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An energy preserving formulation for the simulation of multiphase turbulent flows

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ABSTRACT

In this manuscript we propose an energy preserving formulation for the simulation of multiphase flows. The new formulation reduces the numerical diffusion with respect to previous formulations dealing with multiple phases, which makes this method to be especially appealing for turbulent flows. In this work we discuss the accuracy and conservation properties of the method in various scenarios with large density and viscosity jumps across the interface including surface tension effects.

1. Introduction

Nowadays the simulation of turbulent flows is the object of intense research. Although numerical techniques and models have been already widely investigated in the literature for single phase flows, current studies are still far from a complete understanding of real processes encountered in a countless number of applications involving multiple phases, such as rocket engines injectors, diesel engines or chemical process. When two or more different phases are present in the system we can distinguish not only a range of characteristic length-scales related to the turbulent nature of the flow, but also a range of sizes and shapes of each of the phases present in the system. This fact significantly increases the complexity of the simulations required to investigate such type of problems, which require a continuous development and optimization of the numerical techniques and models. The scientific community has made an important effort developing models for multiphase flows when one of the phases can be considered as disperse (only some examples can be found in Refs. [27,11,29]). However, the extension and evaluation numerical models to situations where the structures of the interfaces is well captured is less prolific. The development of these methods is important in order to evaluate the importance of turbulence in process where any of the multiple phases present on it can be considered as disperse.

Numerical techniques used for the simulation of turbulent flows and multiphase flows have been traditionally different. On one hand, numerical schemes typically used for the simulation of turbulent flows pay an especial attention to the conservation of global properties such as energy. Because we usually want to solve for problems where the smallest scales of the flow cannot be solved (e.g. Large Eddy Simulations) we need to introduce physical models to capture the correct behavior of the system on the resolved scales. Thus, in order to validate the physical models, it is desirable to reduce any numerical dissipation that can interfere with the performance of the subgrid models. On the other hand, the schemes presented for the simulation of multiple phases are designed to guarantee stability. Although they try to reduce the numerical dissipation as much as possible [26], for under-resolved simulations the numerical energy dissipation can become more important than the extra terms added in LES models.

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The selection of the most suitable numerical scheme for the simulation of complex problems involving different phases is not simple. One must evaluate the pros and cons of each numerical scheme for the particular problem that needs to be solved. First of all, one has to be careful on the choice of the numerical method when dealing with multiphase flow with large density ratios [8]. The number of works coupling these methods with turbulent flows is still scarce. Desjardins et al. [9] has proposed a level set/ghost fluid method for simulating turbulent atomization. More recently, Raessi and Pitch [24] have proposed a consistent mass and momentum transport using a level set method. In this work, we propose a new numerical scheme for the simulation of turbulent multiphase flows. The method is based on the discretization procedure followed by Verstappen and Veldman [33,34] for the simulation of single phase flows. This method has been shown to strictly conserve energy irrespective of the mesh resolution in those cases where there is not any physical mechanism of energy dissipation. Indeed, the method is derived in order to reduce numerical dissipation at expenses of the local truncation error. This type of methods has attracted the interest of the scientific community on the simulation of incompressible [33,34] and compressible flows [1,10,15,16], but it has not been extended to systems with multiple phases yet.

When dealing with multiple phases, we need to choose a method to track the interface. Among all the methods available in the literature, the Volume of Fluid (VOF) method is especially suitable for the simulation of under-resolved simulations because it enforces mass conservation and it handles natural topological changes at the interface in the subgrid level. We chose the Gerris Flow Solver [22,23,21] as a platform to implement the new numerical scheme. This code has been well validated for the simulation of multiphase flows in various problems involving interfaces [14,13,2]. Moreover, the method has been designed to reduce the appearance of *parasitic* currents induced by surface tension forces [23], which is an appealing characteristic of the numerical scheme if one wants to reduce any artificial energy dissipation/generation on the system.

This work is structured as follows. First, the basic equations are presented. Then the numerical method is described paying an especial attention to the problems that arise when we account for different phases with arbitrary density and viscosity jumps and also when surface tension effects are included. Finally, we present different test cases to investigate the performance of the method in different situations.

2. Basic equations

The basic equations that need to be solved are the Navier–Stokes equations for incompressible flows [23],

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

$$\partial_t c_i + \nabla \cdot (c_i \boldsymbol{u}) = 0, \tag{2}$$

$$\rho(\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}) + \nabla p - \nabla \cdot \left(2\mu \boldsymbol{D}^T\right) - \sigma\kappa\delta_s \boldsymbol{n} = 0, \tag{3}$$

where $\boldsymbol{u}$ is the fluid velocity vector, c_i is the volume fraction of the i*th* component present in the system, p is the fluid pressure, $\boldsymbol{D}^T$ is the deformation tensor defined as $D^T_{ij} = (\partial_i u_j + \partial_j u_i)/2$, σ is the surface tension coefficient, κ is the curvature of the interface, $\boldsymbol{n}$ is the normal to the interface and δ_s is the Dirac distribution function which is used to express that the surface tension term is concentrated on the interface. The density ρ and viscosity μ represent the averaged fluid properties.

3. Numerical scheme

In this section we describe the numerical scheme developed in this work for the simulation of turbulent multiphase flows. The scheme presented here can be seen as an extension of the previous works presented by Verstappen and Veldman [33,34] for the simulation of turbulence flows in order to extend the applicability of the scheme to multiple phases using the Volume of Fluid techniques (VOF) implemented in Gerris [22,23].

3.1. Skew symmetric formulation for structured meshes

The underlying idea of the skew-preserving formulations is that the discretization scheme must satisfy certain properties in order to preserve mass and energy. Such properties are satisfied at expenses of increasing the local truncation error with respect to other formulations. In incompressible fluids, mass conservation is typically imposed by satisfying condition (1) for the velocity field at each time step. However, this condition is not sufficient to guarantee conservation of other properties such as the total energy. In the absence of thermal effects, the only energy present in the system is the mechanical energy, defined as $E_m = \frac{1}{2}\rho|\boldsymbol{u}|^2$. The evolution of the mechanical energy can be obtained by scalar multiplication of Eq. 3 with the velocity field,

$$\boldsymbol{u} \cdot \left(\rho(\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}) + \nabla p - \nabla \cdot \left(2\mu \boldsymbol{D}^T\right) - \sigma\kappa\delta_s \boldsymbol{n}\right) = 0, \tag{4}$$

which can be written as

$$\partial_t E_m + \nabla \cdot (E_m \boldsymbol{u}) = \nabla \cdot (\boldsymbol{\tau}\boldsymbol{u}) - \phi_v - \boldsymbol{S} \cdot \boldsymbol{u}, \tag{5}$$

where $\boldsymbol{\tau}$ is the total stress tensor, ϕ_v is the viscous dissipation function and $\boldsymbol{S}$ is the source term, that includes surface tension effects. From the mathematical point of view it can be proved that, for an inviscid fluid without any external force, the