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A pressure-based treatment for the direct numerical simulation of compressible multi-phase flow using multiple pressure variables

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ABSTRACT

In this paper we present a pressure-based numerical scheme for the direct numerical simulation of compressible two-phase flows using the stiffened gas equation of state. While for many technical applications, two-phase flows can be treated as incompressible, this assumption fails in cases with high pressure and temperature as they can be found in rocket combustion chambers, for example. Our interest is in the development of a pressure-based method that aims at the extension of an incompressible two-phase code to the compressible regime. The development builds upon an asymptotic pressure decomposition using multiple pressure variables and has originally been designed for single-phase flows. Its adaptation to compressible two-phase flows is presented. This includes the possibility to resolve and track the interface as well as the description of the two phases by different equations of state. It is shown that the pressure-based scheme does not necessitate a cumbersome interface treatment in order to avoid spurious oscillations in the vicinity of the material interface. We do not yet take into account phase changes whose approximation requires a careful thermodynamic consistent procedure. Numerical examples are shown ranging from the one-dimensional transport of a multi-material contact discontinuity to the three-dimensional simulation of shock-droplet interactions. The scheme proves to be able to accurately simulate the propagation of pressure waves in gaseous and liquid phases.

1. Introduction

The direct numerical simulation (DNS) of two-phase flows including the resolution of the material interface is usually performed on the basis of the incompressible Navier–Stokes equations. Typical technical applications concern droplets in an air environment at ambient pressure. In such a configuration, the liquid itself can be considered to be almost incompressible. Often, the droplets are moving at low speed, such that the compressibility of the gas can also be neglected. Under these circumstances, kinetic and internal energy are decoupled resulting in the separation of thermodynamics and hydrodynamics. This separation comes along with different roles of pressure for compressible and incompressible flows. The incompressible pressure is decoupled from density and internal energy, as an equation of state (EOS) is not present. Therefore, pressure is of purely hydrodynamic nature and loses its thermodynamic meaning. Due to the incompressibility assumption thermodynamic effects are not directly coupled to the flow variables and phase changes are modeled as source terms [1]. However, in the context of fuel injection processes, more extreme ambient conditions have to be faced that are characterized by an augmented pressure and temperature and such an incompressible modeling is no longer admissible. Especially for large pressure and temperature gradients in the flow field, the thermodynamic effects have to be fully coupled to the fluid flow requiring the compressible flow equations.

The simulation of multiphase flows is always characterized by large jumps in the material properties across the interface separating two phases. An additional difficulty is the resolution and tracking of the interface itself. Both issues are of great importance for incompressible and compressible flows. A lot of different interface tracking methods have been developed and presented so far. Following [2] they can be grouped into two categories, the first group consists of the so-called moving and adaptive grid methods and the second group comprises the fixed grid methods. For a moving grid method, the grid cell boundaries are always aligned to the interface. Every grid cell only contains one fluid type allowing an accurate separation of the fluids with respect to the solution of the corresponding flow equations [2].

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Fixed grid methods do not align the interface to the cell boundaries, they usually track the interface in an indirect way. Two widespread fixed grid schemes are the volume of fluid (VOF) approach of Hirt and Nichols [3] for incompressible flows and the level set method [4,5]. While the VOF approach is based on the volume conservation and reconstructs the interface topology from the discrete volume fractions, the level set method represents the interface by the zero level set of a continuous function that is often equivalent to a signed distance function in relation to the interface.

Across the interface, the material properties of the fluids are considerably changing and this has to be handled by the numerical approach. For compressible flows special attention has to be paid on the different EOS on either side of the material interface. As the fluids can differ significantly in their properties, their EOS are also very different in nature. Problems may arise due to the numerical smearing of the density across the material interface that represents a contact discontinuity [6]. Numerical schemes for the simulation of compressible two-phase flows are usually density-based flow solvers that use density and energy as primary variables for the solution process. If there is no special remedy applied at the interface location, density-based numerical schemes for multifluid flows are prone to unphysical pressure oscillations when smeared density values are inserted into the EOS [6].

Different strategies can be followed to prevent such oscillations and to handle the jump in the EOS. Based on the way the thermodynamic transition across the interface is addressed, sharp and diffuse interface approaches can be distinguished.

Sharp interface approaches always treat the interface as distinct discontinuity and prevent a density smearing. The well-known ghost fluid approach of Fedkiw et al. [7] is such a sharp interface scheme. It is based on the solution of two independent single-phase Riemann problems at the interface location. Fedkiw uses a level set method to track the interface and ghost cells are introduced in its vicinity. The corresponding ghost values are computed by an entropy based extrapolation and finally a standard Riemann solver can be used to compute the fluxes at the material interface.

For the diffuse interface approaches, the density jump as well as the thermodynamic transition are smeared consistently across the interface. For this purpose, the EOS are modified in such a way that the insertion of the smeared density does not cause unphysical oscillations. Although these methods efficiently eliminate the pressure oscillations some of them suffer from the fact that they are based on the non-conservative flow equations. This limits their range of applicability to the weakly compressible regime as the accurate simulation of shock waves is impossible. For fluids obeying the stiffened gas EOS, Saurel and Abgrall [8] introduced a numerical method that imposes conditions on the energy to guarantee that the pressure stays constant across the interface. This scheme is also not fully conservative, but it allows the simulation of strong shock waves.

Our objective is the extension of the incompressible two-phase flow solver FS3D (Free Surface 3D) [1,9,10] to the compressible regime. Hence, we base our approach on a pressure-based compressible method, which equals the incompressible one when the Mach number tends to zero. The singular incompressible limit of the compressible flow equations can be treated by taking the pressure as primary variable and using the multiple pressure variables (MPV) method [11] that builds upon an asymptotic pressure decomposition. The compressible pressure is decomposed into the sum of a hydrodynamic pressure times M^2 and a thermodynamic background pressure, where M denotes a global reference Mach number. The background pressure has to be constant in space and may vary only in time. In the incompressible limit this pressure is the constant thermodynamic pressure that satisfies the EOS, while the other pressure term is a pure hydrodynamic one and is determined by the incompressible flow equations without any dependency on the EOS. In the compressible regime, the sum of the pressure terms has to satisfy the EOS to be consistent with the compressible flow equations. Using this pressure decomposition, the MPV approach offers the possibility to extend an existing pressure-based incompressible code to the compressible regime. The basis for this development is the conservative MPV formulation as described in the paper [12] for single-phase flows and the EOS of a perfect gas. A similar approach has recently been proposed by Cordier et al. [13] for a general EOS. These authors also verify the asymptotic-preserving property for the incompressible limit.

In this paper we present the extension of the incompressible flow solver to the three-dimensional compressible case and restrict ourselves in this first step to the inviscid case and do not consider phase transitions. The approximation of phase changes needs a thermodynamic consistent modeling of the diffuse interface and is out of the scope of this paper. We basically keep the well-known spatial and temporal discretization of the incompressible flow solver: The flow equations are discretized by a finite volume method on a Cartesian, staggered grid with second order upwind fluxes and a semi-implicit time discretization. The resulting linear system for the pressure is solved by a multigrid method. Both phases are described by a stiffened gas EOS. Due to the use of pressure as primary variable, it is possible to avoid pressure oscillations applying a simple interface treatment: The EOS is sharply switched at the phase interface, while the density is smeared over a few grid cells due to the numerical dissipation. We show that this numerical approach in combination with a pressure-based method is able to handle the propagation of pressure waves in gases and liquids very well. Even in the presence of large density jumps with shock wave interactions the results are free of spurious oscillations.

The outline of the paper is as follows. In the next section, the governing equations are presented. Afterwards, the MPV method and its extension to the treatment of three-dimensional multiphase flows are described. It is shown how the compressible pressure-based flow solver treats the interface and that the first order MPV scheme always guarantees an oscillation-free behavior at the interface. This is followed by the presentation and discussion of computational results that prove the capability of the MPV approach to simulate compressible two-phase flows. Finally, the paper closes with a short conclusion and a perspective on future work.

2. Governing equations

This section gives an overview over the equations that build the basis of our numerical scheme.

2.1. Compressible Euler equations

We use the three-dimensional conservation equations for mass, momentum and total energy for inviscid flows without gravitational and external forces and heat conduction in compressible gas dynamics that are known as the Euler equations

$$\frac{\partial \rho'}{\partial t'} + \nabla \cdot (\rho' \mathbf{v}') = 0, \tag{1}$$

$$\frac{\partial (\rho' \mathbf{v}')}{\partial t'} + \nabla \cdot [(\rho' \mathbf{v}') \circ \mathbf{v}'] + \nabla p' = 0, \tag{2}$$

$$\frac{\partial e'}{\partial t'} + \nabla \cdot [\mathbf{v}'(e' + p')] = 0. \tag{3}$$

Here, ρ' denotes the density, p' the pressure, $\mathbf{v}'$ the velocity vector and e' the total energy per unit volume. Dimensional variables are marked by the superscript $'$. The system (1)–(3) has to be closed