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A path-conservative finite volume scheme for compressible multi-phase flows with surface tension

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ABSTRACT

The accurate simulation of compressible multi-phase flows with surface tension effects is currently still one of the most challenging problems in computational fluid dynamics (CFD). The basic difficulties are the capturing of the correct interface dynamics between the two fluids as well as the computation of the interface curvature. In this paper, we present a novel path-conservative finite volume discretization of the continuum surface force method (CSF) of Brackbill et al. to account for the surface tension effect due to curvature of the phase interface. This is achieved in the context of a *diffuse interface approach*, based on the seven equation Baer–Nunziato model of compressible multi-phase flows. Such diffuse interface methods for compressible multi-phase flows including capillary effects have first been proposed by Perigaud and Saurel. In the CSF method, the surface tension effect is replaced by a volume force, which is usually integrated as a classical volume source term. However, since this source term contains the gradient of a color function that is convected with the flow velocity, we propose to integrate the CSF source term as a non-conservative product and not simply as a source term, following the ideas on path-conservative finite volume schemes put forward by Castro and Parés.

For that purpose, we use the new generalized Osher-type Riemann solver (DOT), recently proposed by Dumbser and Toro and compare it with a path-conservative Roe and Rusanov scheme. Via numerical evidence we can show that if the curvature computation is exact, our new scheme is *well-balanced* for a steady circular bubble in equilibrium according to the Young–Laplace law. This means that the pressure jump term across the interface in the momentum equation is exactly balanced with the surface tension force.

We apply our scheme to several one- and two-dimensional test problems, including 1D Riemann problems, an oscillating droplet, as well as a deforming droplet initially attached to a wall and which is subject to gravity and surface tension forces. Finally, we also check the rising of a gas bubble due to buoyancy forces. We compare our numerical results with those published previously in the literature.

1. Introduction

Multi-phase flow problems including surface tension and capillary effects are of great interest in mechanical, chemical and aerospace engineering. They appear in many industrial processes, such as liquid fuel sprays injected into car, air- and spacecraft

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engines; mixing processes in chemical engineering; breakup of liquid jets; condensation in nuclear reactors; off-shore engineering and bio-medical applications. The simulation of the physics and the mechanics of the interaction of different materials is of vital importance for the application of multi-phase flows, such as in high-speed flows with droplets, bubbles and particles, and high pressure problems with strong shock waves. The interface between the two different fluids is the location where complex phenomena, such as heat and mass transfer and surface tension can occur. Capillary effects are also of increasing interest in nano-mechanics, for example for the design and analysis of the performance of new hydrophobic, non-wetting or self-cleaning surfaces. Therefore, in the current paper the effect of surface tension is carefully studied in the context of compressible multi-phase flows.

In the past, many mathematical models and numerical methods have been developed for compressible and incompressible multi-phase flows. A first problem is to determine the location of the interface where the interactions between different fluids take place. Further difficulties arise when shock waves travel across the interface between two fluids. This is due to the fact that the numerical simulation of compressible multi-phase flows is far more complex than the simulation of single phase flows. The numerical schemes used to solve the interface tracking problem can be classified into three basic categories: tracking methods (moving grid or Lagrangian approach), capturing methods (fixed grid or Eulerian approach) and combined methods. In general, Lagrangian methods [1] explicitly track the interface of the two fluids via a moving mesh and thus always provide the exact location of the interface. However, mesh-based Lagrangian schemes are typically not suitable for multi-phase flows with complex vortex structures or where a complex merging and separation of the phase interface occurs. Thus, a completely different approach for the modeling of multi-phase flows with surface tension is based upon meshless Lagrangian particle schemes, such as the well-known Smooth Particle Hydrodynamics (SPH) method [2]. SPH is well-suited for the simulation of complex interface flows including surface tension, complex vortex flow and separation and merging of the phase interface. The SPH method provides excellent interface tracking capabilities, but it is also well known to exhibit several numerical instabilities, such as the tensile instability, which require artificial viscosity and other stabilization techniques. It is also important to note that SPH is computationally more expensive than most of the other methods. Furthermore, the method in general lacks even zeroth order consistency with the governing PDE. In recent years, novel SPH techniques have been developed to provide accurate and stable solutions for weakly compressible free surface flows, see e.g. [3,4].

In Eulerian schemes based on a fixed mesh there are two very popular methods for the capturing of the phase interface, namely the volume of fluid (VOF) method [5,54] and the level set (LS) method [6]. A combination of VOF and LS proposed in [7,8] has shown to produce a robust method for flows with complex geometries and interface deformations in the setting of incompressible fluids. The disadvantage of Eulerian methods applied to multiphase flow problems is a significant amount of numerical dissipation, which requires proper interface reconstruction techniques to avoid excessive smearing of the phase boundary and to restore a sharp interface. However, this may become rather cumbersome in complex configurations. The level set method also needs a periodic re-initialization to restore the signed distance function property of the level set function, which requires the additional solution of a Hamilton–Jacobi equation. Furthermore, VOF has difficulties in simulating highly compressible multi-phase flows, hence most of the applications of the VOF method are restricted to the simulation of incompressible fluids. While the VOF method is perfectly conservative, the level-set approach is not. Due to the piecewise linear interface reconstruction (PLIC) used in the VOF context and due to the signed distance function property of the level-set method, both approaches are called *sharp interface* methods.

A very recent and completely different method for simulating compressible multi-phase flows is a novel type of model that uses a *diffuse interface* approach based upon extended hyperbolic systems with stiff relaxation. The basic philosophy of this new type of models is similar to the capturing of discontinuities (shockwaves) in gas dynamics. These methods were presented for the first time by Saurel et al. in [9,10]. The diffuse interface approach is stabilized by the numerical diffusion provided by the Riemann solver at the interface, and when the mesh size tends to zero, also the interface thickness is approaching zero. Hence, in the limit, also the diffuse interface model tends to a sharp interface representation, but based on a totally different mathematical formulation. The first applications of the diffuse interface method to compressible multi-phase flows with surface tension in two space dimensions have been presented in [11,12], with a subsequent extension to three space dimensions carried out in [13]. Further recent research on multi-phase flows with surface tension has been presented in [14,15]. A common problem of all Eulerian methods, i.e. for both sharp and diffuse interface approaches, is the correct calculation of the interface curvature.

In this paper, the diffuse interface method of Saurel et al. is used for the capturing of the interface. The interface is identified by a function that represents the volume fraction of one of the two phases. The surface tension effects are included by the continuum surface force (CSF) method [16]. Since the CSF approach produces a source term that contains the gradient of the volume fraction function, we propose to treat this term as a non-conservative product rather than a classical volume source term. This is done in the context of path-conservative schemes forwarded by Parés and co-workers in [17,18]. Within a second order TVD finite volume scheme, the smooth part of the CSF source term is integrated like a classical volume source term, while the contributions due to the jumps in the volume fraction function at the element interfaces are naturally taken into account by the path-conservative finite volume scheme. For that purpose, we use the new generalized Osher-type Riemann solver of Dumbser and Toro [19,20] (DOT) in order to track the material interface accurately with only little numerical dissipation. We also provide a comparison with the more popular path-conservative Roe and Rusanov schemes. For a further recent extension of the DOT method in the framework of polynomial viscosity methods, see [21]. Due to the path-conservative framework, the surface tension force is naturally included into the Riemann solver. The physical properties of the interface with curvature κ are solved by the approximate Riemann solver without spurious oscillations near the material interface. Furthermore, the scheme satisfies the Abgrall condition [22] and is *well-balanced* for a circular bubble at rest that obeys the Young–Laplace relation, i.e. where