Benchmark: LES of particle-laden channel flow

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1 Introduction

Dispersion of particles in a turbulent wall-bounded flow is an important topic in many applications in industry and environment. Think for instance of small particles in exhaust gases which pollute heat exchangers in biomass furnaces or of turbulent mixing processes in chemical and pharmaceutical industry. For numerical simulation of particle-laden turbulent flow various approaches are available. A first distinction can be made in the approach chosen to model the particles. In the *Eulerian* approach particles are modeled by an equation for the particle concentration, whereas in the *Lagrangian* approach individual particles are tracked by solving their equation of motion. The second distinction is the way in which the fluid is described. At one extreme is *direct numerical simulation, DNS* where all relevant length- and time scales of the fluid motion are resolved, which is only possible at low Reynolds numbers and simple geometries. In *Reynolds-averaged Navier-Stokes, RANS* only the mean fluid quantities are solved and the effect of turbulence on the mean flow is modeled by a turbulence model. The computational resources required are negligible compared to DNS, but the predictive capability of the method is limited. Especially in case of the interaction between particles and turbulent flow in boundary layers the isotropy assumed in the most often applied turbulence models might could make the results of RANS questionable. *Large-eddy simulation, LES* could offer a way out. In LES only the larger scales of the flow are resolved and the effect of the smaller scales on the large scales is modeled by a subgrid model. With respect to computational requirements LES is positioned between RANS and DNS. Uncertainty in the model is less than in RANS, since the small scales of the flow are believed to be more universal and presently various subgrid models are available which have proved their validity for several types of flow. However, the treatment of particles in LES is still a relatively new topic. Open or partly open questions can still be found in e.g. the effect of the subgrid scales on particle behavior and the modeling of the interaction between two particles, between particles and fluid and between particles and walls. In this benchmark a Lagrangian-Eulerian model will be chosen, in which the particles are modeled by an equation of motion for each particle and the fluid by LES. The objective of this benchmark is to obtain a large database on results obtained with different numerical methods, subgrid models and physical models in order to resolve questions about the validity of these models.

In the next section a base simulation is described, which should be considered as a starting point for all participants. This specific simulation has been chosen since it has also been used as a benchmark for DNS of particle-laden turbulent channel flow. Therefore, the quality of the LES results can be estimated by comparison with the DNS benchmark results. In the final section possible extensions of the base simulation are suggested. The complete datasets of the DNS benchmark can be downloaded from the web at

`http://cfd.cineca.it/cfd/repository/.`

It is the intention that the complete datasets of the LES benchmark contributions will be made available for download at the same repository.

2 Base Simulation

Fluid

The base simulation is LES of turbulent incompressible flow in a channel with particles of three different sizes. Only one-way coupling is considered. The effect of the particles on the fluid and the effect of collisions between particles is not taken into account under the assumption that the particle concentration is low. Since many particles are simulated, this assumption is perhaps not always true, but a large number of independent particles makes it possible to increase the statistical accuracy by averaging over the particles. The parameters of the base simulation are specified in the table below in a non-dimensionalized way. To this end half the channel height H, the friction velocity u_τ and the fluid mass density ρ_f are chosen as length, velocity and density scale. In real dimensions the parameters correspond for instance to a friction velocity of $u_\tau = 0.11775$ m/s, a fluid mass density of $\rho_f = 1.3$ kg/m^3, a kinematic viscosity of $\nu = 1.57 \times 10^{-5}$m^2/s and a half channel height of $H = 0.02$ m. The friction Reynolds number is defined as $Re_\tau = u_{tau}H/\nu$.

Particles

In the base simulation one-way coupling is applied and only the drag force works on a particle. Hence, the particle equation of motion reads:

$$\frac{d\mathbf{v}}{dt} = \frac{\mathbf{u}(\mathbf{x},t) - \mathbf{v}}{\tau_p}(1 + 0.15 Re_p^{0.687}), \tag{1}$$

where $\mathbf{v}$ is the particle velocity and $\mathbf{u}(\mathbf{x}, t)$ is the fluid velocity at the position of the particle, $\mathbf{x}$. The particle relaxation time is given by: $\tau_p = \rho_p d_p^2/(18\rho_f \nu)$ with ρ_p and d_p the particle mass density and diameter. The standard drag correlation for particles with particle Reynolds number $Re_p = |\mathbf{u} - \mathbf{v}|d_p/\nu$ smaller than 1,000 is applied. The particles are chosen in such a way that the Stokes numbers, i.e. the particle relaxation time in wall units, of the different particles equal 1, 5 and 25. Since the cut-off scale of an LES lies within this regime of typical time scales, it is expected that disregard of the subgrid scales affects the different particles in a different way. The Stokes number is defined as:

$$St = \frac{\rho_p d_p^2 u_\tau^2}{18 \rho_f \nu^2}.$$

Quantity	Symbol	Value
length of channel	L_x	$4\pi H$
width of channel	L_z	$2\pi H$
height of channel	-	$2H$
Reynolds number based on friction velocity	Re_τ	150
particle mass density	ρ_p	$769.23\rho_f$
particle diameter type 1	$d_{p,1}$	$1.019 \times 10^{-3}H$
particle diameter type 2	$d_{p,2}$	$2.280 \times 10^{-3}H$
particle diameter type 3	$d_{p,3}$	$5.099 \times 10^{-3}H$

Table 1: Parameters of base simulation

Boundary and initial conditions

In the streamwise and spanwise direction the fluid flow is periodic. At the solid walls the no-slip condition is applied. Particles collide elastically with the walls at the point where the distance between the particle center and the wall equals the particle radius. If a particle leaves the computational domain through a streamwise or spanwise boundary the fluid velocity at the particle position is found from the periodicity of the velocity field. The simulation is started from a fully-developed statistically stationary solution of the LES equations. Initially the particles are homogeneously distributed over the entire computational domain. The initial velocity of a particle equals the fluid velocity at the particle position, so that the initial acceleration of the particle equals zero. The time step should be chosen sufficiently small compared to the particle relaxation time. In order to obtain accurate statistics, at least 100,000 particles of each kind should be tracked.

Subgrid models

As a basic test case the participants are requested to perform LES on 64^3 grid points without subgrid model (coarse DNS) and with an eddy-viscosity model (either Smagorinsky with wall damping or a variant of the dynamic eddy-viscosity model). Moreover, for the interpolation of the fluid velocity to the position of a particle the participants are requested to use both tri-linear interpolation and a higher order variant. In this basis test case no subgrid model in the particle equation of motion should be applied.

This basic test case serves as a way to see the effects of the different numerical methods used in the LES and the Lagrangian particle tracking on the fluid and particle behavior. The coarse DNS serves as a zero measurement: any useful subgrid model should at least yield better results than the coarse DNS. The tri-linear interpolation for the fluid velocity has shown to be sufficiently accurate for DNS. The LES velocity field is less smooth on the LES grid. Therefore, tri-linear interpolation is not as accurate. However, higher-order interpolation increases the energy contained in the fluid velocity field and therefore acts as a kind of subgrid model in the particle equation of motion. A comparison of the particle velocity statistics of the two methods for interpolation quantifies this effect.

DNS results

The DNS results [1] show that particles tend to move towards the walls of the channel by turbophoresis. The turbophoretic velocity depends on the Stokes number and increases with increasing Stokes number in the regime of Stokes numbers considered in this benchmark. After a long time a statistically stationary situation appears in which the particle concentration has reached a steady state. For $St = 1$ and $St = 25$ this steady concentration is reached at approximately $t^+ = 10,000$, for $St = 5$ near $t^+ = 20,000$. For $St = 1$ the particle concentration close to the wall is then approximately 4 times the initial concentration c_0, for $St = 5$ it equals $70c_0$ and for $St = 25$ approximately $150c_0$.

Required quantities

In order to be able to compare the results at least the following quantities should be provided. All quantities should be given in wall units and for particle concentration scaled with the initial particle concentration and all quantities should be averaged over sufficiently long time.

- Mean fluid velocity, rms's, skewness and flatness of all three velocity components, Reynolds stresses. Do not include subgrid contributions to these fluid properties.
- Mean relative velocity in the wall-normal direction. This quantity is stationary after a small initial transient in the DNS.
- Mean particle velocity in the other two directions, rms's, skewness and flatness of particle velocity and Reynolds stresses.
- Mean, rms's, skewness, flatness and Reynolds stresses of fluid velocity at the particle position.
- Average particle concentration in the steady state.
- Particle concentrations should be given for a hyperbolic tangent bin distribution. The dividing points of the bins are given by:

  $$x_j = Re_\tau \frac{\tanh(\Delta(j_{max} - j)/j_{max})}{\tanh \Delta}$$

  for $j = 0, 1, \dots, j_{max}$, where x_0 is the point on the wall and $x_{j_{max}}$ at the center of the channel, $j_{max} = 32$ and $\Delta = 1.7$.
- Fluid and particle velocity statistics can be given on as arbitrary division of points.

3 Deadlines

- 22-25 March 2010: First results will be presented at the 12^{th} Workshop on Two-Phase Flow, Halle, Germany.
- 7-9 July 2010: More results will be presented at DLES8 in Eindhoven, The Netherlands.
- If possible, a joint paper will be prepared in the second half of 2010.

4 Participating Groups

Presently, the groups participating in the benchmark are:

- Hans Kuerten, Eindhoven University of Technology, The Netherlands
- Cristian Marchioli and Alfredo Soldati, University of Udine and Maria-Vittoria Salvetti, University of Pisa, Italy
- Olivier Simonin and Arthur Konan, IMFT, Toulouse, France
- Christian Gobert and Michael Manhart, Technische Universit"at München, Germany
- Jacek Pozorski, Polish Academy of Sciences, Gdansk, Poland
- Marek Jaszczur, AGH University of Science and Technology, Poland
- Vincenzo Armenio, University of Trieste, Italy
- Bernard Geurts, University of Twente, The Netherlands

5 Possible Extensions

Participants are encouraged to perform apart from the base simulation at least one extension, which concerns the physical model. Several suggestions for extensions are listed below.

- Study other LES grid resolutions and subgrid models.
- Study subgrid models in the particle equation of motion.
- Extend the particle equation of motion with e.g. gravity (preferably in the (opposite) streamwise direction) or lift force.
- Incorporation of two-way coupling (effect of particles on fluid) and four-way coupling (particle-particle interactions). Several questions in this topic are still open: How should the point force exerted by a particle on the fluid be distributed over neighboring grid points?
- Other particle-wall interaction by non-elastic collisions or rough walls.
- Simulations at higher Reynolds number. Useful friction Reynolds numbers are: 300, 395, 590, 950 and 2000.

Especially the first two extensions are recommended.

Reference

[1] C. Marchioli, A. Soldati, J.G.M. Kuerten, B. Arcen, A. Tanière, G. Goldensoph, K.D. Squires, M.F. Cargnelutti and L.M. Portela, Statistics of particle dispersion in direct numerical simulations of wall-bounded turbulence: Results of an international collaborative benchmark test, Int. J. Multiphase Flow **34(9)**, 2008: 879–893.