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Maintaining interface equilibrium conditions in compressible multiphase flows using interface capturing

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ABSTRACT

An accurate treatment of material interfaces in compressible multiphase flows poses important challenges for high-resolution numerical methods. Although high-order interface-capturing schemes have been used to accurately simulate gas/liquid interfaces with the Euler equations, these methods can result in temperature spikes at material discontinuities. While this phenomenon is not problematic for Euler simulations, it gives rise to numerical errors when heat conduction is included. In this work, we identify the source of these errors and propose a methodology to prevent their occurrence for various models used to represent gas/liquid interfaces in compressible flows based on a "single-fluid" formulation, in which interfaces are represented by discontinuities in the material properties. Our focus lies in materials (gases and liquids primarily, but also solids) that can be described by a stiffened equation of state, though our approach is generalizable to other equations. We show that numerical approaches that prevent pressure oscillations at interfaces may generate temperature errors, which affect the energy (and pressure) through the heat conduction term. We demonstrate that the material properties entering the equation of state must be computed according to suitable transport equations in conservative or non-conservative forms; the pressure and temperature must be calculated based on the appropriate properties. To verify the analysis and compute problems with gas/liquid interfaces of relevance, we develop a three-dimensional, high-order accurate, solution-adaptive finite difference framework. In particular, we show that temperatures and pressures may be significantly overestimated in calculations of shock-induced bubble collapse in water if temperature errors are not prevented.

1. Introduction

Compressible multiphase flows are central to a number of engineering applications, including cavitation erosion and high-speed combustion. One of the main challenges in accurately simulating these flows lies in simultaneously representing shock waves, interfaces separating fluids of large density ratios and physical diffusion processes, due to spurious numerical errors commonly generated at interfaces, which may eventually affect the entire flow field. The present work focuses on developing Eulerian approaches to accurately simulate shock waves and gas/liquid interfaces, with viscous and heat diffusion included.

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Numerical methods for Eulerian simulations of compressible flows with interfaces typically fall in one of two categories, tracking or capturing. In this article, we focus on the latter because it is relatively simple to implement even for high-order methods and is a logical approach to treat physical diffusion; tracking, which includes front-tracking [1] and level-set [2] methods, will not be discussed further here. Similarly to shock capturing, interfaces between fluids of different composition can be captured by regularizing them over a few grid points, while maintaining the correct jump conditions. By adding one transport equation for mass conservation of one of the fluids, an extension of the Euler equations to multiple fluids/phases is seemingly straightforward, as such an equation can be solved in conservative form with standard shock-capturing techniques. However, such a naive implementation has long been known to give rise to spurious pressure oscillations for isolated interfaces between fluids of different material properties (i.e., properties entering the equation of state) [3,4]. Furthermore, since material interfaces are linearly degenerate, there is no physical mechanism to steepen interfaces, unlike shock waves. Thus, to prevent interfaces from being overly smeared by numerical diffusion, high-order solution-adaptive [5,6] or sharpening [7–9] techniques are often used in practice.

In this context, Abgrall [3] was the first to recognize that, for interfaces separating two gases of different specific heats ratios γ, an additional transport equation solved for a distinct function of γ in non-conservative (advection) form prevents such oscillations. Shyue [4] later expanded this idea to solving a transport equation for the mass fraction, again in non-conservative form, and to liquids and solids obeying a stiffened equation of state. Johnsen and Colonius [10] further extended these approaches to high-order Weighted Essentially Non-Oscillatory (WENO, [11]) methods to simulate non-spherical bubble collapse [12], which Coralic and Colonius [13] further refined. Such high-order finite volume methods can be computationally expensive in multiple dimensions. To address this difficulty, finite difference (for gases only, [5,14,15]) and discontinuous Galerkin [6] methods have been proposed, in which high-order limiting is applied only at discontinuities. In simulations of the compressible Navier–Stokes equations for two gases with different specific heats ratios, Johnsen and Ham [16] noticed that an inconsistent treatment of temperature causes similar errors and significant temperature undershoots due to the coupling via the heat diffusion term; they proposed approaches to overcome these problems based on γ or mass fraction formulations. Although temperature errors may occur in Euler simulations, they have no influence on the results since temperature is a derived quantity. However, such temperature errors are problematic when accounting for heat diffusion, reacting flows, phase change and other temperature-dependent phenomena.

Recent developments in interface capturing for compressible multiphase flows originated from the seven-equation two-phase flow model [17], in which balance equations for mass, momentum and energy of each phase, as well as an equation for volume fraction evolution, are solved. The additional volume fraction equation prevents the occurrence of spurious pressure oscillations. For many problems of practical importance, five-equation models (e.g., that in [18]) describe the physics accurately, in which pressure and velocity equilibria between the phases are assumed; thus, equations for mass balance of each phase, for total momentum and energy, and for the volume fraction evolution are solved. This latter model and extensions thereof have been used to study a wide range of phenomena [18–26]. With these models, a consistent and efficient high-order extension to accurately include heat diffusion and predict temperature has yet to be proposed.

The objective of the present work is to develop a treatment for temperature in compressible multiphase flows that is physically consistent and efficient, and that does not produce spurious errors in simulations of gas/liquid interfaces and shocks, with viscous and heat diffusion included. Our approach is general in that it applies to γ (as in [3]), mass fraction (as in [4]) and volume fraction (e.g., five-equation, [18]) models. Through our analysis, we identify the causes for numerical errors caused by an inconsistent treatment of temperature using high-order shock-capturing schemes and show how these errors can be prevented so that accurate simulations with physical diffusion can be performed. The resulting 3D finite difference scheme is high-order accurate, conservative and prevents pressure and temperature errors. Our contribution advances the current understanding of compressible multiphase flows in that it generalizes the methodology of Johnsen and Ham [16] for gases, in which temperature errors are prevented, to gas/liquid flows and different capturing approaches and extends the work of Coralic and Colonius [13] to prevent temperature errors in such flows. The article is organized as follows. In Section 2, the physical model is presented, followed by the numerical models (Section 3). In Section 4, we discuss the causes for spurious pressure and temperature errors in the presence of heat diffusion and propose an approach to prevent them. We briefly describe the numerical implementation in Section 5 and verify it with rigorous test problems in Section 6.

2. Physical model

2.1. Equations of motion

Assuming no mass transfer or surface tension, the compressible Navier–Stokes equations govern the gas/liquid flows of interest:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0, \tag{1a}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j + p\delta_{ij}) = \frac{\partial \tau_{ij}}{\partial x_j}, \tag{1b}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}[u_j(E+p)] = \frac{\partial}{\partial x_j}(u_i \tau_{ij} - Q_j), \tag{1c}$$