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Ideal stochastic forcing for the motion of particles in large-eddy simulation extracted from direct numerical simulation of turbulent channel flow

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The motion of small particles in turbulent conditions is influenced by the entire range of length- and time-scales of the flow. At high Reynolds numbers this range of scales is too broad for direct numerical simulation (DNS). Such flows can only be approached using large-eddy simulation (LES), which requires the introduction of a sub-filter model for the momentum dynamics. Likewise, for the particle motion the effect of sub-filter scales needs to be reconstructed approximately, as there is no explicit access to turbulent sub-filter scales. To recover the dynamic consequences of the unresolved scales, partial reconstruction through approximate deconvolution of the LES-filter is combined with explicit stochastic forcing in the equations of motion of the particles. We analyze DNS of high-Reynolds turbulent channel flow to *a priori* extract the ideal forcing that should be added to retain correct statistical properties of the dispersed particle phase in LES. The probability density function of the velocity differences that need to be included in the particle equations and their temporal correlation display a striking and simple structure with little dependence on Reynolds number and particle inertia, provided the differences are normalized by their RMS, and the correlations expressed in wall units. This is key to the development of a general “stand-alone” stochastic forcing for inertial particles in LES. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4745857>]

We focus on the problem of “statistically consistent” particle tracking in high-Reynolds number turbulent flow. Euler-Lagrange simulation of the motion of inertial point particles in turbulence adopts particle acceleration that depends on the fluid velocity at the particle position. In direct numerical simulation (DNS) this velocity is known after interpolation, but in large-eddy simulation (LES) only the spatially filtered fluid velocity is resolved. We use DNS of turbulent channel flow at different Reynolds numbers to extract *a priori* high-Reynolds asymptotics for the “ideal” stochastic forcing that would be required for particles to be dispersed statistically correctly in the LES flow field. This extends recent work ¹ to high Reynolds number flows. The “ideal” high-Reynolds forcing is found to have little dependence on particle inertia and Reynolds number, a prerequisite to developing a successful general “stand-alone” stochastic acceleration term for turbulent dispersion in LES.

The problem of restoring the influence of the unresolved scales in LES on the particle motion stimulated the development of several models. These can be classified into two categories. The first class uses phenomenological stochastic forcing directly added as velocity differences to the equation of motion,² or indirectly, adding broadband forcing to the momentum equations.³ The second class applies approximate deconvolution^{4,5} of the fluid velocity to retrieve some of the small scale energy.⁶

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Using approximate deconvolution one may predict preferential concentration of inertial particles and in particular turbophoresis in wall-bounded flows at relatively modest Reynolds numbers. It turns out that the effects of the sub-filter scales cannot be omitted if the particle relaxation time is of the same order of magnitude as the Kolmogorov time.^{7,8} At larger Reynolds numbers, the deconvolution improvement for the turbulent stresses was found to be insufficient.⁹ Here, we investigate adding an explicit stochastic model term in the particle equation of motion, representing the effect of the unresolved scales more accurately. We propose a “mixed” model; the approximate deconvolution of the resolved velocity field in LES is expected to recover energy at the smaller resolved scales, whereas the stochastic model should provide a model for the smallest, fully unresolved scales. As a first step in the development of a combined deconvolution-stochastic-forcing model we use DNS of particle-laden turbulent channel flow and determine the probability density function (PDF) of the velocity differences and their temporal correlation at various particle sizes.

We consider DNS of turbulent particle-laden incompressible channel flow, in which the particles are represented in a Lagrangian way as point particles. The mass fraction of the particles is considered low enough to safely neglect the effect of these particles on the flow and, in addition, the volume fraction is thought to be sufficiently low to also neglect particle-particle interactions. The fluid satisfies the incompressible flow equations

$$\nabla \cdot \mathbf{u} = 0; \quad \frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\rho} \nabla p = \mathbf{f} - \boldsymbol{\omega} \times \mathbf{u} + \nu \nabla^2 \mathbf{u}, \quad (1)$$

where ρ , ν , and \mathbf{u} denote mass density, kinematic viscosity, and velocity of the fluid, p total pressure, $\boldsymbol{\omega}$ vorticity, and t time. The equations are made non-dimensional using as reference scales the mass density, half the channel height, H , and the friction velocity, u_τ , so that Re_τ is the friction Reynolds number given by $\text{Re}_\tau = Hu_\tau/\nu$. Time is made dimensionless with timescale $\tau = \nu/u_\tau^2$. The friction Reynolds number of the flow is kept fixed by prescribing the mean pressure gradient per unit mass \mathbf{f} in the streamwise direction parallel to the plates. The gas velocity satisfies no-slip conditions at the two plates. In the other two directions periodic boundary conditions are applied for velocity and pressure. We will use x , y , and z for the streamwise, wall-normal, and spanwise coordinates and directions.

The motion of a particle is determined by the forces acting on it. If the particles are small and have a mass density that is high compared to the mass density of the gas, the drag force exerted by the gas is by far dominant.¹⁰ The governing equation for each particle is taken as

$$\frac{d\mathbf{v}}{dt} = \frac{\mathbf{u}(\mathbf{x}, t) - \mathbf{v}}{\tau_p}, \quad (2)$$

completed with the kinematic condition $d\mathbf{x}/dt = \mathbf{v}$. Here $\mathbf{u}(\mathbf{x}, t)$ denotes fluid velocity at the particle position \mathbf{x} at time t and \mathbf{v} the particle velocity. Moreover, τ_p is the particle relaxation time given by $\tau_p = \rho_p d_p^2 / (18\rho\nu)$, where d_p and ρ_p denote diameter and mass density of a particle. The particle relaxation time in wall units is used to define the Stokes number.

In LES, $\mathbf{u}(\mathbf{x}, t)$ is unknown, but ideally a filtered velocity, denoted by $\bar{\mathbf{u}}(\mathbf{x}, t)$ is available. The difference between the unfiltered and filtered fluid velocity at a particle position can be considered as the term which should be added to the particle equation of motion. In particular, we have in *a priori* LES

$$\frac{d\mathbf{v}}{dt} = \frac{\bar{\mathbf{u}}(\mathbf{x}, t) - \mathbf{v}}{\tau_p} + \frac{\delta\mathbf{u}}{\tau_p}, \quad (3)$$

where $\delta\mathbf{u} = \mathbf{u}(\mathbf{x}, t) - \bar{\mathbf{u}}(\mathbf{x}, t)$. Using DNS the statistical properties of $\delta\mathbf{u}$ can be determined when particles are tracked with the actual unfiltered velocity and $\bar{\mathbf{u}}$ is determined by explicit filtering of the DNS velocity field. This allows to infer properties of the “ideal” subfilter forcing that would be required. The explicit filter applied in this work is the top-hat filter, which will be specified momentarily. We will also investigate a possible combination of approximate deconvolution and stochastic forcing. Correspondingly, we rewrite (2) as

$$\frac{d\mathbf{v}}{dt} = \frac{\mathbf{u}^*(\mathbf{x}, t) - \mathbf{v}}{\tau_p} + \frac{\delta\mathbf{u}^*}{\tau_p}, \quad (4)$$

where $\delta\mathbf{u}^* = \mathbf{u}(\mathbf{x}, t) - \mathbf{u}^*(\mathbf{x}, t)$ in terms of the deconvolved fluid velocity field \mathbf{u}^* . From the DNS \mathbf{u}^* can be explicitly computed by applying the approximate inverse of the filter to the filtered fluid velocity field. We approximate the inverse top-hat filter by taking the first five terms in the geometric series approximation for the formal inverse.⁵

The numerical method used to simulate the turbulent channel flow adopts a pseudo-spectral discretization in the periodic directions, whereas the wall-normal direction is treated by a Chebyshev-tau method. For integration in time a combination of a second-order accurate three-stage Runge-Kutta method and the implicit Crank-Nicolson method is chosen.¹¹ The particle equations of motion are integrated in time with the same Runge-Kutta method as the nonlinear terms in the Navier-Stokes equation. In the DNS the fluid velocity is interpolated to the particle position by tri-linear interpolation. More accurate interpolation methods do not lead to significantly different results for the statistical properties we consider in this paper. For the determination of $\bar{\mathbf{u}}(\mathbf{x}, t)$ and $\mathbf{u}^*(\mathbf{x}, t)$ use is made of fourth-order accurate interpolation, since the filtered and deconvolved velocity field are evaluated on a coarser LES grid. This fourth-order interpolation is a combination of Lagrange interpolation in the two periodic directions and Hermite interpolation in the wall-normal direction. In the two periodic directions the explicit top-hat filter is applied in spectral space by multiplication with the Fourier transform of the filter kernel. In the wall-normal direction the integral in the top-hat filter is approximated by the trapezoidal rule.

Simulations are performed at three different values of the friction Reynolds number, 150, 395, and 950. For all three flow conditions the resolution was confirmed adequate by comparison of the results of mean velocity, Reynolds stresses, and turbulent dissipation rate with literature results. The value of Δx^+ , the streamwise grid spacing in wall units, ranges in the DNS between 14 at $Re_\tau = 150$ and 8 at $Re_\tau = 950$. The spanwise grid spacing in wall units is smaller by a factor of 2. The coarse LES grid used for the filtered and deconvolved velocity field satisfies the conditions for resolved LES.¹² This implies that Δx^+ has a value between 60 and 80 and Δz^+ ranges between 15 and 20 and the wall-normal grid spacing near the wall $\Delta y^+ < 2$.

Particles are inserted in a developed, statistically steady turbulent flow using a uniform random distribution. The initial particle velocity equals the fluid velocity at the particle position. Particles of four different Stokes numbers are considered, ranging between 0.2 and 25, and of each type 32 000 particles are tracked. Every ten time steps $\mathbf{u}(\mathbf{x}, t)$, $\bar{\mathbf{u}}(\mathbf{x}, t)$, and $\mathbf{u}^*(\mathbf{x}, t)$ are written to file for later analysis. This makes it possible to calculate moments, time correlation functions and probability density functions of $\delta\mathbf{u}$ and $\delta\mathbf{u}^*$. We turn our attention to these quantities next.

An impression of the RMS of the wall-normal velocity component and wall-normal subfilter velocity differences is given in Fig. 1 using the simulation at $Re_\tau = 950$ and particles with $St = 1$. The chosen filter removes approximately 20% of the peak RMS values, when comparing DNS

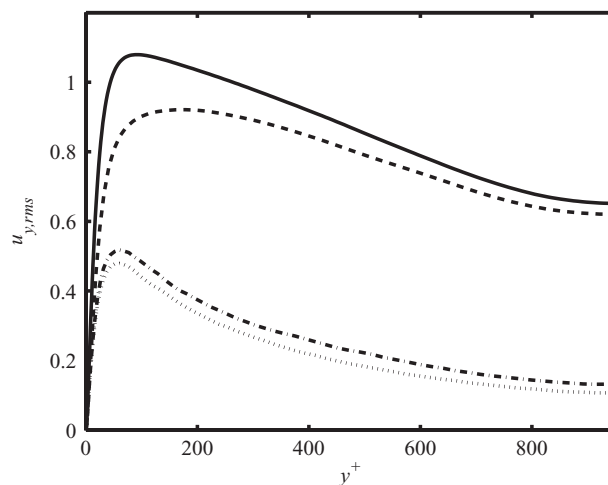


FIG. 1. RMS of wall-normal velocity component as a function of y^+ for $Re_\tau = 950$; solid: DNS result, dashed: filtered DNS result, dashed-dotted: δu_y for particles with $St = 1$, and dotted: δu_y^* for particles with $St = 1$.

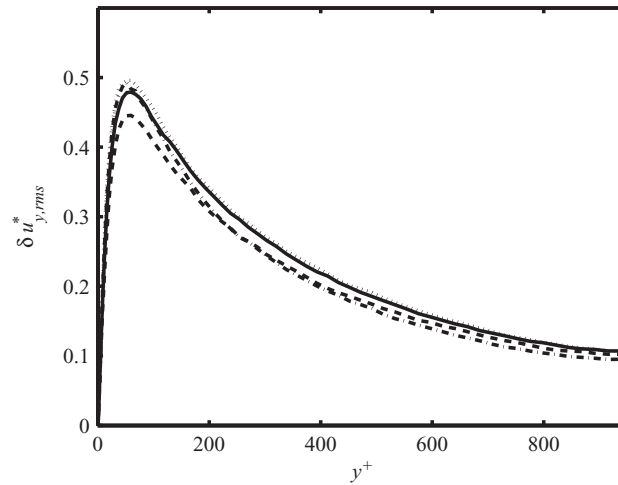


FIG. 2. Root-mean square of δu_y^* as a function of y^+ for $Re_\tau = 950$; solid: $St = 1$, dashed: $St = 5$, dashed-dotted: $St = 25$, and dotted: $St = 0.2$.

and filtered DNS. Also included are the RMS of the subfilter forcing terms δu_y and δu_y^* . The peak RMS of the subfilter forcing term is approximately 50% of the DNS result and application of the deconvolution results in a slight reduction of the RMS. In view of the close agreement between the curves for δu_y and δu_y^* we may infer that the corrections due to approximate deconvolution at this rather high Reynolds number, in combination with the selected filter width, are quite modest. Much of the dynamic consequences for the particle trajectories arising from the small turbulent scales, need to be represented by the (stochastic) forcing model. Incorporating approximate deconvolution as a first step seems nevertheless beneficial since it was also observed that the correlation between u and δu^* is smaller than that between u and δu .

The Stokes number of the particles has a rather modest influence on the velocity differences. Figure 2 illustrates this in terms of the RMS of the wall-normal component of $\delta \mathbf{u}^*$. The results for all four Stokes numbers are quite similar for the flow at $Re_\tau = 950$, each with a maximum at $y^+ = 60$. The result for $St = 5$, which corresponds to particles whose relaxation time is closest to the average Kolmogorov time, deviates somewhat from that of the other three Stokes numbers. Close to the wall, particles with $St = 5$ are, with somewhat higher preference than at the other St , located in positions where δu_y^* has a slightly lower value.⁶

When scaled with the RMS the PDF of $\delta \mathbf{u}^*$ displays a remarkable independence of Stokes number, as illustrated in Fig. 3, taking data where the RMS is maximal, i.e. $y^+ = 60$. The PDF deviates from a Gaussian distribution, which is also included in the figure. Large deviations from the average value of the force are slightly more likely than in a Gaussian distribution. At $y^+ = 60$ the PDF is almost symmetric, but closer to the center of the channel the skewness of the PDF attains values around 0.3. The PDF of the wall-normal *particle* velocity component v_y at $St = 1$ is included as well, showing a close correspondence with the Gaussian distribution. For the other two velocity components similar results are found: the RMS and PDF hardly depend on Stokes number. Also similar deviations from a Gaussian distribution are obtained, a higher value of the flatness, and a mild asymmetry, which depends both on the velocity component and on the wall-normal coordinate.

A further step in the analysis of the stochastic forcing arises by considering the influence of the Reynolds number. We show results for $St = 1$; similar results are found at other Stokes numbers. In Fig. 4 the RMS of δu_y^* is shown for the three Reynolds numbers studied here. The magnitude of the force depends on the filter width and the velocity field. The smaller magnitude of the RMS at $Re_\tau = 150$ could be explained by the fact that in this simulation the filter widths in wall units are smaller than in the other two simulations. The location of the maximum of the RMS is equal to $y^+ = 60$, independent of the Re_τ . The PDF's of δu_y^* are given in Fig. 5 at $y^+ = 60$, displaying a strong collapse of the results for the three different Reynolds numbers, provided we scale by the

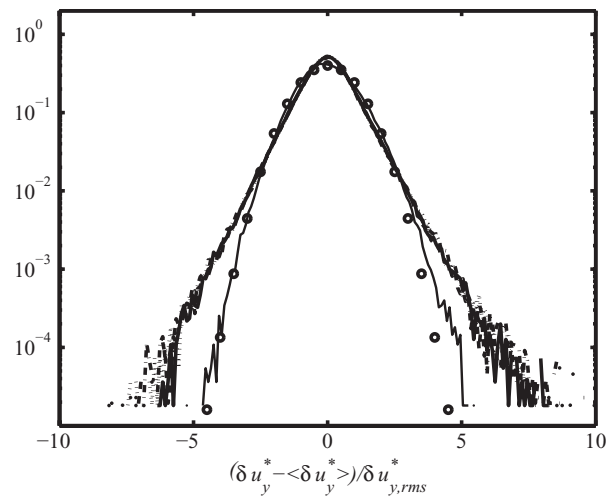


FIG. 3. PDF of δu_y^* at $y^+ = 60$ and $\text{Re}_\tau = 950$; solid: $St = 1$, dashed: $St = 5$, dashed-dotted: $St = 25$, and dotted: $St = 0.2$, circles: Gaussian distribution, thin solid line: PDF of v_y at $St = 1$.

Re_τ dependent RMS. Similar results are obtained for the other two velocity components and at other locations. We can conclude that the PDF's are not only independent of Stokes number, but also of Reynolds number as long as they are considered at the same value of y^+ . This constitutes a strong simplification for the development of a “stand alone” stochastic model for the velocity differences $\delta \mathbf{u}^*$.

Development of a stochastic model needs to incorporate the temporal correlation of the subfilter forcing $\delta \mathbf{u}^*$. Since the subfilter forcing only contains small-scale contributions, it can be expected that the correlation time is smaller than the Lagrangian correlation time. This is shown in Fig. 6, where the temporal correlation functions of δu_x^* are plotted for the four different Stokes numbers together with the temporal correlation function of v_x for $St = 1$. All results are for $\text{Re}_\tau = 950$ and for particles with initial position $y^+ = 60$. The correlation time of the particle velocity is indeed much larger than that of the subfilter forcing term. Moreover, similar as observed for the PDF, the temporal correlation function hardly depends on Stokes number. We also studied other velocity components and other flow conditions and observed the temporal correlation to be quite independent of the

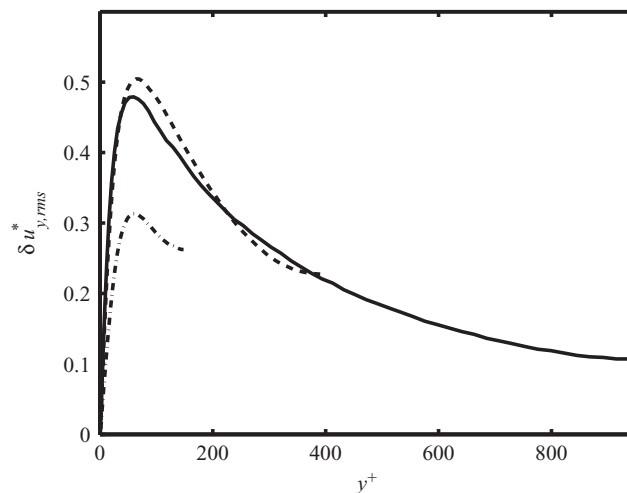


FIG. 4. RMS of δu_y^* as a function of y^+ for $St = 1$; solid: $\text{Re}_\tau = 950$, dashed: $\text{Re}_\tau = 395$, and dashed-dotted: $\text{Re}_\tau = 150$.

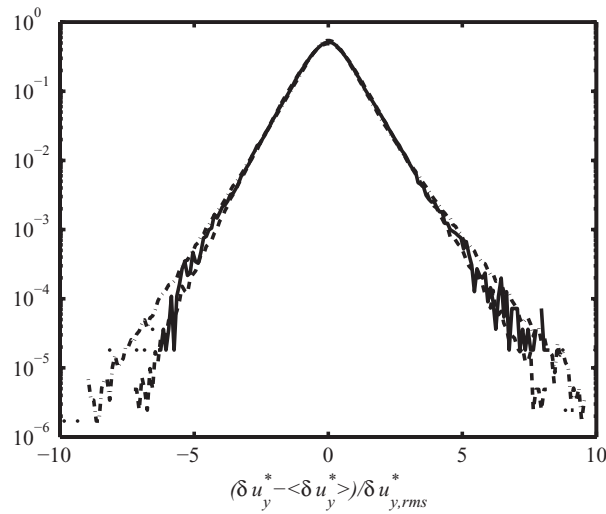


FIG. 5. PDF of δu_y^* at $y^+ = 60$ and $St = 1$; solid: $Re_\tau = 950$, dashed: $Re_\tau = 395$, and dashed-dotted: $Re_\tau = 150$.

particular velocity component that is studied and independent of the particular Reynolds number that is adopted.

Simulation of particle dispersion in LES of high-Reynolds turbulent flow requires explicit stochastic velocity differences to be included in the particle equations of motion. This modeling step allows to enrich the dynamics of the dispersed phase and restore the statistical properties that would be lost if the particles were transported by the spatially filtered LES flow field. Using DNS of high-Reynolds turbulent channel flow we inferred, *a priori*, statistical properties of the “ideal forcing” that should be adopted in order to retain the same dispersive properties in LES, as would arise in fully resolved DNS. We focused on the PDF of the stochastic velocity differences as well as the temporal correlation of these velocity differences. These show little or no dependence on the Reynolds number and particle inertia, when normalized by the RMS of the velocity differences and evaluated at the same distance from the wall, measured in wall units, respectively. Retaining these properties is essential when developing a proper “stand-alone” stochastic forcing model. Next to the PDF and time-correlation of the forcing, also the spatial correlation between \mathbf{u} and $\delta \mathbf{u}^*$ needs attention. The spatial correlation has its own dependence on the distance to the wall, reflecting the

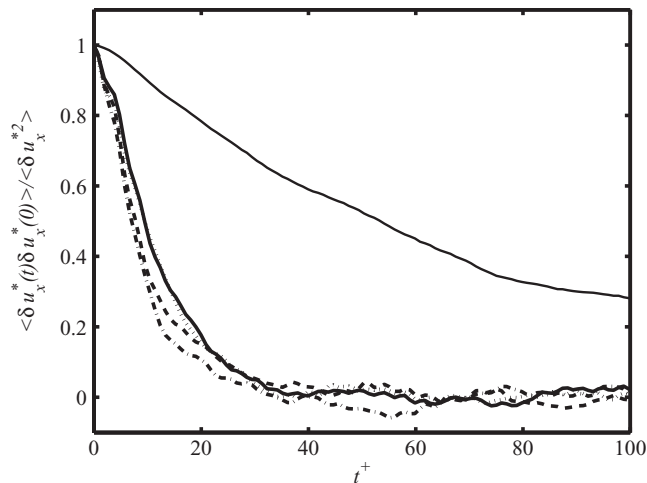


FIG. 6. Temporal correlation function of δu_x^* as a function of t^+ at $y^+ = 60$ and $Re_\tau = 950$; solid: $St = 1$, dashed: $St = 5$, dashed-dotted: $St = 25$, dotted: $St = 0.2$, thin solid line: temporal correlation function of v_x for $St = 1$.

different regimes of near-wall turbulence and the corresponding variations in the spatial coherency in the flow.

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