The Use of Local Solutions to Model Phase Transitions in the Compressible Flow Regime

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Introduction

The idea in a sharp interface approach for two-phase interfaces is based on defining appropriate jump conditions to couple the bulk flows. Hence, local approximate relations are needed, which characterize the local thermodynamics at the interface. We use in the following the solution of the Riemann problem for two-phase flow with phase transition to obtain appropriate jump conditions and to establish the coupling of the macroscopic bulk phase simulations. Molecular interactions, governing the process of phase transition on a microscopic scale, are incorporated through evaporation models that promise a consistent entropy production. The validation of this sharp interface approach is done by comparing the results of a sharp interface macroscopic solution with molecular dynamics simulations. The simulations are based on the compressible flow equations. The viscous terms are neglected in these calculations and we consider the Euler-Fourier system. The heat flux is necessary to model the phase transition properly.

Jump Conditions at the Phase Interface

We restrict ourselves to consider an arbitrary fluid in a liquid and a vapor phase, i.e., a single-component fluid. The phase interface in the macroscopic description is assumed to be infinitesimally thin and to carry no mass nor energy. The phases may exchange mass, momentum and energy, which is based on the application of the conservation laws to the interface, as well as on the thermodynamic modelling. The jump conditions at the phase interface for mass, momentum and energy read as

$$[[\dot{m}]] = 0, \tag{1}$$
$$\dot{m}[[v]] + [[p]] = \Delta p_\Gamma, \tag{2}$$
$$\dot{m}[[e]] + [[vp]] + [[q]] = S^\Gamma \Delta p_\Gamma. \tag{3}$$

Here, $\dot{m} = \rho(v - S^\Gamma)$ is the evaporation mass flux per unit area, the double bracket $[[*]]$ denotes the jump across the interface, Δp_Γ denotes the increase of pressure due to surface tension based on the Young-Laplace law, and S^Γ denotes the velocity of the interface. In addition, the entropy balance has to be satisfied leading to the jump condition

$$\eta_\Gamma = \dot{m}[[s]] + [[\frac{q}{T}]] \geq 0, \tag{4}$$

where η_Γ denotes the entropy production across the interface. Focus of the thermodynamic modelling lies on the fulfillment of the first and second laws of thermodynamics. The first law is covered by the energy jump condition (3). The second law corresponds to the entropy balance and the jump condition (4). To complete these macroscopic jump conditions, local information is needed in form of an evaporation model, e.g., to specify the entropy production term η_Γ.

The Riemann Problem with a Phase Interface

The Riemann problem is the initial value problem with constant data, which jump at one point. It describes locally the situation at an interface assuming a constant state at both sides of an interface. Its solution in time bears the information what happens locally at the interface in short. In bulk flow, it is a basic building block in finite volume schemes to calculate the fluxes between grid cells. It has an exact solution in the inviscid case, i.e. for the Euler equations. Here, we extent this solution of the Riemann problem in the bulk phases to the two-phase case with phase transition. In the following, we restrict ourselves to phase transition from one pure phase to another pure phase and call the phases liquid and gas. We will generally speak of evaporation. However, all considerations also apply to condensation.

We consider the two-phase Riemann Problem as the initial value problem with a constant liquid state on the left and a vapor state on the right. Similar to the classical Riemann Problem, waves emerge from the initial discontinuity to the right and left hand side – into the liquid and into the gas. In the two-phase Riemann problem, the phase interface occurs in the interior region together with the contact discontinuity, which move with the local fluid velocity. A diagram of the Riemann solution is shown in Figure 1. Here, a rarefaction wave travels into the liquid region, while a compression wave goes into the gas. The solution can be obtained iteratively, looking how both states can be connected by the corresponding waves satisfying the appropriate jump conditions. The detailed procedure is described in detail in [1]. We mention that we consider here an inviscid solution, which has a much simpler structure because of the constant states between the waves. However, the jump conditions at the phase interface include

the jump of the heat flux to catch the physical situation in a proper way. The effect of heat conduction is neglected for the waves running into the gas and the liquid to the left and right. Because for the coupling of the bulk simulations the states right and left of the phase interface are needed only and the bulk simulations contain the heat conduction terms this should be of minor importance.
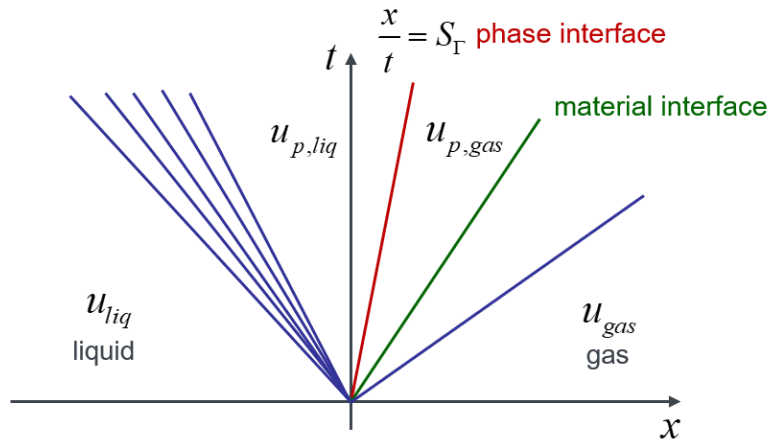

Figure 1. Diagram of the solution of the two-phase Riemann problem for a liquid and a gas interface with phase transition

Numerical Results

For validation, we compared the results of our numerical approach with results of molecular dynamic simulations. Our test problem is the two-phase evaporation shock tube, which was considered by Hitz et al. [2]. They studied the behavior of a saturated liquid that was put in contact with a superheated vapor with molecular dynamics simulations and a sharp-interface method. The vapor densities varied between 90%, 70% and 50% of the saturation density. To keep the interface sharp, we use a grid, moving with the velocity of the phase interface. The numerical method is a finite volume scheme of second order accuracy with a TVD limiter. The numerical fluxes are calculated by solving the classical Riemann problem in the bulk phases. The coupling was established by our two-phase Riemann solver. The evaporation model was based on Cipolla et al. [3]. We also considered an approximate solution of the two-phase Riemann problem. Figure 2 shows a comparison of all the results for 70% saturation density. The numerical results are in a very good agreement in density and velocity. Only directly at the shock wave, at about $x = 700$, the sharp-interface method predicts higher velocities than the molecular dynamics data. This aspect may be related to the absence of viscous terms in the mathematical fluid model while it is inherently contained in the molecular dynamic simulation. In temperature, the value of vapor is too high compared to the molecular dynamics data near the interface. The three Riemann solvers are in excellent agreement with each other, except for the vapor temperature near the interface. Here, both approximate Riemann solvers deviate from the exact solver and predict a slightly lower temperature. In combination with the ghost fluid method to keep the interfaces sharp, multidimensional simulations also show good results and high level of rubustness.
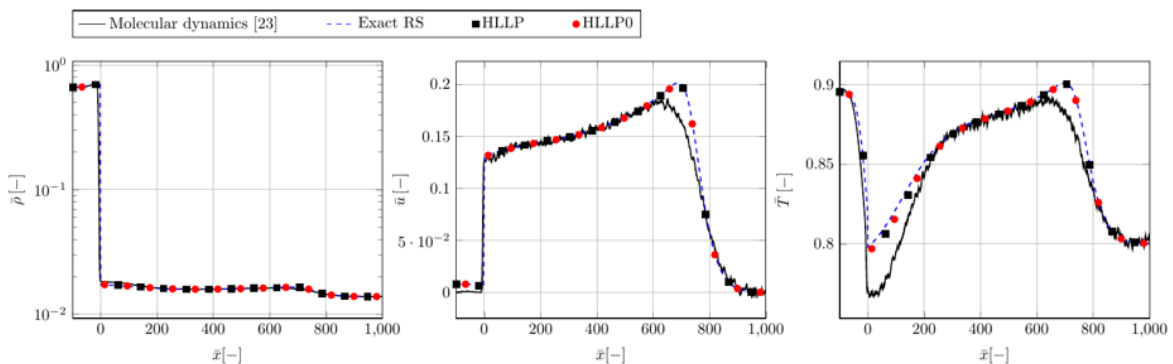

Figure 1. Diagram of the solution of the two-phase evaporation problem for a liquid and a gas interface with phase transition

References

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