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Liquid Vapor Phase Transitions: Modeling, Riemann Solvers and Computation

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The numerical approximation of liquid vapor flows within the compressible regime is a challenging task because complex physical effects at the phase interfaces govern the global flow behavior. In the isothermal case we consider conservation laws

$$\rho_t + \operatorname{div}(\rho\,\boldsymbol{v}) = 0, \qquad (\rho\,\boldsymbol{v})_t + \operatorname{div}(\rho\,\boldsymbol{v}\otimes\boldsymbol{v}) + \nabla p(\rho) = \boldsymbol{0} \tag{1}$$

with unknown density field $\rho = \rho(\boldsymbol{x},t) > 0$, unknown velocity field $\boldsymbol{v} = \boldsymbol{v}(\boldsymbol{x},t)$ and a given non-monotone equation of state $p = p(\rho)$, e.g. the Van-der-Waals pressure.

We develop a sharp interface approach which treats the phase boundary like a shock wave discontinuity and takes capillarity effects into account. The approach relies on the solution of Riemann problems across the interface that separates the liquid and the vapor phase. The Riemann solution accounts for the relevant physics by enforcing appropriate jump conditions

$$[\![\rho(\boldsymbol{v}\cdot\boldsymbol{n}-\sigma)]\!] = 0, \qquad [\![\rho(\boldsymbol{v}\cdot\boldsymbol{n}-\sigma)\,\boldsymbol{v} + p(\rho)\,\boldsymbol{n}]\!] = (d-1)\gamma\kappa\,\boldsymbol{n}, \tag{2}$$

at the phase interface. The propagation speed in normal direction $\boldsymbol{n}$ is denoted by σ. A wide variety of interface effects can be handled in a thermodynamically consistent way. This includes surface tension ($(d-1)\gamma\kappa$) and mass transfer by phase transition ($\rho(\boldsymbol{v}\cdot\boldsymbol{n}-\sigma)$).

For the correct treatment of the interface at any time, an additional level set equation

$$\phi_t + (\sigma\,\boldsymbol{n})\cdot\nabla\phi = 0 \tag{3}$$

has to be solved in the bulk. Since the fluid undergoes a phase transition one can not drive the level set function $\phi = \phi(\boldsymbol{x},t)$ with the fluid velocity $\boldsymbol{v}$.

I will present the main results of my phd-thesis [1]: exact two-phase Riemann solvers for (1), (2), the general coupling of Riemann solvers with bulk solvers for (1), (3) and numerical results in $2d$. To verify the solvers with respect to numerical and thermodynamic requirements, one-dimensional and radially symmetric problems are studied. Furthermore, the Riemann solvers and the sharp interface approach are successfully validated against shock tube experiments of explosively evaporating real fluids (alkanes).

REFERENCES

[1] Zeiler, C.: Liquid Vapor Phase Transitions: Modeling, Riemann Solvers and Computation, Universität Stuttgart, http://dx.doi.org/10.18419/opus-8902