Project Description: Multi-scale Modelling of the Evaporation Process

The goal of the subproject ‘Multi-scale Modelling of the Evaporation Process’ is the simulation of compressible multi-component droplets and their evaporation. The basis of the investigations is the high order, discontinuous Galerkin spectral element (DGSEM) code ‘FLEXI’ that allows to simulate multi-component flows utilizing an EOS tabulation method for efficient calculations. A sharp interface approach, the ghost fluid method, is used to separate liquid and gaseous flow regions with a dynamic boundary condition that can describe the evaporation of the liquid phase. An extensive study of the ghost fluid method with and without evaporation for single component flow is the first step on the road to ultimately implementing respective methods for multi-component flows. Another important aspect is the comparison with analytical (SP-A1) and numerical (SP-A2) investigations as well as diffuse interface simulations (SP-A6). Furthermore, a strong cooperation with SP-A6 is planned, to utilize the advantages of weakly compressible solvers regarding computational effort.

Governing equations and Equation of State

The one-dimensional Euler equation

\[ u_t + F_x = 0 \]  

with

\[ U = \begin{pmatrix} \rho \\ \rho v \\ \rho e \end{pmatrix} \quad \text{and} \quad F = \begin{pmatrix} \rho v \\ \rho v^2 + p \\ (\rho e + p) \end{pmatrix} \]

are used to model both the liquid and the gaseous phase. They are closed by an equation on state (EOS) of the form

\[ p = \rho (\gamma - 1) e + \gamma p \rho e \]

One option is to use a stiffened gas equation \[ \rho = \gamma (\gamma - 1) e + \frac{\gamma p}{\gamma - 1} \] with the parameters \( \gamma \) and \( \rho_e \) for each of the phases.

Numerical framework

The FLEXI solver is based on a DGSEM and allows high order simulations of compressible flows. The method is very efficient in smooth regions of the flow, however it is unable to handle discontinuities such as shocks and sharp material interfaces. As a result, a shock capturing method, based on equidistant finite volume subcells is used.\(^5\)

Thereby a sharp interface is preserved at the cell boundary of a discontinuous Galerkin element or a finite volume subcell respectively\(^1\),\(^2\). It is tracked using a one dimensional level-set equation

\[ \Phi_t + v \Phi_x = 0. \]

Important algorithmic steps are:

- Dynamic boundary condition is defined with the ghost fluid method.
- Riemann solver is used to define ghost states.
- Ghost states define cells that change from one phase to another.

Interaction of shock with air-water interface

Case III from \[4\]:
Shock in air hits air-water interface and is mostly reflected and partly transmitted.

Case IV from \[4\]:
Underwater shock hits air-water interface and is partially transmitted, whereas a rarefaction wave moves into the water region.

Future Work

- Rewriting of CFD code to allow the investigation of alternative ghost fluid methods.
- Extension of method towards evaporation.
- Proof of concept regarding combination of described method with a weakly compressible solver in cooperation with SP-A6.

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