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A new statistical model for subgrid dispersion in large eddy simulations of particle-laden flows.

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Abstract. Dispersed multiphase turbulent flows are present in many industrial and commercial applications like internal combustion engines, turbofans, dispersion of contaminants, steam turbines, etc. Therefore, there is a clear interest in the development of models and numerical tools capable of performing detailed and reliable simulations about these kind of flows. Large Eddy Simulations offer good accuracy and reliable results together with reasonable computational requirements, making it a really interesting method to develop numerical tools for particle-laden turbulent flows. Nonetheless, in multiphase dispersed flows additional difficulties arises in LES, since the effect of the unresolved scales of the continuous phase over the dispersed phase is lost due to the filtering procedure. In order to solve this issue a model able to reconstruct the subgrid velocity seen by the particles is required. In this work a new model for the reconstruction of the subgrid scale effects over the dispersed phase is presented and assessed. This innovative methodology is based in the reconstruction of statistics via Probability Density Functions (PDFs).

Keywords: LES, Lagrangian-Eulerian, SGS Model, Particle-laden flows, PDFs

1. Introduction
Multiphase flows of particles and droplets are a kind of flows characterized by the presence of two (or more) phases, with one continuous phase and another dispersed phase. This flow configuration is present in a large amount of industrial and energy conversion processes like cyclone separators, spray drying, combustion chambers, fluidized beds, etc. Most numerical investigations of particle-laden flows employ a Lagrangian-Eulerian formulation [1] where the continuous phase (the carrier phase) is solved using an eulerian framework, while the dispersed phase is solved employing a point-particle assumption (lagrangian framework), where each particle is tracked individually along his lifetime in the computational domain.

Direct Numerical Simulations (DNS) of multiphase turbulent flows with high Reynolds, like the examples presented before, are not feasible nowadays. In Large Eddy Simulations (LES), the large scale structures of the flow are well resolved and only the subgrid scales (sgs) are modeled. In contrast, in U-RANS, all the energy spectra is modeled. Therefore, LES offer good accuracy and reliable results together with reasonable computational requirements. The

equations governing the fluid-dynamic behavior of the continuous phase are the Navier-Stokes (NS) equations. In LES, the filtered NS equations are:

$$\frac{\partial \bar{\rho}}{\partial t} + \mathbf{M}\widetilde{\mathbf{u}} = \bar{S}_I \tag{1}$$

$$\frac{\partial \bar{\rho}\widetilde{\mathbf{u}}}{\partial t} = -\mathbf{C}(\bar{\rho}\widetilde{\mathbf{u}})\widetilde{\mathbf{u}} + (\mathbf{D} + \mathbf{D_{t,u}})\widetilde{\mathbf{u}} + \mathbf{G}\bar{p} + \bar{\rho}\mathbf{g} + \bar{S}_{II} \tag{2}$$

where $\widetilde{\mathbf{u}}$ is the Favre-filtered velocity vector, $\bar{p}$ the filtered pressure and $\mathbf{g}$ the gravity vector. $\mathbf{C}$ is the convective operator, $\mathbf{D}$ represents the diffusive operator, $\mathbf{D_{t,u}}$ is the modeled turbulent flux, $\mathbf{G}$ the gradient operator and $\mathbf{M}$ is the mass divergence operator. $\bar{S}$ are the source terms due to the dispersed phase effects over the continuous phase.

Regarding the dispersed phase, if this is considered as a large number of discrete spherical particles with density much larger than that of the surrounding ambient gas, the Lagrangian equations governing the motion of the dispersed phase are:

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \tag{3}$$

$$\frac{d\mathbf{v}}{dt} = \frac{\mathbf{u} - \mathbf{v}}{\tau_p} + \left(1 - \frac{\rho_g}{\rho_l}\right)\mathbf{g} \tag{4}$$

where $\mathbf{v}$ is the particle velocity and $\mathbf{u}$ is the velocity of the carrier phase at particle position.

When under the framework of LES modeling, only the large scales of the flow are well-resolved, while the subgrid scales (sgs) are modeled. In equation (4) the velocity of the carrier phase at particle position may be decomposed as $\mathbf{u} = \widetilde{\mathbf{u}} + \mathbf{u}_{sgs}$, where $\widetilde{\mathbf{u}}$ is the resolved velocity field and $\mathbf{u}_{sgs}$ represents the sgs velocity contribution that is lost during the filtering procedure applied in LES modeling.

A key aspect in the development of numerical methods for dispersed multiphase flows is to asses and study the influence and importance of the contribution of the subgrid scales on the dispersed phase. So far, in many studies and simulations the effect of the subgrid velocity over the particles has been directly neglected (it is, $\mathbf{u} = \widetilde{\mathbf{u}}$) [2][3]. This option is reasonable if there is a low residual energy content in the key regions of the computational domain. If this is not the case, and it is required to take into account the influence of the subgrid scales over the particle motion, two main approaches can be employed: deterministic models using Approximate Deconvolution Models (ADM) [4][5] and Stochastic Models [6][7]. The ADM have proven to be favorable correcting the resolved eddies near cut-off scale, but cannot be used to recover the ones below the cut-off scale. Hence, Stochastic models seem a most interesting option.

It is well-known that the instantaneous structures of a turbulent flow influence the motion of the particles depending on their inertia [8]. Some particles tend to correlate with certain eddy structures leading to the effect of preferential concentration. Among other ways to measure the preferential concentration effect present in the literature, one option is the square deviation of the measured number density from the random one [9]: $D = \sum\limits_{n=0}^{\infty} [f_d(n) - f_p(n)]^2$, where $f_d(n)$ is the discrete pdf of the simulated particles distribution and $f_p(n)$ the discrete Poisson (random) distribution. Particle inertia is characterized using the Stokes number, which is defined as the particle relaxation time normalized by the Kolmogorov time scale $St = \frac{\tau_p}{\tau_K}$.

DNS of forced isotropic turbulence tests at $Re_\lambda = 40$ with periodic boundary conditions have been performed in order to study the behavior of the dispersed phase in turbulent cases. The flow field was generated using the linear forcing technique proposed by Lundgren [10]. Particles with different weight and initial velocity equal to the gas velocity at the injected position are randomly injected inside the domain. The domain is a cube of length 2π, periodic in the three
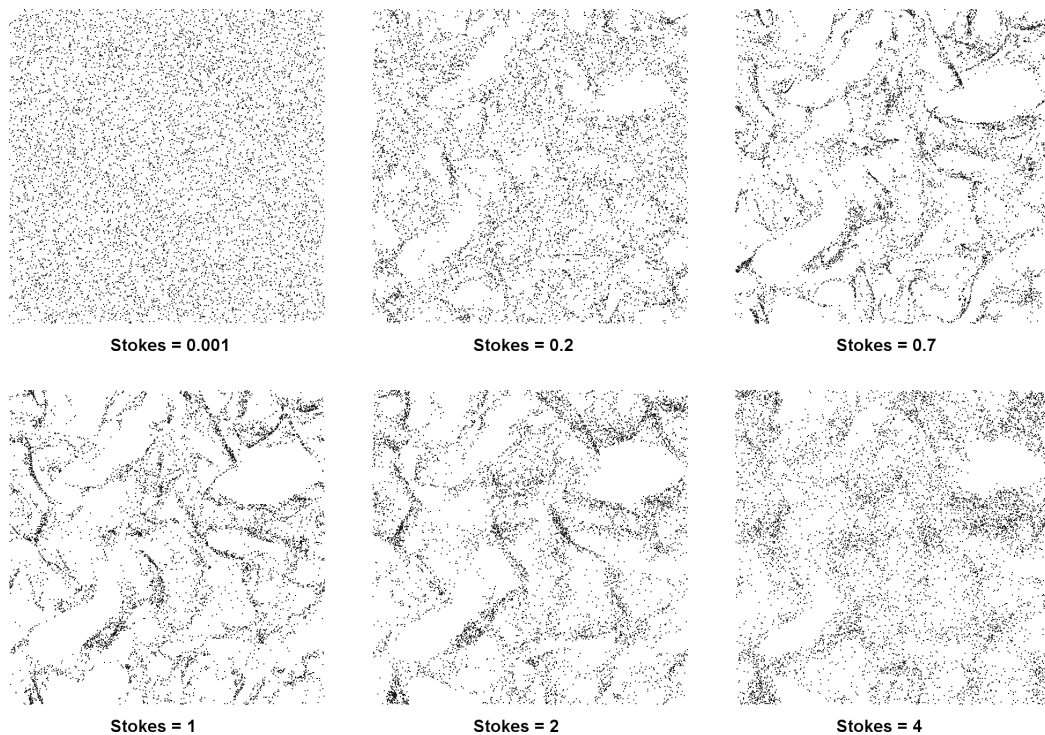
Figure 1. Snapshots of particle positions in DNS simulations.

directions and discretized in 96^3 cells. The computations were done in parallel using 96 CPUs. Each calculated particle field was composed by 64^3 discrete particles. The particle fields are assumed diluted, therefore, one-way coupling is assumed and particle collisions are neglected. The velocity-pressure coupling is solved by means of the Fractional Step Method (FSM). The Poisson equation is solved using the FFT-based Poisson Solver presented by Borrell et al. [11].

Snapshots of particle locations in a slice for different Stokes numbers are depicted in figure 1. As can be seen, particles with a Stokes number close to unity tend to correlate with certain eddy structures. Specifically, particles tend to accumulate in flow regions of low vorticity and high rate of strain, which is in agreement with previous observations [12].

The influence of the unresolved scales of the flow has been studied using two popular stochastic models that are similar in 'flavor' but differ in the mathematical derivation. The first one is the model proposed by Bini and Jones [13, 14] and the second model is the one introduced by Pozorski and Apte [12]. In order to study both models several DNS simulations have been carried out. In these simulations, the instantaneous velocity field has been spatially filtered so as to obtain a LES-like velocity field (FDNS). For each simulation, a particle field is solved using the DNS velocity field, while other particle fields are computed using the LES-like velocity field (FDNS), with and without the subgrid stochastic models and for different filter sizes Δ_f.

For small inertia particles, with Stokes number less than unity (figure 2), the preferential concentration effect is dissipated with filtering. The reason is that small-inertia particles tend to follow all the scales of the flow, including small eddies that are removed in the filtering procedure. The stochastic subgrid models not only do not fix this issue, but also worsen it, since the models tend to introduce a scattering effect.

On the other hand, as depicted in figure 3, for particles with Stokes number larger than one, preferential concentration effect seems to be enhanced by filtering. On that kind of particles inertia dominates, and small scales eddies only have a stirring effect on them, randomizing their distribution. Therefore, for this kind of particles the stochastic models help to restore
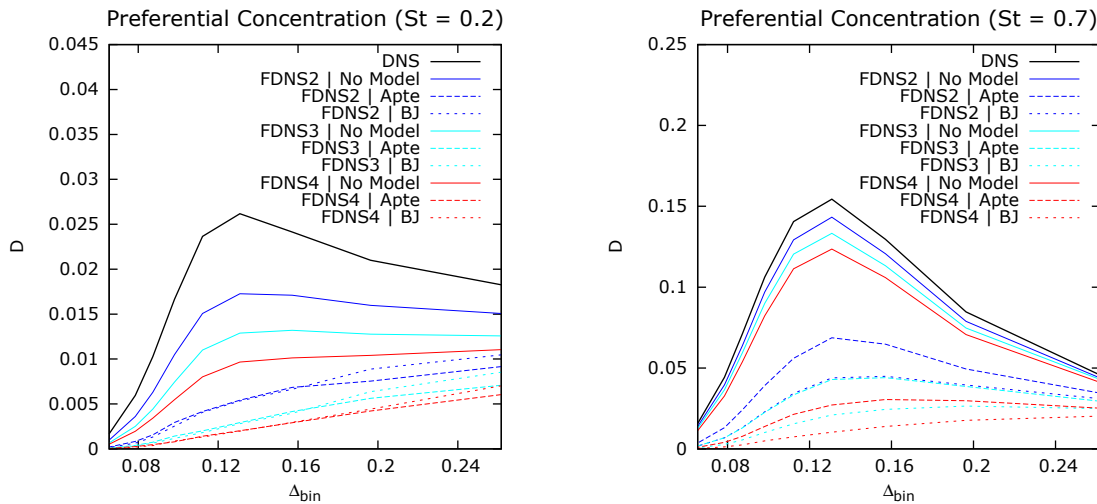
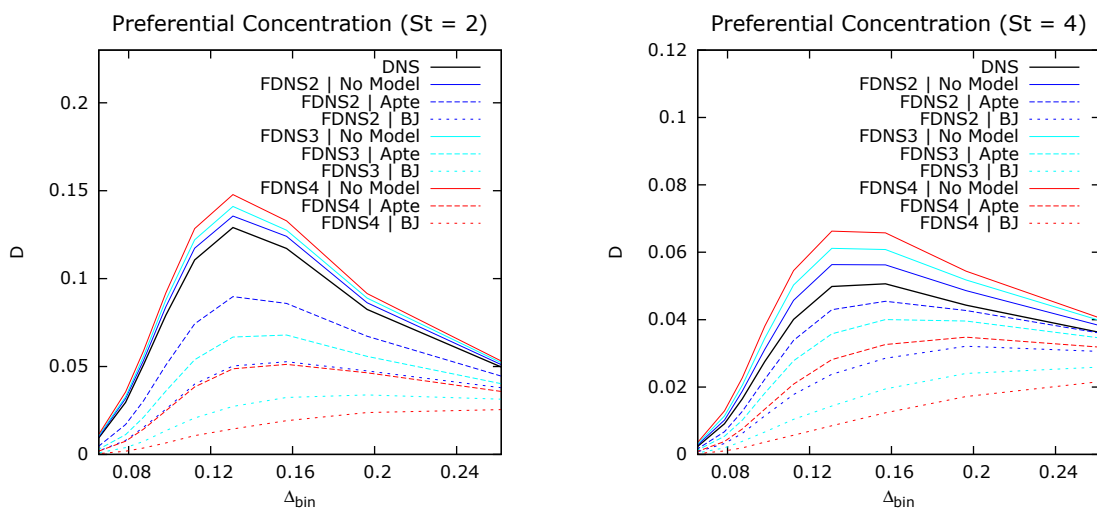**Figure 2.** Prefential concentration for cases $St < 1$.

Figure 3. Prefential concentration for cases $St > 1$.

the randomizing effect lost with filtering. However, in the current simulations, the randomizing effect introduced by the models is bigger than the stirring effect lost by filtering.

Regarding the kinetic energy of the particles, in figure 4 it can clearly be seen how the filtering procedure reduces the kinetic energy of the particles. Both subgrid stochastic models help to recover the kinetic energy level, although the models are not able to retrieve the exact kinetic energy level of the DNS simulation. Hence, at least, a better tuning or adjustment of the model constant C_0 is required. For the present cases, using $C_0 = 1$ for both models, the one of Pozorski & Apte slightly under-predicts the kinetic-energy, while the model of Bini & Jones over-predicts it. In addition, it is worth noting that the model of Bini & Jones seems to be quite more dependent on filter size Δ_f than the model of Pozorski & Apte.
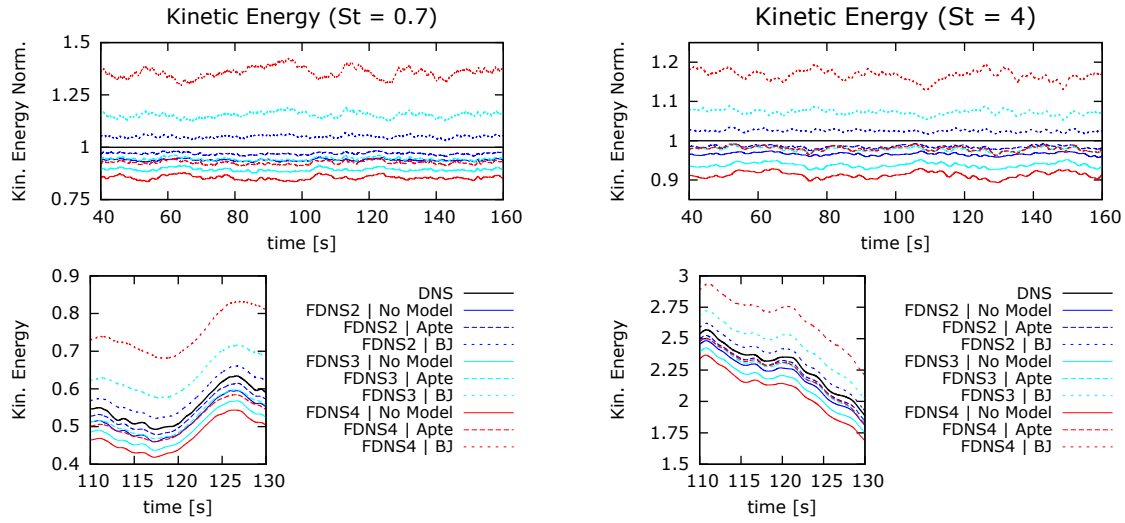
Figure 4. Kinetic Energy.

2. Methodology

Given the shortcomings and deficiencies of the presented methods, the development of a new model for subgrid dispersion of heavy particles without these downsides is investigated. Unlike the previous presented methods, the proposed new methodology is not based in a Langevin-type equation, but in the reconstruction of statistics via Probability Density Functions (pdf). The objective is the reconstruction of the subgrid scales effect over the dispersed phase lost during LES filtering, i.e. recover $\mathbf{u}_{sgs}$. Obviously, this subgrid velocity seen by the particle should be recovered and modeled using values and magnitudes ready-available in LES. In order to do so, the idea is to perform an exhaustive statistical analysis in order to obtain statistical information about how the subgrid velocity seen by the particles is related with values available in LES, like subgrid kinetic energy, vorticity, strain, etc. as a function of different parameters like the Stokes number of the particles or LES filtering size. This statistical analysis is done through DNS simulations of isotropic turbulence where the DNS velocity field is spatially filtered obtaining a LES-like velocity field, where $\mathbf{u}_{sgs}$ is ready available. The particles present in the simulation save at each time step information of the magnitude and direction of the subgrid velocity $\mathbf{u}_{sgs}$ that they see as function of different parameters, like the subgrid kinetic energy or the vorticity. In figure 5 the mean and standard deviation of the subgrid velocity magnitude ($|\mathbf{u}_{sgs}|$) as a function of the subgrid kinetic energy k_{sgs} seen for particles with different Stokes number and various filter size Δ_f are depicted. These results are for a case of isotropic turbulence $Re_\lambda = 40$. Moreover, the discrete pdf for a certain value of subgrid kinetic energy k_{sgs} is shown in figure 6. This discrete pdf can be represented as a $\beta - pdf$. So, the idea is to obtain a function that fits the mean and the standard deviation of the subgrid velocity magnitude ($|\mathbf{u}_{sgs}|$) for a certain Stokes number and a filter size. Then, this information is used in LES to reconstruct dynamically a $\beta - pdf$ representing the statistical information obtained from DNS.

In order to reconstruct $\mathbf{u}_{sgs}$ the method uses three PDFs: one for the subgrid velocity magnitude, and two others for angles θ_i with respect to directions available in LES. Using these three values the subgrid velocity $\mathbf{u}_{sgs}$ is obtained for each particle present in the simulation. Another required value is the subgrid time scale of residual motions seen by the particle τ_{sg}. Currently, this value is estimated using the subgrid kinetic energy k_{sgs} and the filter size Δ_f. However, as detailed by Jin et al. [15], the particle inertia affects the subgrid time scale seen by particles with mass. Therefore, the model should improve when including a better correlation
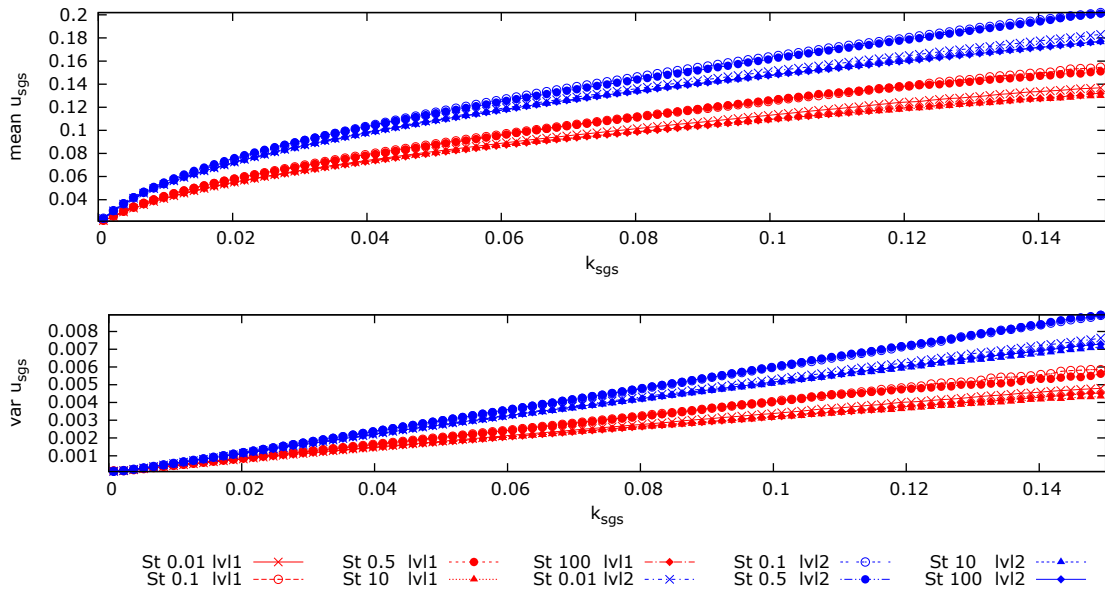
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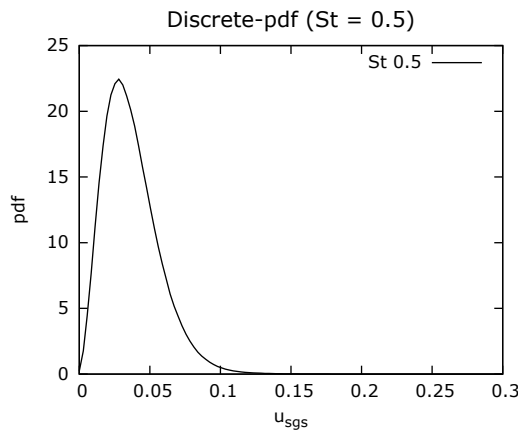**Figure 5.** Mean and Standard Dev. of subgrid velocity magnitude.

Figure 6. Subgrid velocity magnitude discrete-pdf.

to estimate τ_{sg} also using the Stokes number of the particles.

3. Results

Some preliminary simulations have been done in order to test the capabilities and performance of this new methodology. The statistical information for particles with $St = 0.5$ have been analyzed and fitted in an isotropic turbulence simulation of $Re_\lambda = 40$. Afterward, this statistical information has been used as source for the PDFs employed in the presented model. The results obtained using this model are compared against DNS, a LES without any subgrid model, and another LES using the stochastic model introduced by Pozorski & Apte [12]. Figure 7 shows the preferential concentration obtained from the simulations. As can be seen, the presented model performs better than the stochastic method of Pozorski & Apte. This improvement in the results can also be observed in figure 9, where the instantaneous spatial distribution of particles in a 2D slice is depicted. As stated in section 1, filtering dissipates the preferential
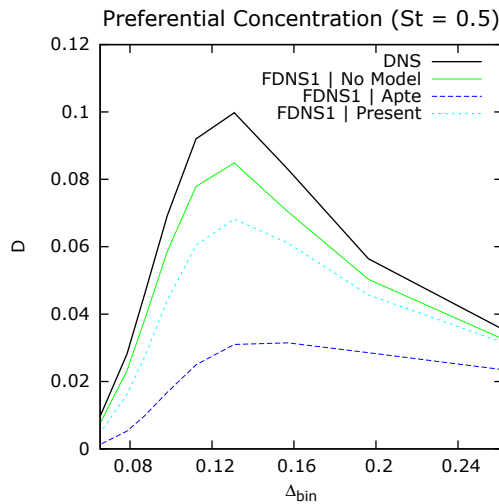
Figure 7. New model results (Preferential Concentration).
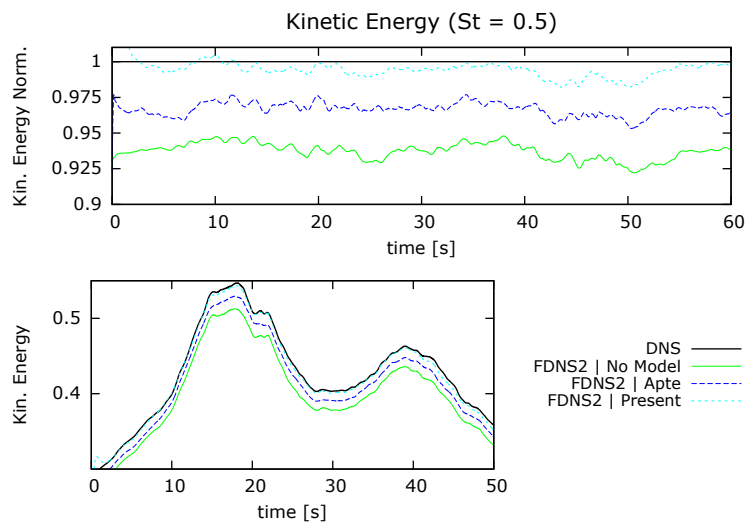

Figure 8. New model results (Kinetic Energy).

concentration effect (*DNS* vs *NO MODEL*). Moreover, the scattering effect introduced by the model of Pozorski & Apte can be clearly observed (since fewer flow structures are followed by the particles). Additionally, the present model is able to improve these results, since more large scales structures can be observed when using the present model than when using the stochastic model of Pozorski & Apte. Therefore, the new model better preserves the preferential concentration effect than the stochastic model. However, it is expected to improve this result, since there is still further work to do in order to find the directions and values best suited to estimate the subgrid velocity direction.

Regarding the kinetic energy, shown in figure 8, the proposed methodology is able to restore fairly well the kinetic energy of the particles lost due to the filtering, since the value obtained using the model is almost matching the DNS value.
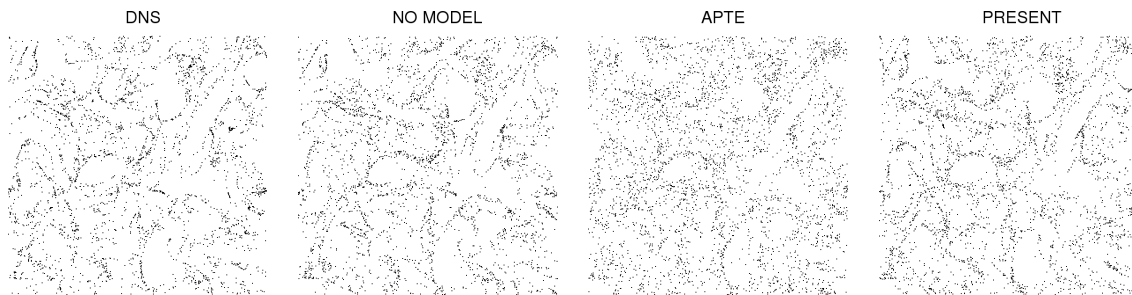
Figure 9. Snapshots of particle positions

4. Conclusions

A new model for subgrid dispersion of heavy-particles in turbulent particle-laden flows using LES has been presented and assessed. This model is based in the reconstruction of the subgrid scales lost due to LES filtering using PDFs. The idea is to employ the PDFs in order to recover statistical information of the sgs from magnitudes ready available in LES. The new model has been tested in an homogeneous-isotropic turbulent case for particles with $St = 0.5$. The obtained preliminary results look really promising and clearly shows the potential of this new method. The model recovers really well the kinetic energy of the particles which is lost with the LES filtering. Furthermore, it is able to preserve more flow scales than stochastic models, conserving better the preferential concentration effect. Nevertheless, the model is still in an embryonic stage and should be further developed. The ongoing and future research is mainly focused in the next points: i) Obtain a bigger amount of statistical information in order to 'feed' the model. ii) Improve the subgrid time scale τ_{sg} estimation. iii) Find better values and directions ready available in LES to reconstruct the subgrid velocity direction.

Acknowledgments

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