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Study of the conservation properties in two-way coupled dispersed multiphase flows using finite volume methods

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Abstract. In order to simulate dispersed multiphase flows, the coupling level must be determined according to the volume fraction in the system. The volume fraction is the ratio of the total volume of the dispersed phases over the total volume of the flow. In dilute flows, with volume fractions smaller than 10^{-6} , only the influence of carrier phase over the dispersed phase is considered which is known as one-way coupling. Nonetheless, in dispersed flows with higher volume fractions, the effect of the dispersed phase over the continuous one should be taken into consideration, known as two-way coupling. This effect normally is applied as a source term in the conservation equations of the carrier phase. Depending on the numerical method and the discrete operators employed, these source terms can lead to some issues when aiming to preserve physical properties like mass, momentum and energy. Moreover, in order to validate the two-way coupling method, a particle-laden turbulent flow benchmark case with a mass loading of 22% is simulated by means of large eddy numerical simulation (LES). The aim of this work is to study the conservation properties of dispersed multiphase flows like momentum, kinetic energy and thermal energy through two-way coupling between dispersed and continuous phases.

1. Introduction

With the purpose of analyzing the phenomena where one phase is continuous and the other ones are dispersed, simulations of dispersed multiphase flow are required.

Aiming toward the numerical simulation of dispersed multiphase flows, several methods can be applied. When the motivation is to simulate two-way coupled dispersed multi-phase flows where up to $\sim O(10^6)$ - $O(10^9)$ particles are present in the studied domain, Eulerian-Lagrangian computational method is the most well suited. This method easily allows capturing and accounting for non-linearities, multi-scale interactions and non-equilibrium effects in poly-dispersed multiphase flows [1].

Accordingly, Navier-Stokes equations and a dynamic equation based on Newton's second law of motion (known as BBO-equation [2]) are applied for the carrier phase and tracking the particles, respectively. The flow field is discretized and solved on a collocated finite volume grid. The pressure-velocity coupling is solved by means of the fractional step method [3]. Moreover, flow field discrete equations are advanced in time using the calculated source terms from the previous time step.

In the present work, numerical simulations of two-way coupled dispersed multiphase flow are presented. It is organized as follows: first section is a brief introduction; second section gives an overview of the background necessary for understanding the numerical methods and presents the main



equations; in third section, first a simple case study is studied and some preliminary results of the conservation properties for the considered numerical methods are presented. Following, in order to validate the two-way coupling method, a benchmark case is studied; finally, some conclusions are drawn in the last section.

2. Methodology

The methods of direct numerical simulation of dispersed multiphase flows have been described comprehensively in the literature [4][5]. So, the goal of this section is to summarize the essential equations and numerical methods that have been applied. The governing equations for determining the n^{th} particle position and momentum in time are respectively [2]:

$$\frac{d\mathbf{x}_p^n}{dt} = \mathbf{v}_p^n \quad (1)$$

$$m_p^n \frac{d\mathbf{v}_p^n}{dt} = \sum_i \mathbf{F}_i \quad (2)$$

where \mathbf{x}_p^n , \mathbf{v}_p^n and m_p^n are center location, velocity and mass of the n^{th} particle. The sum of forces appearing in the right-hand side of equation (2) accounts for all the relevant forces acting over the particles, e.g., drag, gravity, added mass, pressure gradient force, etc.

In order to study the conservation properties of the described numerical algorithm, for simplicity, it is assumed that the drag force is the only significant fluid-particle interaction force. Therefore, equation (2) simplifies to:

$$m_p^n \frac{d\mathbf{v}_p^n}{dt} = m_p^n \frac{\beta^n [\mathbf{u}(\mathbf{x}_p^n) - \mathbf{v}_p^n(\mathbf{x}_p^n)]}{\rho_p}, \quad \beta^n = \frac{3 C_D \rho}{4 d_p} |\mathbf{u}(\mathbf{x}_p^n) - \mathbf{v}_p^n(\mathbf{x}_p^n)| \quad (3)$$

where ρ_p is the density of the particle and $\mathbf{u}(\mathbf{x}_p^n)$ is the velocity of fluid in the position of the n^{th} particle. β is the momentum exchange coefficient. ρ , d_p and C_D are the density of the fluid (assumed constant), the diameter of the n^{th} particle and the drag coefficient, respectively.

The equation for the energy transfer of a single solid particle is determined as [6]:

$$\frac{dT_p^n}{dt} = G \frac{6Nu\lambda_g}{c_{p,p}\rho_p d_p^2} (T_g - T_p^n), \quad Nu = 2 + 0.552 \text{Re}_p^{\frac{1}{2}} \text{Pr}_g^{\frac{1}{3}} \quad (4)$$

where T_p and T_g are the temperature of the n^{th} particle and fluid, $c_{p,p}$ and λ_g are the specific heat for the particle and the thermal conductivity of fluid and $G = 1$. Nu , Re_p and Pr_g are the Nusselt number, the droplet Reynolds number and the gas phase Prandtl number, respectively.

Numerical approximation of the fluid velocity at the particle position $\mathbf{u}(\mathbf{x}_p^n)$ is determined by interpolating the fluid velocity from a stencil of surrounding nodes. Hence, these interpolations can be seen as a weighted sum of the velocities in the computational nodes surrounding particle position.

According to the fact that the volume fraction of particles is relatively small (i.e. less than 0.1%), by neglecting the volume that the particle phase occupies (i.e. dilute approximation) and by considering the two-way coupling between particles and fluid, the equations of motion for the fluid can be approximated by:

$$\nabla \cdot \mathbf{u} = 0 \quad (5)$$

$$\rho \left[\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) \right] + \nabla p = \mu \nabla^2 \mathbf{u} + S_u \quad , \quad S_u = - \sum_{n=1}^{N_p} \frac{m_p^n \beta^n [\mathbf{u}(\mathbf{x}_p^n) - \mathbf{v}_p^n(\mathbf{x}_p^n)]}{\rho_p} \quad (6)$$

where p , μ and S_u are the pressure, the dynamic viscosity and the momentum source term. The thermal energy equation is defined as:

$$\rho \frac{\partial h}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) - h \nabla \cdot (\rho \mathbf{u}) = \frac{Dp}{Dt} - \nabla \cdot \dot{\mathbf{q}} + \boldsymbol{\tau} \nabla \cdot \mathbf{u} + \dot{Q} + S_e \quad (7)$$

where h , $\dot{\mathbf{q}}$, $\boldsymbol{\tau}$, \dot{Q} and S_e are the enthalpy, the conduction heat flux, the viscous stress tensor, a heat source term and the thermal source term due to the two-way coupling, respectively.

$$S_e = - \sum_{n=1}^{N_p} m_p^n c_{p,p} conv_{ht}^n \quad , \quad conv_{ht}^n = G \frac{6Nu\lambda_g}{c_{p,p}\rho_p d_p^2} (T_g - T_p^n) \quad (8)$$

As expressed in the work of Sundaram et al. [7], the dynamic equation for the total kinetic energy in a fluid phase considering a periodic system is:

$$\frac{dE}{dt} = -\Phi_v - \sum_{n=1}^N \frac{m_p^n \beta^n \mathbf{u}(\mathbf{x}_p^n) \cdot [\mathbf{u}(\mathbf{x}_p^n) - \mathbf{v}_p^n(\mathbf{x}_p^n)]}{\rho_p} \quad (9)$$

where E and Φ_v are the total kinetic energy of the fluid and the viscous loss term. The dynamic equation for the kinetic energy of a single particle is found by dotting equation (3) with the particle velocity. Summing over the total number of particles then yields:

$$\frac{dE_p}{dt} = \sum_{n=1}^N \frac{m_p^n \beta^n \mathbf{v}_p^n(\mathbf{x}_p^n) \cdot [\mathbf{u}(\mathbf{x}_p^n) - \mathbf{v}_p^n(\mathbf{x}_p^n)]}{\rho_p} \quad (10)$$

where E_p is the total kinetic energy of the particles.

If we sum equation (9) and (10), the total kinetic energy in the system can be expressed as:

$$\frac{dE}{dt} + \frac{dE_p}{dt} = -\Phi_v - \sum_{n=1}^N \frac{m_p^n \beta^n |\mathbf{u}(\mathbf{x}_p^n) - \mathbf{v}_p^n(\mathbf{x}_p^n)|^2}{\rho_p} \quad (11)$$

As discussed in the work of Sundaram et al. [7], and according to equation (11), the total kinetic energy of the system is dissipated by two mechanisms, a homogeneous term due to viscous losses throughout the system and a term that results from the drag imparted by one phase on the other. The drag forces, although conservative in their momentum exchange, are dissipative in terms of the total kinetic energy.

3. Preliminary results

3.1. Simple test case

A cube with a length $L = 1m$ with periodic boundary condition is considered. 10^5 - 10^6 particles with density and diameter of $\rho_p = 1500 kg.m^{-3}$ and $d_p = 3 \times 10^{-4}m$ are distributed randomly in the domain. $\mathbf{v}_p = (1,0,0)m.s^{-1}$, $\mathbf{u} = (0,0,0)m.s^{-1}$, $T_p = 40^\circ C$ and $T_g = 25^\circ C$ are the initial velocity and temperature for the particles and fluid.

As it is shown in figure 1, figure 3 and figure 4 due to the two-way coupling approach, the total momentum and thermal energy of the system are almost conserved. figure 2 shows that the total kinetic energy of the system is almost equal to the expected one due to the dissipation.

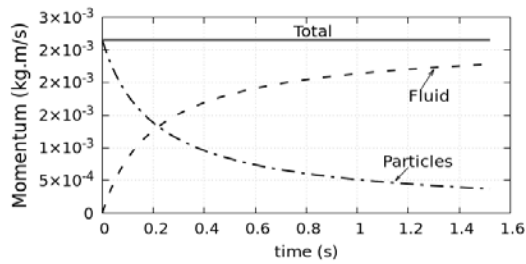


Figure 1. Momentum conservation versus time.

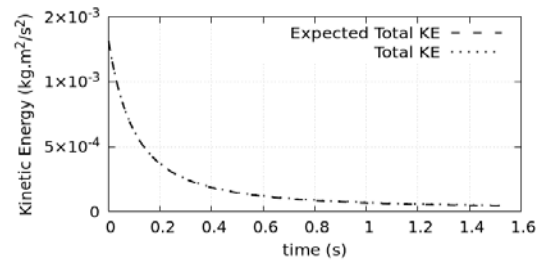


Figure 2. Total kinetic energy and the Expected total kinetic energy.

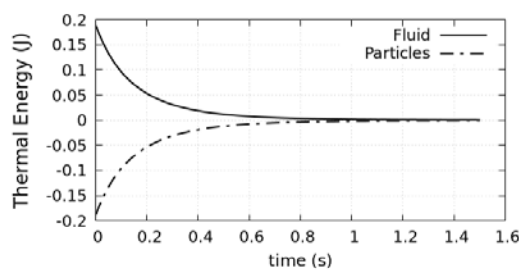


Figure 3. Variation of thermal energy in each time step for particles and fluid.

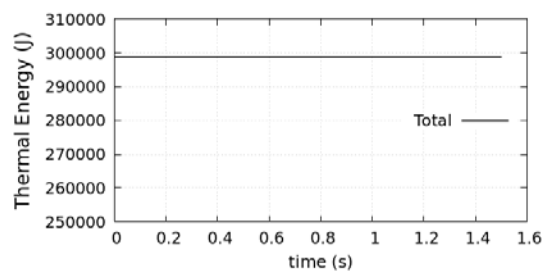


Figure 4. Total thermal energy in the system.

3.2. Real test case

In this section, a real test case of a particle-laden turbulent flow using two-way coupling approach is simulated. The selected case is the flow loop Hercule of Borée et al. [8] which generates an axisymmetric confined bluff body flow.

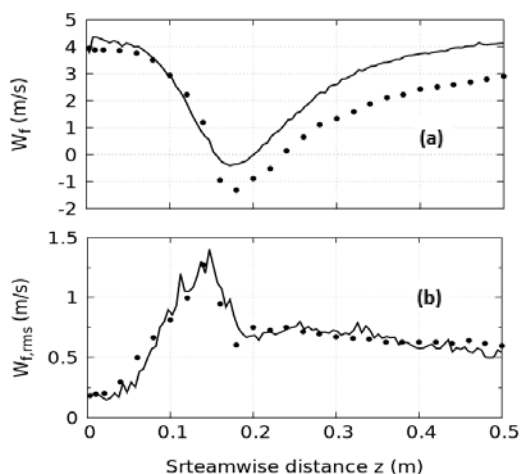


Figure 5. Streamwise profiles of fluid (a) mean velocity and (b) RMS velocity for the particle-laden configuration ($M=22\%$). Circle: Experiment; solid line: Numerical simulation.

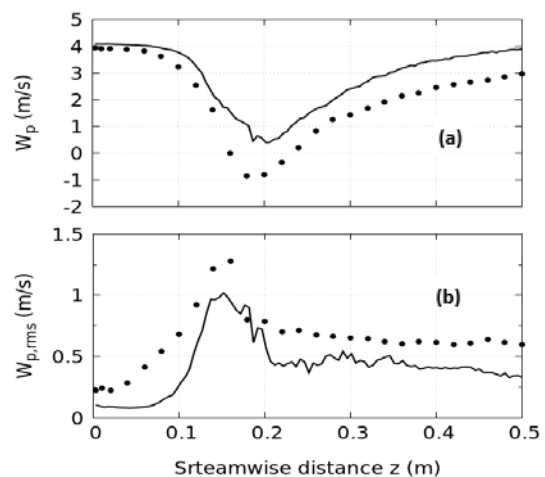


Figure 6. Streamwise profiles of particle ($dp=20\mu\text{m}$) (a) mean velocity and (b) RMS velocity for the particle-laden configuration ($M=22\%$). Circle: Experiment; solid line: Numerical simulation.

As it is seen in figure 5 and figure 6, the preliminary results show a good agreement for the continuous phase velocities, although some discrepancies can be seen for the velocities of the dispersed phase. Nonetheless, the trend is well-captured. Further studies are being carried out to assess the source of discrepancies.

4. Conclusion

The present work is focused on the study and development of numerical methods in order to enhance the conservation properties of the numerical methods for two-way coupled dispersed multiphase flows. According to the presented preliminary results, the developed numerical method presents an almost constant value for the total momentum and thermal energy of the system. Moreover, the total kinetic energy of the system almost matches the theoretically expected one, considering the inherent dissipation due to the drag force.

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