DNA of Gravity-Driven Bubbly Flows  
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Abstract

Present research is focused in combining High-Performance Computing (HPC) and Direct Numerical Simulation (DNS) of gas-liquid multiphase flows, in order to study gravity-driven flows and thermocapillary instability (g ≠ 0). Bubbly flows in a vertical channel. The Navier-Stokes equations and energy equations are discretized by means of the finite-volume approach, the pressure-velocity coupling is solved using a fractional-step-projection method, whereas the conservative scale level (CSE) methodology is used for interface capturing, thus, mass conservation issue that is known to affect standard LS methods, is circumvented. On the other hand, one of the disadvantages of interface capturing methods is the numerical and potentially unphysical coalescence of the fluid interfaces. In this work, a novel multiple marker-level-set methodology is used in order to avoid the numerical coalescence of the bubbles, instead, long-time simulations of bubbly flows including bubble collisions can be simulated.

Introduction

Gravity-driven and thermocapillary-driven bubbly flows are found in many natural and industrial processes, for instance boiling heat transfer in heat exchangers, bubble columns, bubble reactors in the chemical processes industry and micro-devices. While experiments are difficult due to limitations in optical access and analytical methods can be applied for the most simple cases, the development of supercomputers have promoted Direct Numerical Simulation (DNS) of the Navier-Stokes equations as another method to carry out controlled experiments of bubbly flows, although computationally demanding.

Mathematical model and numerical methods

Following the work of [3], the Navier-Stokes equations for the disordered fluid and continuous fluid, are written as:

\[ \frac{\partial \rho_{f} \mathbf{v}}{\partial t} + \rho_{f} \nabla \cdot \mathbf{v} = \nabla \cdot (-p 
abla \mathbf{v}) + \rho_{f} \mathbf{g}, \quad \text{and} \quad \nabla \cdot \mathbf{v} = 0 \]  

where \( \rho_{f} \) is the disordered fluid density at the interface, \( H_{f} \) is the Heaviside step function that is one in \( U_{2f} \) and zero elsewhere, \( g \) is the gravity vector, \( \mathbf{v} \) is the velocity field, \( p \) is the pressure. The energy equation is written for the temperature \( T \) as follows:

\[ \frac{\partial \rho_{f} T}{\partial t} + \nabla \cdot (\rho_{f} \mathbf{v} T) = \frac{\sigma}{\rho_{f}} \nabla \cdot (\nabla \cdot \mathbf{v} T) + \rho \mathbf{g} \cdot \nabla \mathbf{v} \]  

where \( \sigma \) is the thermal conductivity and \( \rho \) is the thermal conductivity. Interface capturing is performed by means of a unstructured CFSM [12, 13], furthermore a coupled VOF/LES method [5] has been designed. A multiple marker approach [3, 15] is used to represent each fluid particle. In CFSM method [2, 12], the interface is implicitly represented by the 0.5 iso-surface of an indicator function \( \phi_{j} \):

\[ \phi_{j}(x, t) \sim \frac{\text{tanh} \left( \frac{d_{j}(x, t)}{2} \right)}{2} + 1, \quad i = 1, \ldots, n_{f} \]  

where \( d_{j} \) is the signed distance function of the \( i \)-th fluid particle, \( c = 0.5 d_{j} / \Delta x \) is a parameter that sets the thickness of the profile, and \( h \) is the grid size [2]. The interface transport equation is written in conservative form provided the velocity field is solenoidal, \( \nabla \cdot \mathbf{v} = 0 \):

\[ \frac{\partial}{\partial t} \nabla \cdot \mathbf{v} + \nabla \cdot (\mathbf{v} \mathbf{v}) = 0 \]

A re-initialization equation is solved in order to keep a sharp and constant interface profile [2, 3, 12, 13], extended to the multiple-marker CFSM method [3] and variable interface tension [3, 10]:

\[ \frac{\partial}{\partial t} \phi_{j} + \nabla \cdot (\phi_{j} \mathbf{v}) = 0, \quad i = 1, \ldots, n_{f} \]

Surface tension is calculated by the continuous surface force (CSF) model (Brackbill, 1982), extended to the multiple-marker CFSM method [3] and variable interface tension [3, 10]:

\[ \mathbf{f}_{i} = \sum_{i=1}^{n_{f}} \left( \frac{\partial \mathbf{v}}{\partial t} \phi_{i} \mathbf{n} + \phi_{j} \left( \frac{\partial \mathbf{v}}{\partial t} \mathbf{n} \right) \right), \quad \text{with} \quad \mathbf{f}_{i} = \frac{\partial \mathbf{v}}{\partial t} + \nabla \phi \mathbf{n}, \quad \mathbf{v} = 0 \]

Interface curvature \( k_{i} \) and normals \( \mathbf{n}_{i} \) are computed as follows [2, 3, 10]:

\[ \phi_{j}(x) \sim \frac{1}{2} \nabla \cdot \nabla \phi_{j}(x), \quad \mathbf{n}_{i} = \frac{\nabla \phi_{j}(x)}{\nabla \phi_{j}(x)} \]

The mathematical model is discretized by means of the finite-volume method on a collocated unstructured grid, according to [3]. For \( \rho_{f} \mathbf{g} \) and \( \mathbf{v} \), Runge-Kutta4 schemes are used for convective terms [3], whereas the pressure-velocity coupling is solved with the fractional-step method (Chorin 1967). The numerical algorithms are implemented in the framework of an in-house parallel C++/MPI code called TermoFluids. Simulations have been performed on the supercomputer MareNostrum III (BCS), Barcelona-Spain. Verifications, validations, further details on the numerical methods and finite-volume discretization of the governing equations are reported in [3, 12, 13, 2].

Numerical experiments

Isotropical gravity-driven bubbly flows are characterized by the density ratio \( \rho_{f} / \rho_{d} \) or \( \rho_{f} / \rho_{l} \), viscosity ratio \( \mu_{f} / \mu_{d} \) or \( \mu_{f} / \mu_{l} \), and the ratio of the disordered fluid density at the interface, \( \rho_{f} \), to the disordered fluid density, \( \rho_{f} \). Thermocapillary instabilities with \( g = 0 \) are characterized by the thermal conductivity ratio \( K_{t} = \lambda_{f} / \lambda_{d} \), or \( K_{t} = \lambda_{f} / \lambda_{l} \), the heat capacity ratio \( c_{p,f} / c_{p,d} \), or \( c_{p,f} / c_{p,l} \). The heat capacity ratio \( c_{p,f} / c_{p,d} \), or \( c_{p,f} / c_{p,l} \) is the ratio of the disordered fluid density at the interface, \( c_{p,f} \), to the disordered fluid density, \( c_{p,f} \). Capillary number \( \mathbf{Ca} = \mu_{f} / \rho_{f} \), and Reynolds number \( \mathbf{Re} = \mu_{f} / \rho_{f} \).

Isotropical gravity-driven bubbly flows

The domain \( \mathbf{D} \) is defined as a vertical circular cylinder bounded by a rigid wall, with \( (D_{h}, H_{f}) = (5, 5) \), \( D_{f} = 10 \), \( D_{d} = 20 \), \( D_{c} = 10 \), \( D_{r} = 20 \), \( D_{s} = 20 \). The disordered fluid density at the interface, \( \rho_{f} \), is distributed in smooth CR > 0. The disordered fluid density at the interface, \( \rho_{f} \), is distributed in smooth CR > 0. The domain \( \mathbf{D} \) is defined as a vertical circular cylinder bounded by a rigid wall, with \( (D_{h}, H_{f}) = (5, 5) \), \( D_{f} = 10 \), \( D_{d} = 20 \), \( D_{c} = 10 \), \( D_{r} = 20 \), \( D_{s} = 20 \). The disordered fluid density at the interface, \( \rho_{f} \), is distributed in smooth CR > 0.

Conclusions

* Robust and accurate interface capturing methods have been introduced for simulating isolatomical and non-isotropical bubbly flows on unstructured grids [3, 12, 13], including interface heat transfer and variable interface tension [3]. A multiple marker approach has been introduced for simulating bubble swarms [3, 15], without numerical coalescence of the fluid interfaces.
* Future work is focused in the introduction of complex transport phenomena at the fluid interfaces, including mass transfer, phase change and chemical reactions.

References


Acknowledgements

The authors acknowledge the financial support of the MINECO (RTI2018-99728-P) Spain, Núria Rigola acknowledges the financial support of the Programa Genera Excel, ADIFREDO (ITD-101768-I), Spain. Compute time awarded by PRACE, ECB-F00-C01 (project 2.3.112060) on the supercomputer MareNostrum III based in Barcelona Spain is acknowledged. The Implementation Phase of PRACE receives funding from the EU’s Seventh Framework Programme (2007-2013) under grant agreement INFSO-ICT-216903 and from the EU’s Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 6332763.