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Statistics of particle dispersion in direct numerical simulations of wall-bounded turbulence: Results of an international collaborative benchmark test

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ABSTRACT

In this paper the results of an international collaborative test case relative to the production of a direct numerical simulation and Lagrangian particle tracking database for turbulent particle dispersion in channel flow at low Reynolds number are presented. The objective of this test case is to establish a homogeneous source of data relevant to the general problem of particle dispersion in wall-bounded turbulence. Different numerical approaches and computational codes have been used to simulate the particle-laden flow and calculations have been carried on long enough to achieve a statistically steady condition for particle distribution. In such stationary regime, a comprehensive database including both post-processed statistics and raw data for the fluid and for the particles has been obtained. The complete datasets can be downloaded from the web at HTTP://CFD.CINECA.IT/CFD/REPOSITORY/. In this paper the most relevant velocity statistics (for both phases) and particle distribution statistics are discussed and benchmarked by direct comparison between the different numerical predictions.

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1. Introduction

Turbulent particle dispersion in wall-bounded flows is a fundamental issue in a number of industrial and environmental applications. Direct numerical simulation (DNS) and Lagrangian particle tracking (LPT) may be a useful tool to provide physical insights, new modeling ideas and benchmark cases (Moin and Mahesh, 2002; Yeung, 2002). Despite the large number of published works, however, it is extremely difficult to gather a uniform and complete source of data that can be used to perform a phenomenological study of some, still not well-established features of particle transport in turbulent flows or to assess the effectiveness of computer simulation models on the accuracy of predicted particle deposition rates (Sergeev et al., 2002; Tian and Ahmadi, 2007).

Lack of uniformity and of completeness in the available numerical data is connected to several reasons (associated with the intrinsic complexity of turbulent transfer phenomena) and is accompanied to uncertainty in methodologies, mostly due to the large number of physical and computational parameters involved and to the unclear influence of several of them. The main physical parameters that will influence the simulation results are the particle Stokes number, which quantifies the response of the dispersed phase to the perturbations produced by the underlying turbulence, and the flow Reynolds number. Other important parameters are related to modeling of fluid–particle interaction (one-way/two-way coupling); particle–particle interaction (collision models); particle–wall interaction (reflecting or absorbing wall, wall effects); particle rotation and modeling of forces acting on particles (e.g., the lift force). On the computational side, the treatment of discrete particles in DNS fields poses open or partly open questions on the assessment of the performance of flow solvers that use different numerical methods and on the accuracy of the interpolation scheme used to obtain the fluid velocity at the instantaneous particle location. In this context, the proper choice of parameters such as the grid resolution and the time-step size required for advancement of the governing balance equations becomes extremely important.

This paper is the result of the first necessary step towards a rigorous, systematic analysis of these issues. Specifically, the objectives of this analysis are to have a large number of people working independently on the same test case problem (DNS of particle dispersion in turbulent channel flow) and to establish a large validated database including (i) reliable and accurate velocity

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statistics for the fluid, for the particles and for the fluid at the particle position (mean and rms velocities, skewness and flatness, Reynolds stresses and quadrant analysis); (ii) particle concentration profiles and deposition rates; (iii) one-particle statistics (particle velocity auto-correlations, particle turbulent diffusivity, particle mean-square displacements, Lagrangian integral time scales); (iv) two-particle statistics (rms particle dispersion). Datasets come from five independent simulations and include not only the post-processed statistics just listed but also the corresponding raw data providing the evolution of the fluid velocity field and the time behavior of the particle position and velocity components: these data are made available to users who need to compute specific statistics other than those included in the database. Besides providing a homogeneous source of data on DNS and LPT not previously available, the database can be used as benchmark either to compare directly different numerical approaches or to validate engineering models for particle dispersion (e.g., two-fluid Eulerian models). The need for this type of data could be extended also to commercial softwares for computational fluid dynamics: these softwares, even though usually exploited for high-Reynolds-number flows in complex geometries, fail predictions of multiphase flows due to the lack of appropriate physical models for particle dispersion, resuspension and deposition.

The test case was conceived in 2004 at the IUTAM Symposium on Computational Approaches to Multiphase Flow (Balachandar and Prosperetti, 2006) and it was first advertised in 2005 at the 11th Workshop on Two-phase flow predictions (Sommerfeld, 2005). During the workshop, common base guidelines for participant groups were provided. The following groups (listed in random order) joined the test case calculations: (1) C. Marchioli and A. Soldati (Group UUD hereinafter), (2) J.G.M. Kuerten (Group TUE hereinafter), (3) B. Arcen and A. Tanière (Group HPU hereinafter), (4) G. Goldensoph and K. Squires (Group ASU hereinafter), (5) M.F. Cargnelutti and L.M. Portela (Group TUD hereinafter). As starting point of the test case, a DNS of dilute particle-laden turbulent channel flow at low Reynolds number has been performed by all groups following the base guidelines. Aim of this benchmark calculation is to build a thorough statistical framework including both statistically developing and statistically steady conditions for the distribution of the dispersed phase. To quantify the collaborative effort required by the test case, it should be noted that the simulation time taken for each group to achieve a statistically steady condition for the particle distribution was of the order of eight to ten months, mostly depending on the availability of computational resources. This is equivalent to an overall simulation time of about four years on standard production machines.

The present paper is organized as follows: first the physical problem and the numerical methodology adopted by each group are briefly outlined, then the performance of the different numerical approaches is benchmarked through direct comparison of the most relevant statistics for both phases. In the final section, conclusions and implications for future developments of the test case are drawn.

2. Physical problem and numerical methodology

2.1. Particle-laden turbulent channel flow

The flow into which particles are introduced is a turbulent channel flow of gas. In the present study, we consider air (assumed to be incompressible and Newtonian) with density $\rho = 1.3\ \mathrm{kg\ m^{-3}}$ and kinematic viscosity $\nu = 15.7 \times 10^{-6}\ \mathrm{m^2\ s^{-1}}$. The governing balance equations for the fluid (in dimensionless form) read as:

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial u_i}{\partial t} = -u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j^2} - \frac{\partial p}{\partial x_i} + \delta_{1,i}, \tag{2}$$

where u_i is the ith component of the dimensionless velocity vector, p is the fluctuating kinematic pressure, $\delta_{1,i}$ is the mean dimensionless pressure gradient that drives the flow and $Re_\tau = u_\tau h/\nu$ is the shear Reynolds number based on the shear (or friction) velocity, u_τ, and on the half channel height, h. The shear velocity is defined as $u_\tau = (\tau_w/\rho)^{1/2}$, where τ_w is the mean shear stress at the wall. In this benchmark calculation, the shear Reynolds number is $Re_\tau = 150$; the corresponding bulk Reynolds number is $Re_b = u_b h/\nu = 2100$ based on the bulk velocity $u_b = 1.65\ \mathrm{m\ s^{-1}}$. All variables considered in this study are reported in dimensionless form, represented by the superscript +[2] and expressed in wall units. Wall units are obtained combining u_τ, ν and ρ.

The reference geometry consists of two infinite flat parallel walls: the origin of the coordinate system is located at the center of the channel and the $x-$, $y-$ and $z-$ axes point in the streamwise, spanwise and wall-normal directions, respectively (see Fig. 1). Periodic boundary conditions are imposed on the fluid velocity field in x and y, no-slip boundary conditions are imposed at the walls. The calculations were performed on a computational domain of size $4\pi h \times 2\pi h \times 2h$, corresponding to $1885 \times 942 \times 300$ wall units in x, y and z, respectively. For ease of reading, details on the Eulerian grid used to discretize the flow domain and on the time-step size, Δt^+, employed by each group are given in Section 2.2. Here, we just mention that the base simulation requirements prescribe a minimum number of grid points in each direction to ensure that the grid spacing is always smaller than the smallest flow scale[3] and that the limitations imposed by the point-particle approach are satisfied.

Particles with density $\rho_p = 1000\ \mathrm{kg\ m^{-3}}$ are injected into the flow at concentration low enough to consider dilute system conditions (particle–particle interactions are neglected). Furthermore, particles are assumed to be pointwise, rigid and spherical. The motion of particles is described by a set of ordinary differential equations for particle velocity and position at each time step. For particles much heavier than the fluid ($\rho_p/\rho \gg 1$) Elghobashi and Truesdell (1992) have shown that the only significant forces are Stokes drag and buoyancy and that Basset force can be neglected being an order of magnitude smaller. In the base simulation, the aim is to minimize the number of degrees of freedom by keeping the simulation setting as simplified as possible; thus the effect of gravity has also been neglected. With the above assumptions the following Lagrangian equation for the particle velocity is obtained:

$$\frac{d\mathbf{u}_p}{dt} = -\frac{3}{4}\frac{C_D}{d_p}\left(\frac{\rho}{\rho_p}\right)|\mathbf{u}_p - \mathbf{u}|(\mathbf{u}_p - \mathbf{u}), \tag{3}$$

where $\mathbf{u}_p$ and $\mathbf{u}$ are the particle and fluid velocity vectors, d_p is the particle diameter and C_D is the drag coefficient given by Rowe and Enwood (1962):

$$C_D = \frac{24}{Re_p}(1 + 0.15 Re_p^{0.687}), \tag{4}$$

where Re_p is the particle Reynolds number ($Re_p = d_p|\mathbf{u}_p - \mathbf{u}|/\nu$). The correction for C_D is necessary because Re_p does not necessarily remain small, in particular for depositing particles.

For the simulations presented here, three particle sets were considered, characterized by different relaxation times, defined

[2] The superscript + has been dropped from Eqs. (1) and (2) for ease of reading.

[3] In the present flow configuration, the non-dimensional Kolmogorov length scale, η_K^+, varies along the wall-normal direction from a minimum value $\eta_K^+ = 1.6$ at the wall to a maximum value $\eta_K^+ = 3.6$ at the centerline. In terms of time scales, the Kolmogorov time scale, τ_K^+, varies along the wall-normal direction from a minimum value $\tau_K^+ = 2$ at the wall to a maximum value $\tau_K^+ = 13$ at the centerline (Marchioli et al., 2006).

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