

# Parallelization of a DEM/CFD code for the numerical simulation of particle-laden turbulent flows

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**Abstract:** The interaction between a turbulent fluid flow and particle motion is investigated numerically. A complete direct numerical simulation (DNS) is carried out to solve the governing equations of the fluid phase, to investigate the behavior of inter-particle collision and its effects on particle dispersion, the discrete element method (DEM) is employed to calculate the particle motion. The parallelization strategy of the DNS part is based on a domain decomposition method and uses a hybrid MPI+OpenMP approach. On the other hand, the OpenMP is used for the parallelization of DEM: the total number of particles to be tracked are equally distributed among processors. Finally, the method is tested for a turbulent flow through a square duct.

*Keywords:* Parallelization, Direct Numerical Simulation, Discrete Element Method, Particle-laden Turbulence, OpenMP

## 1 Introduction

Turbulent dispersed multiphase flow are common in many engineering and environmental applications. The stochastic nature of both the carrier-phase turbulence and the dispersed multiphase distribution makes the problem of turbulent dispersed multi-phase flow far more complex than its single phase counterpart [1]. Through the literature, it can be found that there have been many experimental and numerical studies of fluid-solid two-phase turbulent flows over the past decades, early work that ignored the inter-particle collisions can be found in [2, 3, 4], for instance. While there are some studies [5, 6, 7] showing that the inter-particle collisions may play an important role and the effects cannot be neglected. However, in all the above-mentioned simulations, either a Lagrangian Particle Track (LPT) method or the deterministic hard-sphere model was used to predict the trajectory of the particles. The LPT method is difficult to deal with problems when solid volume loading is high since interaction between particles is neglected, while in deterministic hard-sphere model, the post-collision velocity of the particles were directly obtained by solving the equations of impulsive motion, no interaction force informations can be obtained. In the present study, the particle-particle interaction rules are based on the theoretical contact mechanics described in discrete element method (DEM) proposed by Cundall [8]. DEM simulations can provide dynamic information, such as the trajectories and transient forces acting on individual particles, the force is extremely difficult to obtain by physical experimentation at this stage of development.

For the fluid calculation, a direct numerical simulation is performed, where two-way coupling effects between fluid and solid are considered.

## 2 Governing equations and numerical methods

### 2.1 Navier-Stokes equations

We consider the simulation of turbulent, incompressible flows of Newtonian fluids. Under these assumptions, the governing equations in primitive variables read

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon u) = 0 \quad (1)$$

$$\frac{\partial(\varepsilon u)}{\partial t} + \nabla \cdot (\varepsilon u \otimes u) = \nu \nabla^2 u - \nabla p - F_{pf}/\rho_f \quad (2)$$

where  $u$  and  $p$  are the velocity and pressure fields, respectively.  $\nu$  is the kinematic viscosity and  $\rho_f$  is the fluid density. The void fraction,  $\varepsilon$ , is obtained from the DEM computations and  $F_{pf}$  represents the particle-fluid interaction force per unit volume. Notice that once discretized in space,  $F_{pf}$  is given by the sum of forces of all particles in a fluid computational cell,

$$F_{fp} = \frac{1}{V_{cell}} \sum_{i=1}^{N_{cell}} f_{fpi} \quad (3)$$

where  $V_{cell}$  is the volume of the cell,  $N_{cell}$  is the number of particles in that cell and  $f_{fpi}$  is the fluid force on particle  $j$ , detailed description of  $f_{fpi}$  was given in Eq. (6).

Navier-Stokes equations are discretized on a staggered grid in space by a fourth-order symmetry-preserving scheme by [9]. For the temporal discretization, a fully explicit second-order one-leg scheme [10] has been used. This method allows to increase the time step to a value that is about twice than the standard second-order Adams-Bashforth scheme. The use of the fourth-order symmetry-preserving scheme for the convective and diffusive terms of the equations implies that the Laplacian operator in the Poisson equation must be also fourth-order (otherwise the symmetry-preserving property is lost). This is the most problematic aspect from a parallel computing point-of-view. In the companion work [11], we have focused on the improvement of the parallel Poisson solver by means of a hybrid parallelization strategy. The previous version [12] was conceived for single-core (also dual-core) processors and therefore, the distributed memory model with message-passing interface (MPI) was used. The irruption of multi-core architectures motivated the use of a two-level hybrid MPI+OpenMP parallelization with the shared memory model on the second level. Advantages and implementation details for the additional OpenMP parallelization are presented and discussed in the companion paper [11].

### 2.2 Modelling of particle-fluid and particle-particle interactions

When the particles are not in direct contact among themselves but driven only by the fluid flow and body force, their motion can be determined by Newton's equation of motion:

$$ma = f_{fpi} + mg \quad (4)$$

$$I \frac{\partial^2 \theta}{\partial t^2} = \tau \quad (5)$$

where  $m$  and  $I$  are respectively the mass and the moment of inertia of a particle,  $\theta$  is the angular position,  $a$  is the acceleration,  $g$  is the gravitational acceleration if considered,  $\tau$  is the torque, and  $f_{fpi}$  is the particle-fluid force given as:

$$f_{fpi} = 0.5\rho_g A_p C_D |u_f - u_p| (u_f - u_p) \quad (6)$$

where  $A_p$  is the cross-sectional area of the particle as  $A_p = 0.25\pi d_p^2$ , and  $C_D = (24/Re_p)f$  is the drag coefficient,  $f$  is the modified factor for the Stokes drag force, described as  $f = 1 + 0.15Re_p^{0.687}$  when  $Re_p \leq 1000$  [13], the particle Reynolds number  $Re_p = |u_f - u_p|d_p/\nu$  ( $d_p$  is the particle diameter,  $\nu$  is the kinematic viscosity of the fluid), and the particle Stokes number  $St$  is defined as  $St = (\rho_p d_p^2 / (18\mu)) / (d/U_0)$  ( $\rho$  is the density of the particle,  $\mu$  is the fluid dynamic viscosity). When direct contact occurs between the particles and/or between particles and wall, there should be an additional term at the right-hand side of Eq. 4, namely the contact force  $ma = f_{fpi} + mg + f_c$ . In this study, the discrete element method (DEM) [8] was adopted to account for the interaction forces. The particles and walls were directly specified by material properties such as density, Young's modulus and friction coefficient. The theory of Hertz [14] was used for modeling the force-displacement relationship while the theory of Mindlin and Deresiewicz [15] was employed for the tangential force-displacement calculations.

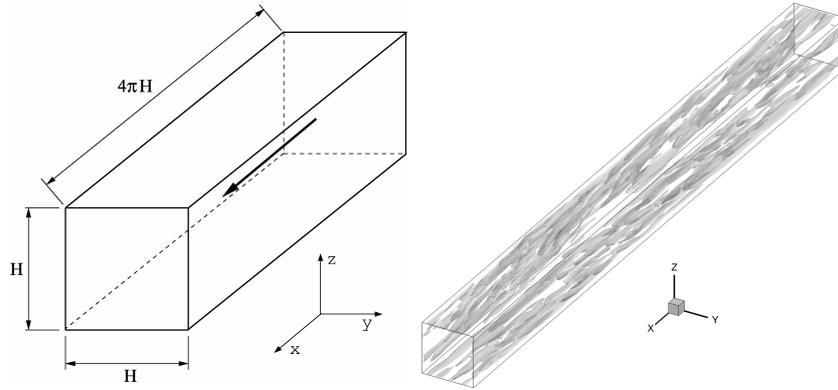


Figure 1: Square duct schema (left) and instantaneous isosurfaces of  $Q = 2$  (right).

### 3 On the parallelization of particle interactions

The incompressible Navier-Stokes equations together with the Newton's second law and the Hertz theory for impacts form an excellent mathematical model of particle-laden turbulent flows. Unfortunately, attempts at performing direct numerical simulations (DNS&DEM) with the available computational resources and numerical methods are limited to relatively low-Reynolds numbers. Anyhow, DNS is nowadays an essential tool to provide new insights into the physics of turbulence and indispensable data for the development of better turbulence models. The progress in DNS is closely related with the efficient use of modern High Performance Computing systems that offer a rapidly growing computing power. Since the irruption of multi-core architectures, this trend is mainly based on increasing both the number of nodes and the number of cores per node.

The parallelization strategy for the DNS code is based on a domain decomposition method (see the companion papers [11, 16], for details) whereas for the DEM code it is based on dividing the total number of particles to be tracked among the processors. The latter, basically consist on a main loop over all the particles that can be easily parallelized by means of OpenMP directives. However, the shared memory parallelization is limited by the number of available cores per processor. On the other hand, depending on the number of particles being tracked, the computational cost of the DEM part of the

algorithm can even exceed that of the DNS of the fluid flow. In this context, a hybrid OpenMP+MPI parallelization leaves the problem open to further scalability.

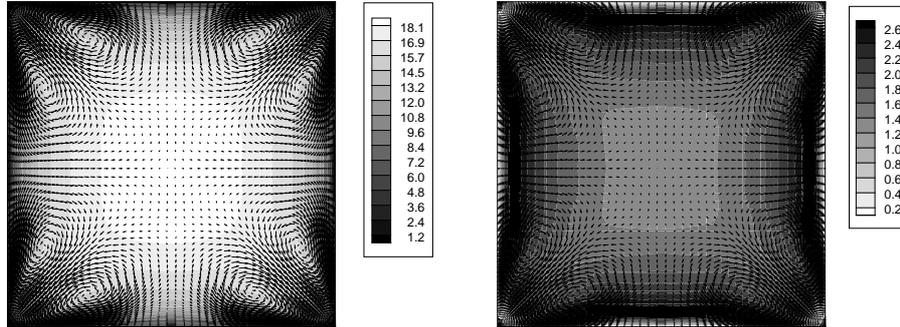


Figure 2: Left: mean secondary velocity vectors and contours for the mean streamwise velocity component,  $\langle u \rangle / u_\tau$ . Right: contours for  $u_{rms} / u_\tau$ .

A direct numerical simulation of a turbulent flow through a square duct has been chosen as a first demonstrative application of the DEM/CFD code. The geometry is displayed in Figure 1 (left). The computational domain is  $4\pi H \times H \times H$  in the streamwise and wall-normal directions. The Reynolds number based on the friction velocity,  $u_\tau$  and the hydraulic diameter,  $H$ , is  $Re_\tau = 300$ . Periodic boundary conditions are applied in the streamwise direction. The flow is driven by means of a constant pressure gradient in the streamwise direction,  $dP/dx = 4Hu_\tau^2$ . Finally, no-slip boundary condition is imposed at the walls. Since, the pioneering work by [17] in the early 90s, this configuration has been widely used for benchmarking purposes to validate turbulence models. Here, we propose to study the fluid-particle interaction in detail for this case. Figures 1 (right) and 2 show results for a preliminary DNS simulation. In this case, we have used a  $512 \times 128 \times 128$  staggered grid to cover the computational domain. Results are in very good agreement with those obtained by [17]. Figure 3 shows the instantaneous distribution

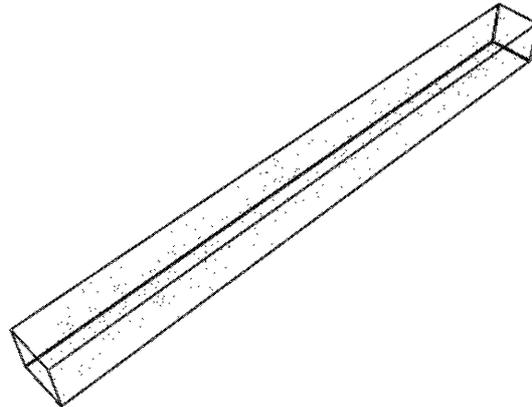


Figure 3: Instantaneous distribution of the particles.

of 150000 particles. Further results will be presented in the final paper and in the conference.

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