Large Eddy Simulations of particle-fluid interaction in a turbulent channel flow

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Abstract. This paper presents a comparison between results obtained using Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) in particle-laden turbulent channel flow. In the case of LES method computations were performed using the dynamic model, Smagorinski model, with and without Van Driest damping at the wall, and without sub-grid scale turbulence modelling. The focus is on the difference in the computed forces acting on a particle in the particle equation of motion. Results for turbulent flow in a channel at $Re_\tau = 150$ are presented, focusing on point-particle statistics. DNS provides a point of reference for assessing LES with different sub-filter eddy-viscosity models.

1. Introduction

Turbulent flows laden with a large number of small particles is fundamental to a large number of environmental and industrial processes. Accurate prediction of the behavior of particles in a turbulent flow can be obtained using Direct Numerical Simulation (DNS) Elghobashi (2004); Jaszczur et al. (2008). However, such simulations are too costly for frequent application in problems of realistic complexity.

In recent years, large-eddy simulation for turbulent flow has become focused on multiphase applications, including particle-laden flow Portela et al. (2003); Kuerten et al. (2005). This poses new challenges to the representation of small-scale turbulent motion, as the aim shifts toward capturing the dispersion of inertial particles that are embedded in the flow.

The motion of particles that respond slowly to the flow because of their large inertia, i.e., large relaxation time, will not be influenced much by the small turbulent scales at their seems to be easy to model. For very fast responding particles that closely follow details in the flow modelling will require a highly resolved turbulent velocity field which is not the case for LES. With decreasing relaxation time, the dependence of the particle motion on small scales in the flow increases. An numerical analysis investigate to what extent an increase in accuracy and can be used for simulated flow most accurately. In cases where the motion of the particles also depends to a large extent on scales that are smaller than the LES resolution, or in case the LES field does not capture important flow structures near the wall, some models are not expected to yield improvements. In such situations additional sub-filter scale modelling special for discrete phase may be required Marchioli et al. (2008).

The presented simulation of wall-bounded turbulent particle-laden flow are based on the Euler-Lagrange point-particle approach Portela et al. (2003). Particles are dispersed in a
pressure-driven fluid flow, assumed to be incompressible and Newtonian. Restrict to very small volume fractions and assume that the size of the particles is considerably smaller than the local Kolmogorov length-scale in the turbulent flow. In such situations the particles have a negligible feedback coupling on the turbulence and the one-way coupling formulation for the particle phase can be employed Elghobashi (2004).

2. Mathematical model

The motion of the particles in the turbulent flow is obtained by time-accurate tracking of their trajectories. The instantaneous transfer of momentum from the continuous fluid phase to the discrete particle phase is dominated by Stokes drag. This is determined by the velocity of the particle and that of the surrounding fluid at the location of the particle.

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\[
\frac{d\vec{x}(t)}{dt} = \vec{v}(t) ; \quad \frac{d\vec{v}}{dt} = C_d \frac{Re_p}{24} \frac{1}{\tau_v} (\vec{u}(\vec{x}(t), t) - \vec{v}(t))
\]

where \( \vec{u}(\vec{x}(t), t) \) is the velocity of the fluid at the location of the particle. The particle drag coefficient \( C_d \) and the hydrodynamic particle relaxation time \( \tau_v \), are defined as:

\[
C_d = \frac{24}{Re_p}, \quad \tau_v = \frac{\rho_p D_p^2}{\rho_f 18 \nu}
\]

in terms of the particle Reynolds number \( Re_p = (|\vec{u} - \vec{v}|) D_p / \nu \). In these expressions \( \rho_p \) and \( \rho_f \) are the particle and fluid mass densities, \( D_p \) is the diameter of the particles. The expression for \( C_d \) is valid only for small \( Re_p \).

![流体と粒子の運動](image.png)

- 流体の流れ方向
- 党細胞

Figure 1. Computational domain.

The continuous-phase, represented by conservation of mass and momentum, is solved using DNS and LES Portela et al. (2003) for incompressible flow. We adopt a geometry of the problem as sketched in Fig. 1. The position, flow, and particle quantities are normalized by the channel half-width, \( \delta \), and the friction velocity, \( u_* \). The particle motion is obtained using a second-order Adams-Bashforth scheme for the time-advancement, and a tri-linear interpolation for the velocity. Periodic boundary conditions are imposed in streamwise and spanwise directions.
The filtered continuity and Navier-Stokes equations, that are the basis for LES of the continuous phase are:

\[ \nabla \cdot \overline{\vec{u}} = 0 \]  

(3)

\[ \frac{D \overline{\vec{u}}}{Dt} = -\nabla P + \frac{1}{Re} \nabla^2 \overline{\vec{u}} - \nabla \cdot \overline{\tau} \]  

(4)

where the overbar denotes the spatially filtered flow variable, \( \rho_f \) is the fluid density and \( Re \) is the fluid Reynolds number, while \( P \) denotes the pressure. The influence of the subgrid motion on the resolved fluid-velocity is represented by the turbulent stress-tensor, \( \overline{\tau} \). In components this tensor is given by

\[ \tau_{ij} = \overline{u_i u_j} - \overline{u_i} \overline{u_j} \]  

(5)

In LES the tensor \( \overline{\tau} \) is parameterized by a sub-filter model. Here we will consider eddy-viscosity models in which

\[ \tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2\nu_t \overline{S_{ij}} \]  

(6)

The trace \( \tau_{kk} \) of the turbulent stress tensor is incorporated in the pressure term. In the Smagorinsky model the turbulent eddy-viscosity \( \nu_t \) is model by analogy to the mixing length hypothesis:

\[ \nu_t = C_S \Delta^2 |\overline{S}| \]  

(7)

where \( C_S \) is the Smagorinsky coefficient, \( \Delta \) is the filter width, and \( |\overline{S}| \) is the magnitude of the strain rate tensor defined as:

\[ |\overline{S}| = \left( 2\overline{S_{ij} S_{ij}} \right)^{1/2} \]  

where \( \overline{S_{ij}} = \frac{1}{2} \left( \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) \)  

(8)

The Smagorinsky model used here contributes to the dissipative fluxes in the LES equations. Near the solid walls of the channel this model is known to exaggerate the dissipation, up to the point of preventing transition to turbulence. To counteract this tendency, the turbulent eddy-viscosity \( \nu_t \) may be directly damped near the walls. One of the example of this strategy is van Driest damping in which the constant \( C_S \) is replaced by \( C_S (1 - \exp(-y^+ / A)) \) where \( y^+ \) measures the wall-normal distance in terms of wall-coordinates and \( A = 25 \) Moin et al. (1982).

A more elegant method tested here is to damp the overly dissipative Smagorinsky model in a turbulent boundary layer obtained as a by-product of the dynamic procedure Germano et al. (1991). The dynamic procedure yields a self-adaptive dynamic eddy-viscosity coefficient. This eddy-viscosity reduces to zero in the viscous sub-layer near a solid wall, thereby avoiding the excessive dissipation that arises with the Smagorinsky model.

3. Results

Simulations using presented models were performed in a computational domain as sketched in Fig. 1 with up to 64 \( \times \) 64 \( \times \) 64 control volumes for LES and up to 256 \( \times \) 256 \( \times \) 128 in case of DNS. For the streamwise and spanwise directions the grid spacing is uniform, and for the wall normal direction a hyperbolic-tangent stretching has been used. The shear Reynolds number of the flow was \( Re_{\tau} \) = 150 based on the shear velocity and half channel height. In order to obtain good statistics for particles in these simulations we used \( 1.5 \times 10^6 \) particles for the DNS and up to one order less for LES.

The simulations were started from arbitrary conditions (random flow and temperature field) and flow field was time advanced to get a statistically-steady state for velocity and
temperature. When a statistically steady state was reached particles were injected uniformly over the computational domain. Their initial velocity was assumed to be the same as the fluid in the center of the particles’ location. The particles need to adapt to the new velocity and temperature, which usually takes a few particle response times and then much longer time is required to ensure a statistically-steady state for the particle conditions required to produce reliable statistics (to obtain a statistically steady state for particles takes much longer than it does for the flow field; it also takes longer for particles with larger response times). After an initial big change in the particle concentration profile, particles continue to very slowly process of accumulate near the walls. As Portela Portela et al. (2003) has shown, this process can take an enormous amount of time. In the present computations, the time before particles start to be averaged takes at least $t^* = 200$. The statistics for the fluid and particles were averaged for $100d/u_\tau$ at $Re_\tau = 150$. The particle properties were obtained by averaging over rectangular slices using a simple linear model based on centre of particle locations and distance from reference points, which correspond to flow computational grid points.

In Fig. 2 the streamwise fluid velocity component and its fluctuations are presented as a function of the wall normal coordinate for various sub-filter models. The Smagorinsky model yields considerable errors (Fig. 2), which are mainly due to the overestimated near wall dissipation as can be seen by comparison with the results obtained with the dynamic and the Van Driest damped case (Fig. 2). The streamwise velocity fluctuations are slightly under-predicted in case no sub-filter model is used ($C_S = 0$). Better results are obtained using the dynamic model and the Van Driest damped model at $C_S = 0.05$ and 0.1 (Fig. 2). Too large values of $C_S$ in combination with Van Driest yield too high fluctuation levels.

![Figure 2](image-url)  

**Figure 2.** Fluid velocity (top) and fluctuations (bottom) for the streamwise component comparing various sub-filter models with DNS results at $Re_\tau = 150$. 
In Fig. 3 Particle concentration are presented for Stokes number $St = 1$. It can be seen that all models under-predict the particle accumulation. The highest concentration was observed for the case when no sub-filter model was used; apparently the small-scale turbulent fluctuations near the wall are very important for proper prediction of turbophoresis.

![Particle concentration graph](image)

**Figure 3.** Particle concentration. For particle Stokes number $St = 1$ and compare various LES models with DNS.

4. Conclusion

In this paper the Euler-Lagrange framework has been used to simulate the point-particle dynamics with fluid flow represented using LES and DNS. The relevance of the near-wall velocity fluctuations was studied in relation to the particle clustering. At low Stokes numbers the use of accurate model for turbulent was found to be important for the particle statistics. Van Driest damping and the dynamic procedure proved to be quite reliable while the Smagorinsky model was found less accurate. In contrast to other work in literature low order (linear) of interpolation for particle velocity was used.

It is known that articles tend to be highly concentrated in the region close to the wall. The particles also agglomerate in the form of long strikes; behavior known as preferential concentration is very strong close to the wall but it can also be observed across nearly the entire domain. It has been shown that this phenomena is very difficult to reproduce using LES modeling. Mean streamwise velocity fluctuation in the boundary layer is different for the fluid and for the particle, and decorrelates with the increasing time response. Increasing in particle concentration close to the wall as well as particle clustering have to be capture very accurately.
because this mechanisms can be very important in many fields and industrial processes. Non-homogenity in particle concentration can have a strong negative affect on numerous chemical processes.

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