Computers and Fluids 000 (2017) 1–17

Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/compfluid

Approximate Riemann solver for compressible liquid vapor flow with phase transition and surface tension

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ARTICLE INFO

Article history:
Received 6 December 2016
Revised 21 March 2017
Accepted 27 March 2017
Available online xxx

Keywords:
Compressible two-phase flow
Discontinuous Galerkin scheme
Phase transition
Surface tension
Realistic equation of state
Level-set
Rapid evaporation
Approximate Riemann solver

ABSTRACT

The sharp-interface resolution of compressible liquid–vapor flows is cumbersome due to the necessary tracking of the interface. The global dynamics are governed by local interface phenomena like surface tension effects as well as mass and energy transfer across the interface. These effects impose subtle jump conditions that have to be resolved locally at the interface. The exact solution of the two-phase Riemann problem is done by a complicated time-consuming iteration process. In addition most of the detailed knowledge of the Riemann pattern is not used in the overall algorithm such that the development of a much simpler approximative Riemann solver is desirable. The concept in this paper is to use an approximate solution of a two-phase Riemann problem at the phase interface. Extending the classical HLL Riemann solver for compressive shock waves, an additional intermediate state is introduced to distinguish between the liquid and vapor phase and to resolve the phase interface accurately. To get a thermodynamically consistent approximation a kinetic model is applied that determines the phase transition rate. The suitability of this approximative Riemann solver is validated by comparing the numerical results to the exact solution in one- and three-dimensional frameworks. The evaporation rates are compared to experiments with rapid evaporation and boiling. The two-phase approximative Riemann solver is then used in a compressible two-phase code with a sharp-interface resolution based on a ghost fluid approximation with data from this novel approximative two-phase Riemann solver. For a shock-droplet interaction this method provides a fast and accurate resolution of phase transfer and surface tension effects at much lower costs than the exact solution.

1. Introduction

Compressible two-phase flow is of practical relevance for several applications in high pressure and high temperature environments as found e. g. in rocket engines or diesel injection systems. Its numerical simulation is still challenging due to the fact that strong density changes occur at the interface which are driven by local phenomena as surface tension and phase transition. Furthermore strong pressure waves may propagate in the domain and interact with the fluid interfaces. Besides the different spatial scales the time evolution may also vary within several orders of magnitude.

To handle these phenomena, three different numerical approaches are discussed in the literature: The first two approaches handle the interface as a diffuse profile such that is smeared out over a couple of grid cells by the numerical discretization method. The challenge for these models is to obtain at the interface a thermodynamically consistent description of the mixture states, which may be even non-physical. The first approach is to consider the whole flow in each phase as a homogeneous mixture, often denoted as Baer–Nunziato-type models, see e. g. [1,2]. In this context the first exact Riemann solver has been presented in [3]. Another approach leads to phase field or second-gradient models as e. g. the Navier–Stokes–Korteweg equations, see [4,5] for instance. The third approach is to consider the interface as a discontinuity within the flow field that separates the phases. This necessitates the tracking of the interface during the simulation. The inherent assumption here is that the width of the physical interface is smaller than that of a grid cell and that a proper model exists to establish physically consistent interface jump conditions. The focus of this paper is on the latter topic with a physically motivated model to connect the states on both sides of the interface. Appropriate jump conditions are provided by an approximate solution of a two-phase Riemann problem.

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http://dx.doi.org/10.1016/j.compfluid.2017.03.026
0045-7930/

Let us note that the analysis of the Riemann problem for two-phase problems has been a very active field of research in the past decade (see [6] for a general theory and e.g. [7–12] for more specific examples). But, the analysis is mostly restricted to either the isothermal case or to homogeneous coupling conditions neglecting surface tension, latent heat, and entropy production. For the isothermal case approximate Riemann solvers based on a relaxation procedure can be found in [13,14] and based on the HLL approximation in [15]. An interface Riemann solver based on the linearization of the Lax-curves has been introduced by Fechter, Jaegle&Schleper [16]. For the Baer–Nunziato model a HLL approximation has been suggested by Furfaro & Saurel [17]. Let us note that we account explicitly for surface tension via integrating the dynamical Young–Laplace law into the approximate Riemann solver. For homogenized models capillarity effects enter directly into the equations. Corresponding Riemann solvers can be found in e.g. [18–20].

We use the ideas of the HLL approximation, introduced in [21] for single-phase flows. Several authors extended the basic HLL approximation to include more complex wave patterns. A classical issue is the improvement of the resolution of contact waves in the compressible Euler equations. Einfeldt [22] replaced the constant intermediate state by a linear one in the HLLEM Riemann solver, Toro et al. [23] developed an explicit reconstruction of the contact wave in their HLLC framework. Some recent extensions of the HLLEM scheme to multiple linearly degenerate characteristic fields are obtained by Balsara & Dumbser in [24].

In this paper we describe the development and numerical validation of the approximate interface Riemann solver. To account for phase transition waves we follow here the approach of Toro et al. [23] and adapt it to the occurrence in multi-phase flows. We denote the resulting approximate Riemann solver as *HLLP Riemann solver*, where *P* stands for phase transition. Let us mention here the related HLLC solvers in [25,26] which have been designed for the homogenized Baer–Nunziato models. The quality of any HLL-type approximation depends on the a priori estimation of the wave speeds. For single-phase flows improvements have been proposed e. g. in [22,27]. The description gets more difficult in the case of a liquid–vapor interface. Based on the Roe linearization for general equations of state Hu, Adams & Iaccarino [28] introduced estimations that take into account phase interfaces without phase transition and surface tension effects.

We present a HLL approximation, that is based on the sharp-interface model for two phase flows with phase transition, introduced in [29]. This model consists of the Euler equations in the bulk phases and jump conditions at the interface. The model has been validated against experimental results for shock tube problems of evaporating alkanes. The comparisons show a good agreement on the qualitative level as long as temperature differences remain small. In other situations, however, the solutions show unphysical large temperature jumps at the contact wave. Note that, using Euler equations heat conduction is neglected and temperature jumps can be arbitrary large at contact waves. The comparison using the HLLP approximation will compare better to the shock tube experiments. The reason is, in particular, that the contact wave, which is the potential source for the unphysical behavior, is averaged.

The proposed coupling by the approximate two-phase Riemann solver has to be combined with any interface tracking method. Here, we use a ghost fluid approach that is described without phase transitions in [30]. It is based on the ghost fluid method, proposed in [31] and extended by Merkle & Rohde [9]. Techniques to handle the interface resolution by the use of a moving grid are considered, e. g., by Nguyen et al. [32] and by Chalons et al. [33]; in Hu et al. [34] cutted cells are introduced.

The structure of the paper is as follows. In Section 2 the physical and mathematical model of the Riemann problem with phase transition and surface tension effects is described. In Section 3 the single-phase HLL approach is extended to approximate the effects at the phase interface. In Section 4 the numerical approach for the simulation of compressible two-phase flows is described that is based on the approximate Riemann solver. The approximate Riemann solver is then validated in Section 5 using several test cases with resolved surface tension and phase transition effects.

2. Mathematical and physical model

For the simulation of compressible liquid–vapor flows we consider the compressible Euler equations as model for the dynamics of the bulk (Section 2.1). The two-phase setting is explained in Section 2.2. The jump conditions at the interface are resolved sharply by the solution of the interface Riemann problem. For this Riemann problem in interface-normal direction the jump conditions are provided in Section 2.3 within a one-dimensional setting. The application and the coupling algorithm of the one-dimensional interface model within a three-dimensional flow solver is detailed in Section 4.2.

2.1. Bulk model: Compressible Euler equations

We assume that the interface $\Gamma(t)$ at time t divides the computational domain $\Omega \subset \mathbb{R}^3$ into two regions, the liquid region $\Omega_{\text{liq}}(t)$ and the vapor region $\Omega_{\text{vap}}(t)$. In both regions the mathematical model is given by the Euler equations

$$\begin{aligned} \varrho_t + \operatorname{div}(\varrho \boldsymbol{v}) &= 0, \\ (\varrho \boldsymbol{v})_t + \operatorname{div}(\varrho \boldsymbol{v} \otimes \boldsymbol{v} + p\boldsymbol{I}) &= \boldsymbol{0}, \\ (\varrho e)_t + \operatorname{div}((\varrho e + p)\boldsymbol{v}) &= 0, \end{aligned} \tag{1}$$

together with suitable initial and boundary conditions.

The vector of the conservative variables is denoted by $\boldsymbol{U} = (\varrho, \varrho\boldsymbol{v}, \varrho e)^t$, in which ϱ is the fluid density, $\boldsymbol{v} = (v_1, v_2, v_3)^t$ is the velocity vector and e is the specific total energy, which is related to the specific internal energy ε via $e = \varepsilon + \frac{1}{2}\boldsymbol{v}\cdot\boldsymbol{v}$. The superscript ^{t} denotes the transposed vector and $\boldsymbol{I}$ the 3-dimensional unit matrix. The system (1) is closed by a general equation of state (EOS) that relates the pressure to the conservative variables. To facilitate the thermodynamic description, we restrict ourselves in the following to the case of a single species in the bulk phases.

2.2. Two-phase thermodynamics

The pressure p, temperature T, specific entropy s, specific enthalpy h and specific Gibbs energy g of the fluid are considered to be given by a suitable EOS. Here we assume that the EOS is given as a (implicit) function of the conservative variables. For instance, the pressure-law is given as general function $p = p(\varrho, \varepsilon)$ of the variables density ϱ and internal energy ε. Similar approximations are available for the other thermodynamic quantities.

We consider solely subsonic, subcritical phase transitions and require that the saturation curve exists. This curve can be parametrized by a single thermodynamic quantity, e. g. using the temperature T or the pressure p. Along these curves the pressure, temperature and specific Gibbs free energy g are equal in both phases.

A schematic visualization of a generic EOS is plotted in Fig. 1 showing the isotherms for two different temperatures. The space of admissible states in the vapor and liquid region is indicated by shaded areas. In between these regions, the spinodal region is found, see e. g. [35,36], without physically meaningful sound speed. This region is the main reason for the complicated construction algorithm of the Riemann problem. The effects that may take

Please cite this article as: S. Fechter et al., Approximate Riemann solver for compressible liquid vapor flow with phase transition and surface tension, Computers and Fluids (2017), http://dx.doi.org/10.1016/j.compfluid.2017.03.026