Lagrangian simulation of large and small inertial particles in a high Reynolds number flow: Stochastic simulation of subgrid turbulence/particle interactions

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This report is focused on simulation of the solid particle motion in the turbulent flow. The objective is to account for the contribution of fluid velocity fluctuations at unresolved scales in LES (Large Eddy Simulation) to the particle dynamics. To this end, we suggest that the instantaneous force acting on the particle along its trajectory is made up of a net drag force in the resolved velocity field, and a random fluctuating force, which represents the force of reaction to changes in the flow velocity at unresolved scales. Both parts represent the decomposition of the instantaneous particle acceleration on resolved and residual parts; The latter is random and needs to be modeled. Two models are developed. The first model addresses a particle, which is bigger than the Kolmogorov scale. Here we focus on the stochastic simulation of the fluctuating response time along the path of such a particle. The simulation is based on the stochastic properties of the dissipation rate in the framework of the lognormal process. The model is tested against experimental measurements, as well as against LES with standard tracking of particles. The second model is addressed to small particles subjected to strongly intermittent turbulence at subgrid scales. Here the model for the subgrid part of the particle acceleration is given by the product of two independent stochastic processes: one for the acceleration norm, the other one for its orientation. The proposed model is assessed by comparison with DNS (Direct Numerical Simulation) of Bec *et al.* (2010), and with LES using the usual tracking of particles with various spatial resolution. The advantages and drawbacks of the proposed models are discussed.

1. Introduction

Practical interest in turbulent flows laden with dispersed solid (or liquid) particles underlies mutliple laboratory studies. The numerical part of these studies is often aimed at describing the interaction between an individual particle and the carrier flow. Of the various numerical approaches, Eulerian-Lagrangian simulations (Dukowicz 1980) have demonstrated accurate results overall. In this approach, the trajectories of an ensemble of point particles moving in the fluid are given by Newton's law. For particles with a large density ratio, the simplest and, probably, the most widely used approximation is to consider the steady drag force as the only force acting on the particle

$$\mathbf{a}_p = \frac{d\mathbf{u}_p}{dt} = \frac{\mathbf{u}_f - \mathbf{u}_p}{\tau_p} \quad ; \quad \tau_p = \frac{\rho_p}{\rho_f}\frac{d_p^2}{18\nu} \ . \tag{1.1}$$

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Here $\mathbf{u}_p$ is the particle velocity, $\mathbf{u}_f$ is the flow velocity at the particle position, τ_p is the Stokes response time of a particle to changes in the relative velocity, d_p is the particle diameter, ρ_p is the particle density, and ν and ρ_f are the kinematic viscosity and the fluid density, respectively.

In turbulent flows, the velocity of the droplet motion relative to the fluid is a random quantity. Along the particle trajectory, the main contribution to the statistics of this random quantity comes from turbulent fluctuations with frequencies of the order $1/\tau_p$ and higher. Part of those frequencies is unresolved in simulation. Assuming that all turbulent frequencies along the particle path belong to the inertial range of the turbulent spectrum, the following estimate is obtained for the relative velocity (Kuznetsov & Sabel'nikov 1990)

$$\left\langle (\mathbf{u}_f - \mathbf{u}_p)^2 \right\rangle \sim \langle \varepsilon \rangle \, \tau_p \tag{1.2}$$

where $\langle \varepsilon \rangle$ is the mean viscous dissipation rate. In fact, this expression does not account for the fact that the mean viscous dissipation rate along the particle path may depend on the Stokes response time: a particle with τ_p of order of the Kolmogorov time scale is present preferentially in zones of high dissipation more often than a particle with larger τ_p, and the mean dissipation rate along the particle path is likely to be different for these two particles. However, with a certain reservations, hereafter we have adopted Eq. (1.2), assuming that the mean dissipation rate is the same along particles of different response time.

When the Large Eddy Simulation (LES) approach is used to compute the turbulent flow, the fluctuations of relative velocity $\mathbf{u}_f - \mathbf{u}_p$ are classically obtained from the filtered velocity field $\overline{\mathbf{u}}_f$, i.e.

$$\frac{d\mathbf{u}_p}{dt} = \frac{\overline{\mathbf{u}}_f - \mathbf{u}_p}{\tau_p}, \tag{1.3}$$

whereas velocity fluctuations at subgrid scales are usually discarded. The justification for this is that subgrid scales have only a minor impact on the motion of the inertial particle. However, at large Reynolds number, the flow structure at small unresolved scales may be strongly intermittent. Consequently, along the particle path, the unresolved gradients of the fluid velocity, and the kinetic energy dissipation rate, ε, may fluctuate widely at high frequencies and with large amplitude. This is illustrated in figure 1. The left-hand side of figure 1 shows the evolution of the dissipation rate along the particle trajectory computed by Bec. et al. (2010) from Direct Numerical Simulation (DNS) of homogeneous isotropic turbulence (HIT) at $\mathrm{Re}_\lambda = 400$, with immersed solid particles with Stokes number $\mathrm{St} = \tau_p/\tau_\eta = 0.1$ (τ_η being the Kolmogorov time scale). The large fluctuations of ε are observed to span over few Kolmogorov time scales. As observed in the right-hand side of figure 1, computation of the same flow by the LES approach with a quite coarse resolution (64^3 nodes) shows a much smoother evolution without any signature of intermittency. Let us consider a stochastic process giving the evolution of ε along the particle trajectory from the large-scale dynamic obtained by LES. Following the Oboukhov lognormality conjecture of the stochastic field ε (Monin & Yaglom 1981), we use the Pope & Chen (1990) stochastic equation

$$d\varepsilon = -\varepsilon \left(\ln \frac{\varepsilon}{\overline{\varepsilon}} - \frac{\sigma_\chi^2}{2} \right) T_\chi^{-1} dt + \varepsilon \sqrt{2\sigma_\chi^2 T_\chi^{-1}} dW(t) \ , \tag{1.4}$$

where $dW(t)$ is the increment of standard Brownian process, i.e., $\langle dW(t) \rangle = 0$, $\langle dW(t)^2 \rangle = dt$. Note that in contrast to the equation of Pope & Chen (1990), the locally resolved

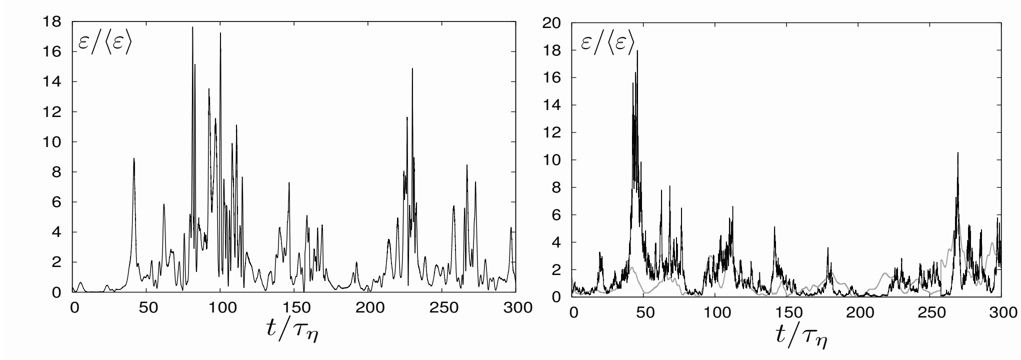

FIGURE 1. Right: evolution of the turbulent dissipation rate $\varepsilon = \nu S_{ij}S_{ij}$ (S_{ij} is the deformation rate tensor) along a particle trajectory, at St = 0.1 and $\mathrm{Re}_\lambda = 400$ (data are obtained from DNS of Bec *et al.* (2010)). Left: evolution of the dissipation rate from LES $\overline{\varepsilon} = (\nu + \nu_t)\overline{S}_{ij}\overline{S}_{ij}$ ($\overline{S}_{ij}$ being the resolved deformation rate tensor) at $\mathrm{Re}_\lambda = 400$ with a 64^3 nodes resolution (grey line) and a realization of the stochastic model given by Eqs. (1.4)-(1.5) (black line).

dissipation rate $\overline{\epsilon}$ is used instead of its mean value, and the parameters are chosen as a function of the mean eddy-viscosity $\langle\nu_t\rangle$, the Kolmogorov scale η and the spatial resolution Δ

$$T_\chi = \frac{\nu_t}{\Delta^2}\ ,\ \sigma_\chi^2 = \ln\frac{\Delta}{\eta}\ . \tag{1.5}$$

The right-hand side of Fig. 1 presents a sample path of the stochastic process (1.4) with $\overline{\epsilon}(t)$ obtained from the LES. It is seen that the signal is strongly intermittent, similar to that in the DNS and in contrast to the dissipation in the LES $\overline{\epsilon}(t)$. It is to be expected that the particle along its path may be responsive to some extent to the subgrid flow fluctuations. But how then can we account for the contribution of such fluctuations on the particle dynamics? To introduce the influence of the subgrid scale fluctuations, we propose to decompose the instantaneous force acting on a particle in a drag force given by the velocity field at resolved scales, and a randomly fluctuating force, which represents the force due to the fluctuations of the flow velocity at unresolved scales. In other words, we suggest that, in the LES framework, the instantaneous acceleration of the particle is the sum of two parts

$$\frac{d\mathbf{u}_p}{dt} = \overline{\left(\frac{d\mathbf{u}_p}{dt}\right)} + \left.\frac{d\mathbf{u}_p}{dt}\right|_\varepsilon\ , \tag{1.6}$$

where the first terms on the right hand side denotes for the particle acceleration in the resolved fluid velocity field, and the second term is random and represents the particle acceleration conditionally averaged on the instantaneous dissipation rate ε along the particle path. The latter needs to be modeled from the presumed statistical properties of ε. In our work, we propose such a model along with its assessment.

Our work also focus on particles of finite size compared to the Kolmogorov length scale η. The underlying question is to characterize the motion of such an inertial particle, when $d_p > \eta$, where, consistent with the LES framework, d_p is still assume much smaller than the resolved length scale. As a brief introduction to this model, let $d\mathbf{P}/dt$ be the momentum exchanged per unit of time between a particle and the fluid. Assuming that $d\mathbf{P}$ is determined as the mass of the fluid entrained by the moving particle $\rho_f u'\pi d^2/4\ dt$ (where according to Kolmogorov scaling $u' \sim \langle\varepsilon\rangle^{1/3}d_p^{1/3}$) multiplied by the relative velocity $\mathbf{u}_f - \mathbf{u}_p$, we write Newton's law in the following form

$$\frac{\pi d_p^3}{6}\rho_p \frac{d\mathbf{u}_p}{dt} = \rho_f \frac{\pi d_p^2}{4} \left(\mathbf{u}_f - \mathbf{u}_p\right) \langle\varepsilon\rangle^{1/3} d_p^{1/3} \ , \tag{1.7}$$

which reduces to

$$\frac{d\mathbf{u}_p}{dt} = \frac{3}{2}\frac{\rho_f}{\rho_p}\frac{\langle\varepsilon\rangle^{1/3}}{d_p^{2/3}} \left(\mathbf{u}_f - \mathbf{u}_p\right) \ . \tag{1.8}$$

It can be seen from (1.8) that because $d_p > \eta$, the fluctuations of the response time may also contribute to statistics of the particle acceleration.

In section 2, we will first focus on the contribution of the fluctuating response time for particle larger than the Kolmogorov scale, in connection with Eqs. (1.6) and (1.8). The derivation of the model is given and compared to results from a standard LES approach as well as from experimental results Then in section 3, in view of Eqs. (1.2) and (1.6), we present a model that includes the contribution of fluid velocity fluctuation at unresolved scales in the motion of particles that are much smaller than the Kolmogorov scale.

2. Statistics of the acceleration for a particle with a fluctuating response time

First, we suggest that when the particle diameter is larger than the Kolmogorov scale, $d_p > \eta$, the particle equation of motion Eq. (1.1) is controlled not only by laminar viscous effects, but also by the eddy viscosity $\nu_{p,t}$, which is "seen" by a moving particle, and is defined by turbulent length scales $\ell_{turb} \leq d_p$. Thus, we rewrite the particle response time as follows

$$\tau_{p,t} \sim \frac{\rho_p}{\rho_f}\frac{d_p^2}{\nu + \nu_{p,t}} \ . \tag{2.1}$$

Note that the 1/18 factor in Eq. (1.1) has been omitted for sake of brevity. Estimation of the turbulent viscosity in terms of the Kolmogorov's scaling gives

$$\nu_{p,t} \sim u' d_p \sim \langle\varepsilon\rangle^{1/3} d_p^{4/3} \ , \tag{2.2}$$

and inserting Eqs. (2.1) and (2.2) into Eq. (1.1), we find (consistent with Eq. (1.8)):

$$\frac{d\mathbf{u}_p}{dt} = \frac{\overline{\mathbf{u}}_f - \mathbf{u}_p}{\tau_p} + \frac{\rho_f}{\rho_p}\frac{\langle\varepsilon\rangle^{1/3}}{d_p^{2/3}} \left(\overline{\mathbf{u}}_f - \mathbf{u}_p\right) \ . \tag{2.3}$$

Here again, the over line denotes the filtered velocity at the particle location, and the filter width imposed much larger than the particle diameter. We now consider Eq. (2.3) in view of the decomposition given in Eq. (1.6):

$$\frac{d\mathbf{u}_p}{dt} = \overline{\left(\frac{d\mathbf{u}_p}{dt}\right)} + \left.\frac{d\mathbf{u}_p}{dt}\right|_{\varepsilon} \ . \tag{2.4}$$

where

$$\left.\frac{d\mathbf{u}_p}{dt}\right|_{\varepsilon} = \frac{\rho_f}{\rho_p}\frac{\varepsilon^{1/3}}{d_p^{2/3}} \left(\overline{\mathbf{u}}_f - \mathbf{u}_p\right) \ . \tag{2.5}$$

To estimate the value of $\varepsilon^{1/3}$ "seen" by the particle in Eq. (2.5), we apply the Ito transformation to the Pope & Chen (1990) Eq. (1.4) to obtain the following stochastic equation

$$d\varepsilon^{1/3} = -\varepsilon^{1/3}\left(\ln\frac{\varepsilon^{1/3}}{\overline{\varepsilon}^{1/3}} - \frac{\sigma_\chi^2}{18}\right) T_\chi^{-1} dt + \frac{1}{3}\varepsilon^{1/3}\sqrt{2\sigma_\chi^2 T_\chi^{-1}} dW(t) \ . \tag{2.6}$$

Note that the use of the local value $\overline{\varepsilon}$, provided by the LES of the fluid, introduces spatial correlations in the solution of Eq. (1.5). In order to assess the model given by Eq. (2.4)-(2.6) along with parameters from Eq. (1.4), we ran a set of simulations corresponding to five particle diameters: $d_p/\eta = 0.3$, 0.6, 1, 1.5, and 2 and with density ratio $\rho_p/\rho_f = 900$. The fluid phase is simulated by LES using the Smagorinsky model for the eddy-viscosity ν_t. The Reynolds number based on the Taylor scale is $Re_\lambda = 400$, and the mesh consists of 64^3 nodes. Each particle is tracked according to Eq. (2.4) - (2.5), where the instantaneous dissipation rate is determined from the stochastic process (2.6). In figure 2, the probability density function (PDF) of the particle acceleration, for the five particle diameters, is compared with the PDF obtained when the force acting on the particles is given by the classical Stokes drag law (1.3). Those PDFs are also compared to the relation:

$$P(x) = \frac{e^{3s^2/2}}{4s\sqrt{3}} \left[1 - \text{erf}\left(\frac{\ln\left(|x/\sqrt{3}|\right) + 2s^2}{\sqrt{2}s} \right) \right] , \tag{2.7}$$

with parameter s, associated with the lognormal distribution of the acceleration amplitude (Mordant *et al.* 2004). Qureshi *et al.* (2008) performed an experimental measurement of the acceleration of particles larger than the Kolmogorov scale. They found that the PDFs of the normalized acceleration collapse onto a single curve for all the parameter values considered in their experiments (d_p/η ranges from 12 to 25 and the density ratio from 1 to 65, along with $\text{Re}_\lambda \sim 160$). In addition, they observed that the experimental measurement of Ayyalasomayajula *et al.* (2006) for a much smaller and heavier particles ($d_p/\eta \sim 0.05$ and $\rho_p/\rho_f = 1000$) also collapses on the same curve, which is very well approximated by the previous relation with $s = 0.62$. They conclude that the statistics of inertial particle acceleration exhibit finite size effect even for very small particles. Figure 2 indicates that the model allows stretched tails to be developed in the PDFs, in remarkable agreement with the experimental fit, while results from the standard Stokes law (1.3) exhibit narrow distributions, becoming narrower with increasing particle diameter. Note that the non-linear drag correction for finite particle Reynolds number proposed in Clift *et al.* (1978) does not significantly alter the shape of the distribution, but is not shown for the sake of clarity. As observed in the experiment of Qureshi *et al.* (2008), when the model (2.4)-(2.6) is used, the shape of the PDF remains unchanged if particle size is modified.

3. Statistics of the acceleration of a small particle accounting for fluid velocity fluctuations at unresolved scales

In this section we propose a model to account for the fluid fluctuations at unresolved scales in the dynamics of small inertial particles. The model is based on the expression of the particle acceleration resulting from the subgrid scale of the flow $\left.\frac{d\mathbf{u}_p}{dt}\right|_\varepsilon$ in Eq. (1.6), as the product of two independent stochastic processes

$$\left.\frac{d\mathbf{u}_p}{dt}\right|_\varepsilon = a'_p \mathbf{e}_p , \tag{3.1}$$

where a'_p is the random modulus of acceleration at subgrid scales, and $\mathbf{e}_p$ is its random unit vector of orientation. Following the estimation provided by Eq. (1.2), the stochastic

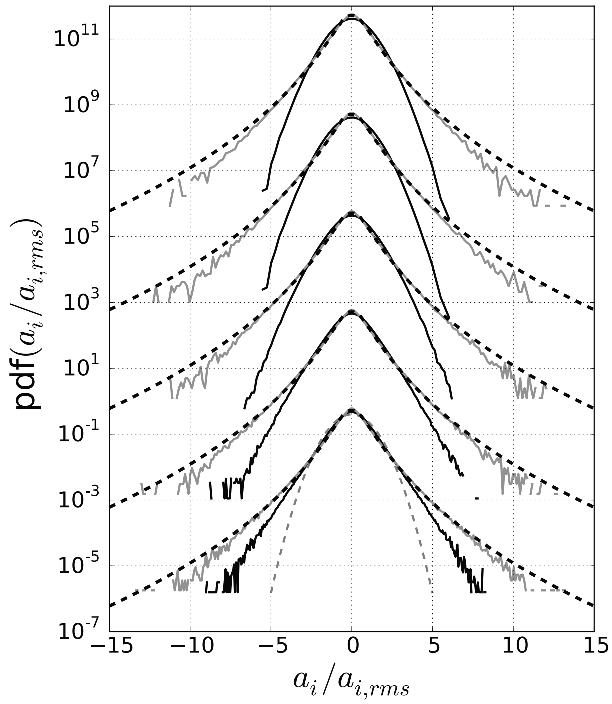

FIGURE 2. PDF of the particle acceleration, for 5 particle diameters (equal to 0.3, 0.6, 1, 1.5 and 2 times the Kolmogorov length scale from bottom to top) for a density ratio of 900. PDF are normalized by the particle acceleration variance. Comparison between the regular LES (black lines), LES with the stochastic model (grey lines), the normal distribution (grey dashed line) and the experimental fit from Qureshi *et al.* (2008) (black dashed lines).

process for a'_p is defined by the stochastic process for ε

$$a'_p \sim \sqrt{\frac{\varepsilon}{\tau_p}} \ . \tag{3.2}$$

Here again, applying the Ito transformation to the Pope & Chen (1990) equation (1.4) to have a stochastic estimate of $\sqrt{\varepsilon}$ at the particle position, we have

$$d\varepsilon^{1/2} = -\varepsilon^{1/2} \ln \frac{\varepsilon^{1/2}}{\overline{\varepsilon}^{1/2}} - T_\chi^{-1} dt + \frac{1}{2}\varepsilon^{1/2}\sqrt{2\sigma_\chi^2 T_\chi^{-1}} dW(t) \ . \tag{3.3}$$

We used the same parameters as thos used previously in Eq. (1.5). The second stochastic process is for the unit vector of orientation $\mathbf{e}_p$ of the particle subgrid acceleration. The components of this vector $e_{p,i}(t)$ are assumed to be correlated over a Kolmogorov time scale τ_η, and $e_{p,i}e_{p,i} = 1$. The following stochastic equation, representing a Brownian motion on the unit sphere, models the evolution of $\mathbf{e_p}(t)$:

$$d\mathbf{e}_p = \left(\frac{2}{\tau_\eta}\right)^{1/2} \mathbf{e}_p \times \circ d\mathbf{W} \ , \tag{3.4}$$

where $\mathbf{W} = (W_1, W_2, W_3)$ is the standard Brownian motion, and $\circ d$ denotes the use of Stratonovich calculus. To assess the coupling of Eq. (2.4) and Eqs. (3.1)-(3.4) with LES, we simulate $\mathrm{Re}_\lambda = 400$ with a 64^3 mesh for four Stokes numbers $\mathrm{St} = 0.16$, 0.6, 1 and 2.

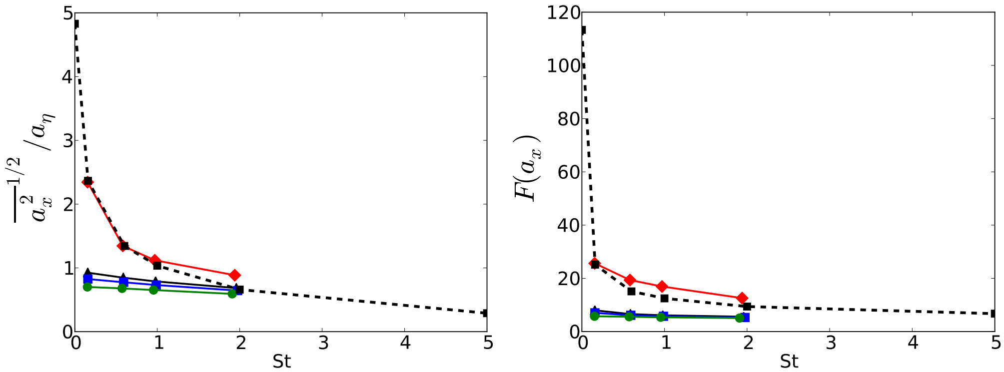

FIGURE 3. Evolution of variance (on the left-hand side) and of flatness (on the right-hand side) of the particle acceleration with the Stokes number. Comparison between LES with 64^3 grid nodes with use of stochastic model (2.4), (3.1)-(3.4): red diamonds; LES linked to (1.3) for three resolutions (64^3: green circles, 96^3: blues squares, 128^3: black triangles), and DNS form Bec *et al.* (2010): dashed lines.

These simulations are compared with the DNS of Bec *et al.* (2010), and with a reference LES (without the second term in Eq. (1.6)) for three resolutions (64^3, 96^3 and 128^3). In the DNS and the reference LES, the particles are dragged by Eq. (1.3).

In figure 3, the variance and flatness of the particle acceleration are shown for the different Stokes numbers. According to the DNS, both statistical moments decrease sharply with increasing the Stokes number. A similar behavior is observed in figure 3 when the LES are supplemented by Eq. (2.4) and Eqs. (3.1)-(3.4), whereas the LES along with Eq. (1.3) reproduces this effect of the Stokes number much less accurately even when the resolution is increased significantly. From other side, it is to note that when the LES is supplemented with the stochastic model, the flatness of the particle acceleration is overestimated compared with the DNS. In figure 4, the PDFs of the particle acceleration from the LES with Eqs. (2.4), (3.1)-(3.4) are shown for the different Stokes numbers, and are compared with the reference LES for the three resolutions and with the DNS of Bec *et al.* (2010). In this figure, the PDFs are normalized by the particle acceleration variance. Although for $\mathrm{St} = 0.16$ and $\mathrm{St} = 0.6$, the stochastic model Eqs. (2.4), (3.1)-(3.4) matches quite well the PDF from DNS, for the two higher Stokes numbers, $\mathrm{St} = 1$ and $\mathrm{St} = 2$, this model leads to PDF with wider tails than the DNS. In figure 5 the autocorrelation of the particle acceleration along its trajectory are presented to $\mathrm{St} = 1$ and $\mathrm{St} = 2$ for the LES supplemented with Eqs. (2.4), (3.1)-(3.4), for the DNS and for the reference LES at three resolutions. The autocorrelation obtained with the use of the stochastic model is closer to the autocorrelation given by the DNS, in contrast to the LES with Eq. (1.3). Nevertheless, at short time lags (on the order of a few Kolmogorov times), it is observed that the decorrelation is too fast with the stochastic model; this is a manifestation of excessive forcing provided by the model in the unresolved high-frequency part of the spectra.

4. Conclusion

The main objective of this work has been to account for turbulent fluctuations at unresolved scales in LES of particle laden flow. To this end, we propose that the instantaneous acceleration of the particle may be decomposed in the sum of two parts: the first part is

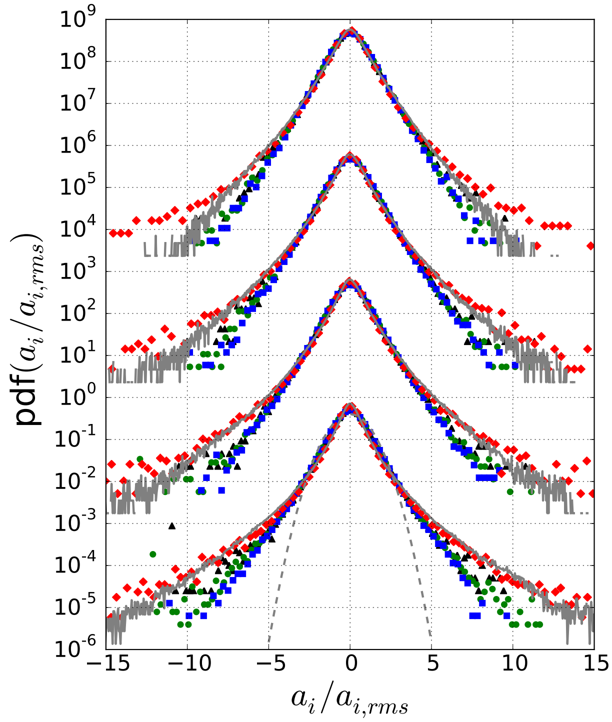

FIGURE 4. PDF of the particle acceleration, for four Stokes number: St = 0.16, 0.6, 1 and 2 from bottom to top, respectively. Comparison between LES linked to (1.3) for three resolutions (64^3: green circles, 96^3: blues squares, 128^3: black triangles); DNS form Bec *et al.* (2010): grey lines; and LES with stochastic model (2.4), (3.1)-(3.4) and 64^3 resolution: red diamonds. PDF are normalized by the particle acceleration variance. Grey dashed line represents the normal distribution.

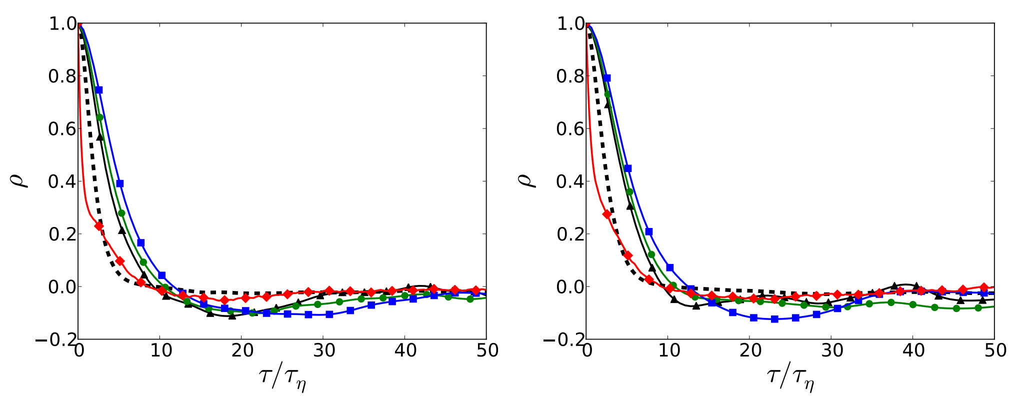

FIGURE 5. Autocorrelation of the particle acceleration along the particle trajectory for St = 1 (on the left-hand side) and St = 2 (on the right-hand side). Comparison between LES with 64^3 grid nodes with use of stochastic model (2.4), (3.1)-(3.4): red diamonds; LES linked to (1.3) for three resolutions (64^3: green circles, 96^3: blues squares, 128^3: black triangles), and DNS form Bec *et al.* (2010): dashed lines.

given by particle acceleration due to the resolved fluid velocity field, and the second part is random. The random part represents the particle acceleration conditionally averaged on the instantaneous dissipation rate along the particle path. Two models have been studied.

The first model considers that for particles larger than the Kolmogorov scale, the relaxation time of the particle (or equivalently, its drag coefficient) is random. In the model proposed, this random response time appears in the subgrid part of the particle acceleration as a function of the dissipation rate on scales of the size of the particle. To model the latter we propose a stochastic equation. The LES of HIT with particles using this stochastic equation assesses by experimental data from the literature, and the advantage of the proposed model is shown. The strongly non-Gaussian PDFs, invariant to the fluid-to-particle density ratio and to the diameter-to-Kolmogorov scale ratio, were obtained in agreement with experimental measurements, in contrast to the case of standard tracking of the particles.

The second model focus on the contribution of unresolved turbulent frequencies of the fluid velocity to the motion of small particles. We propose that the subgrid part of the particle acceleration is given by the product of two independent processes. One is for the modulus, which is also expressed by the stochastic properties of the dissipation rate. The other is for the orientation of the particle acceleration and is given by a Brownian motion on the unit sphere with correlation in time controlled by the Kolmogorov time. The proposed model is assessed by comparison with the DNS, and with the LES using the usual particle tracking. The behavior of the acceleration variance with increasing Stokes number is predicted fairly well compared to the case of standard tracking of particles. The detailed statistics also showed that this model successfully predicts the DNS particle statistics when the Stokes number is less than unity. However, for Stokes numbers larger than one, the model leads to an excessive contribution at subgrid scales: too extended tails in PDF of acceleration and a too fast decay of the acceleration autocorrelation are observed. This implies that the model needs to be improves for short times of order of the Kolmogorov time scale. In future researches, it is anticipated that the viscous effect in Eq. (3.3) will be introduces as well as accounting for the particle inertia in Eq. (3.4).

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