the cross-corelation of SGS velocity components accounted for. A priori and a posteriori results are presented, showing the model's ability to reconstruct SGS velocity fluctuations. The idea of a mixed variant of the model is also reported. In this variant the defiltering of the fluid scales near the cutoff (through the approximated deconvolution) is coupled with the stochastic treatment of small scales.

*Key words: turbulence, dispersed phase, particles, LES, SGS model*

## INTRODUCTION

Turbulent flows with small particles are of great interest for both physicists and engineers. Dispersed phase is involved into a range of physical phenomena like clustering, aggregation, deposition at the walls and fractal patterns of preferential concentration, being vital for industrial applications, e.g., the dynamics of droplets or particles in combustion chambers. Since experiments are costly and usually limited to simple geometries, there is a need for a physics-capturing model that would simulate behaviour of the dispersed phase. Direct Numerical Simulations (DNS) allow to explicitly resolve all scales of turbulent motion, but computational cost can be met only by supercomputers. To develop a more applicable engineering tool, we consider the fluid being modelled by Large Eddy Simulation (LES), where only large scales of motion are resolved, and the effect of small scales, mainly dissipation of kinetic energy, needs to be accounted for. The basis of the method is filtering operation, where fluid fields, say velocity $\boldsymbol{U_f}$, are convoluted with filter function $G$ of width $\bar{\Delta}$: $\overline{\boldsymbol{U_f}} = G * \boldsymbol{U_f}$ to result in a large-scale field $\overline{\boldsymbol{U_f}}$; symbol $\overline{(.)}$ denotes filtering with $G$. Under assumption of commutativity of filter and differential operator, filtering is applied to the Navier-Stokes equations (NSE). As a result, the subgrid-scale (SGS) stress tensor is added to the equation to reconstruct effects of the small scales on the resolved flow. Still, only the filtered field is solved, so no small-scale information about fluid is available. On the plus side, LES is less costly than DNS, and still gives time-dependent fluid field. Nevertheless, adding dispersed phase to the flow, we observe that small scales of fluid motion may have a considerable effect on preferential concentration patterns of particles, deposition velocity and kinetic energy, which, if neglected, leads to unphysical behaviour. Therefore, the effect of SGS velocity fluctuations on particles should be considered (Fede et al., 2006).

## GOVERNING EQUATIONS

In order to explore effects of the wall on the particle movement, channel geometry is chosen. The carrier phase is described by the Navier-Stokes equations for incompressible fluid with no-slip and no-penetration conditions at the walls. Point, heavy particles (drag only) move in the flow according to equations:

$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{V}_p; \frac{d\boldsymbol{V}_p}{dt} = f_D \frac{\boldsymbol{U}_f^* - \boldsymbol{V}_p}{\tau_p}$$

where $\boldsymbol{x}_p, \boldsymbol{V}_p$ are particle location and velocity, $\tau_p$ is the particle momentum relaxation time and $f_D$ is a semi-empirical drag correction factor. The Stokes number of particle is defined as the ratio of particle relaxation time and a fluid time scale: $St = \tau_p/\tau_f$. The mass and volume load of the dispersed phase are low, so one-way momentum coupling is assumed. Here, $\boldsymbol{U}_f^* = \boldsymbol{U}_f(\boldsymbol{x}_p, t)$ is the exact fluid velocity at particle position. Since in LES full information on fluid fields is not available, $\boldsymbol{U}_f^*$ is decomposed into the resolved part and the SGS component, $\boldsymbol{U}_f^* = \overline{\boldsymbol{U}_f} + \boldsymbol{u}^*$. Here, $\overline{\boldsymbol{U}_f}$ is the fluid velocity in LES computations, and $\boldsymbol{u}^*$ represents fluctuations of fluid velocity at particle position that need to be modelled.

## SGS PARTICLE DISPERSION MODEL

To model the effect of SGS flow velocity on particles, we use the Langevin equation:

$$(1)\ d\boldsymbol{u}^* = -\frac{\boldsymbol{u}^*}{\tau_f^*}dt + \boldsymbol{\sigma} \cdot d\boldsymbol{W}_t$$

where $d\boldsymbol{W}_t$ is a vector of independent increments of the Wiener process, $\boldsymbol{\sigma}$ is a diffusion matrix and $\tau_f^*$ is a time scale of SGS fluid velocity at particle position. In general, stochastic modeling has been used both in the PDF approach for single phase turbulence and for dispersed flows considered in the statistical way as in RANS, cf. (Minier & Peirano, 2001). We are faced with two problems. First, defining $\tau_f^*$ and $\boldsymbol{\sigma}$, and second, extracting data necessary for previously defined $\tau_f^*$ and $\boldsymbol{\sigma}$ from LES computations. In this paper, three approaches to the first problem will be presented, and, to the authors knowledge, new solutions are proposed to the latter.

The first attempt to model the effects of subgrid fluid velocity on particles is to take a diagonal matrix $\boldsymbol{\sigma}$ with $\sigma_{ii}{}^2 = 4k_{sg}/(3\tau_f^*)$ and $\tau_f^* = C_{sg}\bar{\Delta}/\sqrt{2/3\,k_{sg}}$, where $C_{sg}$ is a model constant representing level of damping of $\boldsymbol{u}^*$, $k_{sg}$ is residual kinetic energy, and $\bar{\Delta}$ is width of the filter imposed by LES (Pozorski & Apte, 2009). Subgrid-scale (residual) kinetic energy is obtained from the Yoshizawa estimation $k_{sg} = C_I\bar{\Delta}^2|\bar{S}|^2$, where $|\bar{S}|$ is the norm of the strain tensor, $C_I$ is a dynamically estimated parameter:

$$(2)\ C_I = \frac{1}{2}\frac{\langle \widehat{\bar{U}_k\bar{U}_k} - \hat{\bar{U}}_k\hat{\bar{U}}_k\rangle}{\langle \bar{\Delta}^2|\bar{S}|^2 - \hat{\bar{\Delta}}^2|\hat{\bar{S}}|^2\rangle}.$$

Symbol $\widehat{(.)}$ represents filtering with test filter of higher than LES filter width. The average $\langle . \rangle$ is then taken in homogeneity directions of the flow.This approach gives acceptable results in homogeneous isotropic turbulence, where fluctuations of SGS fluid velocity are statistically the same in all three directions. However, it performs worse in wall-bounded flows (Pozorski & Łuniewski, 2008).

Recently (Pozorski et al., 2012), a promising improvement of this model was proposed. Correlation matrix $\boldsymbol{\sigma}$ is still kept diagonal, but the components are proportional to the r.m.s. of SGS fluid velocity fluctuations in respective directions $\sigma_{jj}{}^2 = 2\overline{u_{jj}^2}/\tau_f^*$. Here $\overline{(.)}$ represents average over realizations of stochastic process $\boldsymbol{u}^*$. We assume that fluctuation intensity of fluid velocity at particle position is the same as that of fluid itself. The estimation of $\overline{u_{jj}^2}$ is done in a similar way that in the model above, only parameter $C_I$ in Eq. (2) is substituted by direction-dependent proportionality factors (no summation over $j$):

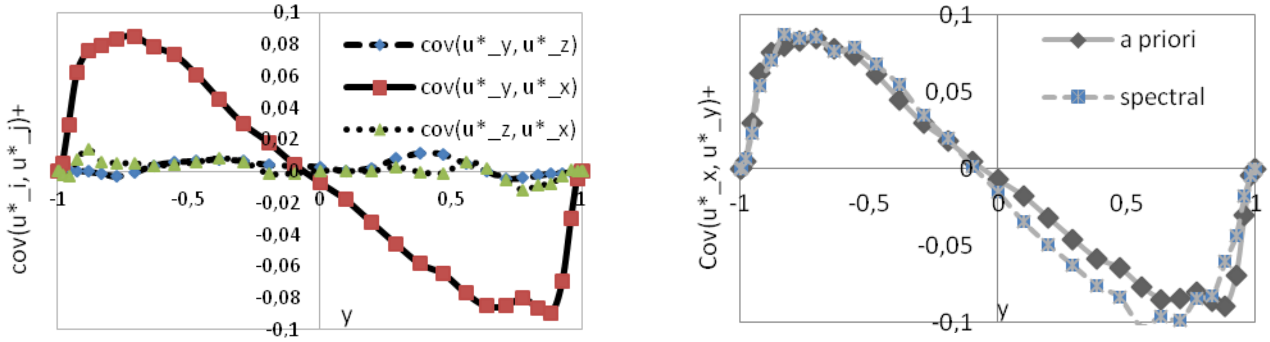


Fig.1: The covariance of SGS fluid velocity components in Large Eddy Simulation of turbulent channel flow: a) computed in *a priori* simulation (filtered DNS); b) estimated *a priori* and computed with the dynamic procedure (spectral code).

$$\overline{u_{jj}^2} = \frac{1}{2}\frac{\langle \overline{\bar{U}_j\bar{U}_j} - \bar{\bar{U}}_j\bar{\bar{U}}_j\rangle}{\langle \bar{\Delta}^2\overline{|\bar{S}|^2} - \bar{\bar{\Delta}}^2|\bar{\bar{S}}|^2\rangle}\bar{\Delta}^2|\bar{S}|^2$$

In the basis of this idea lies the Bardina model, where $\overline{u_{jj}^2} = C_m\langle \overline{\bar{U}_j\bar{U}_j} - \bar{\bar{U}}_j\bar{\bar{U}}_j\rangle$. Here, the idea is developed further, so that $C_m$ becomes a parameter depending on the norm of the large-eddy strain tensor $\bar{S}$. That approach enhances anisotropy of near-wall turbulent flow.

In the third approach, the correlation of SGS velocities is added, and $\boldsymbol{\sigma}$ becomes a lower-triangular matrix. Following the literature and our results (Fig. 1), in channel flow, the correlation between streamwise (*x*) and wall-normal (*y*) velocity is one order of magnitude higher than the two remaining. On this basis we assume $\sigma_{ik} = 0$ for other combinations of directions.

Considering the properties of the Langevin equation, components of $\boldsymbol{\sigma}$ are:

$$\sigma_{jj} = \sqrt{2\overline{u_{jj}^2}/\tau_f^*},\ j = 2{,}3;\ \sigma_{11} = \sqrt{2\left(\overline{u_{11}^2} - \overline{u_1u_2}/\overline{u_{22}^2}\right)/\tau_f^*}\ ;\ \sigma_{21} = \sqrt{2\overline{u_1u_2}\Big/\left(\tau_f^*\sqrt{\overline{u_{22}^2}}\right)}$$

Here, cross-correlations of velocity are also computed with the dynamic procedure based on the Yoshizawa estimation

$$\overline{u_ku_j} = \frac{1}{2}\frac{\langle \overline{\bar{U}_k\bar{U}_j} - \bar{\bar{U}}_k\bar{\bar{U}}_j\rangle}{\langle \bar{\Delta}^2\overline{|\bar{S}|^2} - \bar{\bar{\Delta}}^2|\bar{\bar{S}}|^2\rangle}\bar{\Delta}^2|\bar{S}|^2$$

To validate this approach, we compare the covariance of streamwise and wall-normal SGS velocity component in *a priori* computations and the full LES (Fig. 1a).

The last model considered here has a bit different idea behind. Partial solution to insufficient intensity of fluctuations of fluid velocity at particle position is the Approximate Deconvolution Method (ADM), which provides an estimation of exact fluid velocity $\boldsymbol{U}_f^*$ (Kuerten, 2006). Performed on a coarser grid, ADM behaves as a low-pass filter, cutting off fluctuations of velocity with higher wavenumbers (Stolz et al., 2001). Then, since we have separation of scales, we can add a SGS stochastic part of the model, independent of larger scales $\boldsymbol{U}_f^* = \widetilde{\boldsymbol{U}}_f + \boldsymbol{u}^*$, where $\widetilde{\boldsymbol{U}}_f = g^{-1} * \overline{\boldsymbol{U}_f}$ and $g^{-1}$ is an approximate inverse of the filtering operator. Statistics of the ideal forcing from a priori LES with ADM alone for particles have recently been computed (Kuerten & Geurts, 2012).

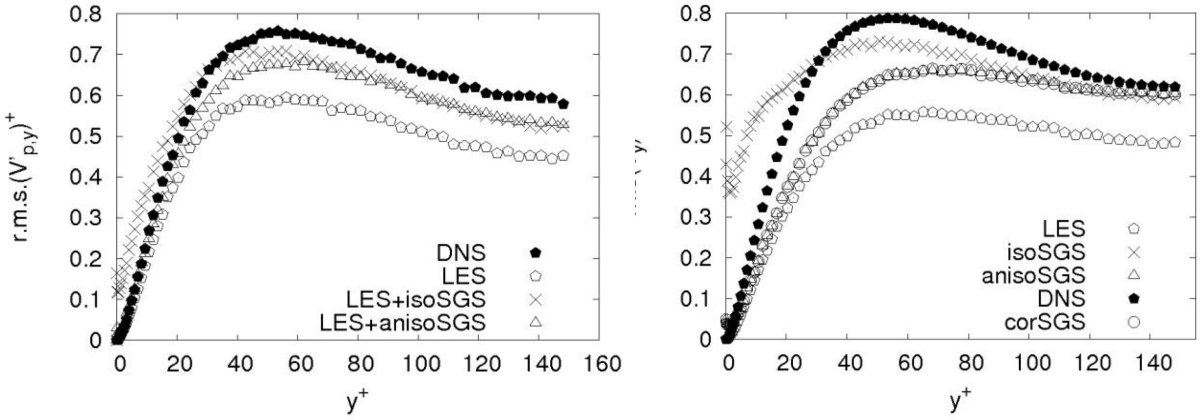


Fig.2: The r.m.s. of wall-normal particle velocity (St = 1, $C_{sg} = 0.1$): a) a priori LES; b) LES.

**RESULTS**

The channel geometry is used to test the model. The Reynolds number based on friction velocity equals $Re_\tau = 150$. Numerical code used (courtesy of Prof. J.G.M. Kuerten) is spectral in periodic flow directions and Chebyshev in the wall-normal direction. Fluid velocity at particle position is interpolated with 2$^{nd}$ order Lagrange scheme. Particles evolution is computed with 2$^{nd}$ order Runge-Kutta scheme.

In order to evaluate impact of the model for the SGS fluid velocity at particle position, we perform two types of simulation. In first one, the *a priori* LES, fluid velocity field obtained with DNS is filtered at every time step. Particles evolve in filtered field, and the model of SGS fluid velocity, based on explicitly computed loss of kinetic energy, is added. The purpose is to check whether the proposed form of $\boldsymbol{\sigma}$ is correct. Also, real LES computations are performed, and the evaluation of both, equations and method of modeling fluctuations, is presented.

Figure 2 presents the fluctuation intensity of wall-normal particle velocity for several variants of the model: isotropic (isoSGS), anisotropic, but with diagonal matrix $\boldsymbol{\sigma}$ (anisoSGS), and third -  with correlation of wall-normal and streamwise velocity (corSGS) for *a priori* and real LES computations. We observe that, for the same model constant, fluctuations in the center of the channel are better reconstructed in real LES (Fig. 2b), where the curve representing every variant of the model meets DNS (filled pentagons). Meanwhile, in a priori LES (Fig. 2a) only about half of the lost intensity of fluctuations is retrieved. The other observation is that, for isotropic model, near-wall fluctuations are strongly overestimated in the vicinity of the wall. The probable explanation is that particles from regions further from the wall do not have enough time to relax SGS fluid velocity at particle position $\boldsymbol{u}^*$ while getting near the wall. In other words, the isotropic model implies unrealistic long-time memory. This excessive fluctuations may be also due to lack of spatial correlation in equation (1). Particles do not have joint information about underlying SGS velocity field.  That leads to unphysical behavior and over-excitation of particles. One way to overcome this is to set different relaxation time $\tau_f^*$ for different directions. Still, other models based on Langevin equation improve the LES results (anisoSGS, corSGS).

Too generous input of near-wall fluctuations is also visible in Fig. 3a, where streamwise r.m.s. of velocity fluctuation for St = 1 particles is shown. Anisotropic model distributes SGS kinetic energy proportionally to estimated level of component's velocity fluctuation. Therefore, since streamwise velocity has the highest fluctuations, we see lower values for isotropic model. Slightly different situation occurs for heavier particles (St = 5, cf. Fig.3b).

Stochastic model is not that effective far from walls, and its isotropic version gives the highest errors at the walls. This behavior might be due to more effective damping of fluctuations.
As expected, statistics computed from anisotropic and correlated models statistics behave similarly except for the covariance between streamwise and wall-normal fluid velocity (cf. Fig 4). Structure of velocity correlation seems to be well reconstructed, though; for particle velocity the model gives better results for St = 1 (Fig. 4a) for chosen model constant $C_{sg} = 0.1$. It should be observed that correlation of fluid velocity at particle position (Fig. 5) gives almost the same level of reconstruction for smaller (St = 1) and bigger (St = 5) particles. Detailed results of the mixed model (variant 4) will be presented at the conference.

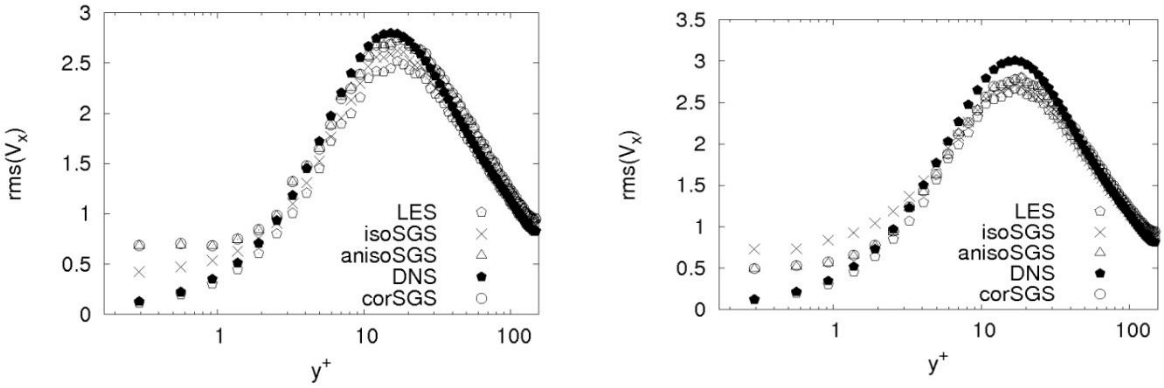


Fig.3: The r.m.s. of streamwise particle velocity from real LES ($C_{sg} = 0.1$): a) S =5; b) St=1.

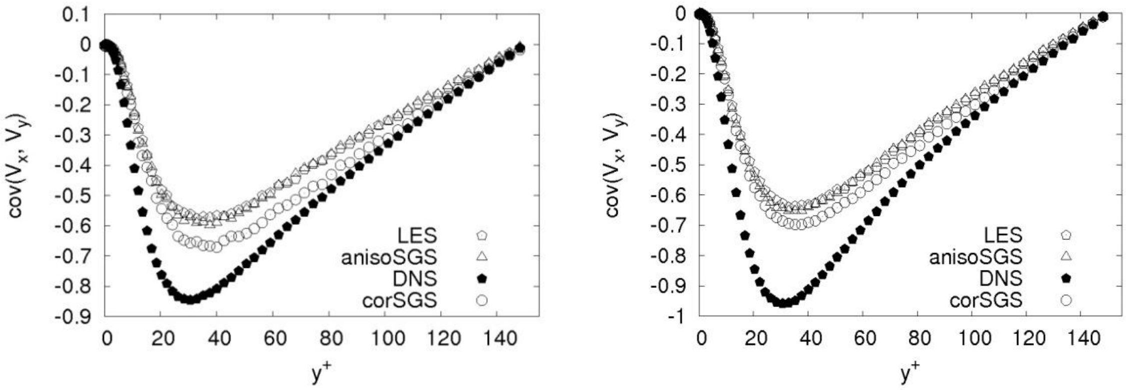


Fig.4: Covariance of streamwise and wall-normal particle velocity from LES simulations ($C_{sg} = 0.1$): a) St = 1; b) St = 5.

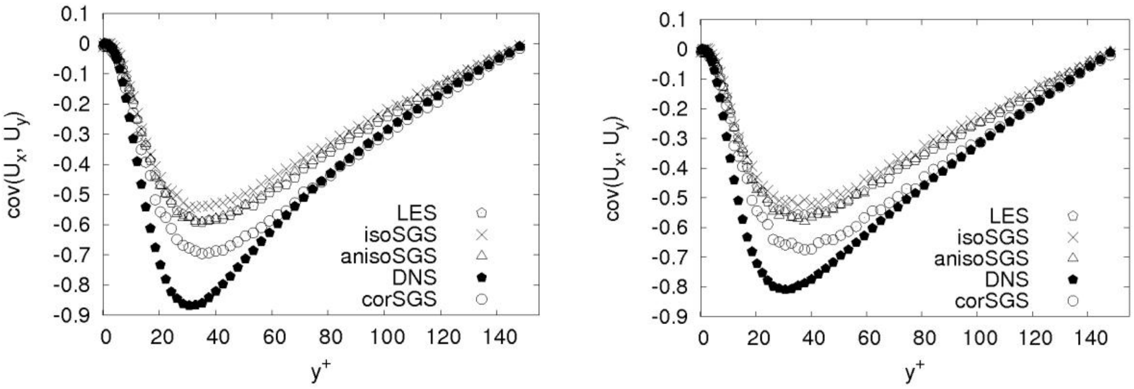


Fig.5: Covariance of streamwise and wall-normal fluid velocity at particle position from LES simulations ($C_{sg} = 0.1$): a) St = 1; b) St = 5.

## Conclusion

A stochastic model for SGS fluid velocity at particle position was presented. Four formulations were introduced and compared. Results show that for anisotropic flow, such as channel flow, model restores part of the kinetic energy lost in small scales. Formulation of correlation matrix, including covariance of the most correlated components shows to be promising, while the difference in computational effort between three formulations of the model is insignificant. The near-wall region, though, still needs attention and there is room for improvement.

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