Accurate Simulation of Rayleigh-Taylor-Instabilities

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1 Introduction

The accurate incorporation of source terms into high-resolution methods for hyperbolic conservation laws and the treatment of multicomponent gas flows are two import topics of current numerical research.

In [7] R. J. LeVeque proposes a modification of the wave propagation method to accurately capture the behaviour of quasi-steady flows.

In this paper, we derive the method for the case of the Euler equations under gravitational influence and apply it to flows of two nonmixing ideal gases. We present results of a numerical simulation of the behaviour of an instable interface between two gases driven by the standard gravitational field (Rayleigh-Taylor-instability).

The wave propagation method is a high resolution finite volume method of Godunov-type. By solving Riemann problems normal to the cell interfaces the flux-difference at each interface is split into a left-going and a right-going part. The update of a cell is defined by summing up all flux-difference fractions entering the particular cell. Second-order accuracy for smooth solutions is achieved by applying standard limiters to the waves. See [4] for details of the method.

An import property of the wave propagation method is it's applicability to hyperbolic equations that are not in conservation form. Instead of following the common approach to seperate the two gases by two continuity equations, we use a transport equation for the adiabatic coefficient γ [8][9]. Roe's approximate Riemann solver, based on multiple continuity equations, tends to create numerical oscillations at contact-discontinuities. For Euler equations without source terms, it has been proven, that these oscillations can be avoided by applying the γ-based model [9].

2 Treatment of source terms in quasi-steady flows

We consider the hyperbolic conservation law with source term

$$q_t + f(q)_x = \psi(q)\,. \tag{1}$$

A common approach to incorporate source terms into numerical methods is to use a fractional step method that alternates between solving the homogenous PDE

$$q_t + f(q)_x = 0 \tag{2}$$

and the ODE

$$q_t = \psi(q)\,. \tag{3}$$

These splitting schemes have the advantage, that the PDE can be treated with a high resolution method, while the ODE can be solved seperately with a standard ODE-solver.

But, fractional step methods must fail for quasi-steady flows, because they are based on the assumption $|q_t| \approx |\psi(q)|$. Near steady state, the relations

$$|q_t| \ll |f(q)_x| \approx |\psi(q)|$$

hold and the source term nearly has to be balanced by the flux gradient [7].
A splitting-like approach for the quasi-steady state can be based on the equations

$$f(q)_x = \psi(q) \tag{4}$$

$$q_t + f(q)_x = 0\,. \tag{5}$$

Fractional step methods make use of intermediate values of q in time. A numerical method based on (4) and (5) naturely uses intermediate values of q in space. Such a method has to fulfill the implicit condition (4) and must remain conservative on the original space discretization.

The quasi-steady version of the wave propagation method is based on the above idea [6][7]. Instead of employing the discrete value q_i to solve Riemann problems at the interfaces between neighboring cells, two intermediate values, q_i^+ and q_i^- are introduced. The Riemann problem at the right cell interface is solved using q_i^+, while the Riemann problem at the left uses q_i^-. A half cell is assigned to each intermediate value.
As a first order approximation to (4) we set

$$f(q_i^+) - f(q_i^-) = \Delta x \psi(q_i)\,. \tag{6}$$

To get a conservative scheme, the intermediate values q_i^+ and q_i^- have to fulfill the relation

$$\frac{1}{2}(q_i^+ + q_i^-) = q_i\,. \tag{7}$$

This condition is true for $q_i^\pm = q_i \pm \tilde{\delta} q_i$.

The flux difference $f(q_i^+) - f(q_i^-)$ of the newly-introduced Riemann problem equals the source term $\psi(q_i)$. Hence, the effect of $\psi(q_i)$ is exactly canceled out by the waves resulting from solving the Riemann problem between q_i^+ and q_i^-. By ignoring the source term and the Riemann problem, the required steady state balance is achieved. As the indermediate Riemann problems are omitted, the quasi-steady wave propagation method is stable up to Courant number 1 [7].

The jump magnitude $\tilde{\delta} q_i$ could be calculated from (6) by an iterative method. But, for particular cases, sufficient approximations can be derived directly.

3 One-dimensional Euler equations with gravity

We consider the one-dimensional Euler equations under influence of the standard gravitational field

$$\begin{aligned} \rho_t + (\rho u)_x &= 0 && (8)\\ (\rho u)_t + (\rho u^2 + p)_x &= -\rho g && (9)\\ E_t + [(E+p)u]_x &= -\rho u g && (10) \end{aligned}$$

with the ideal-gas-law $\quad p = \rho(\gamma - 1)(E - \rho u^2/2) \quad .$

We apply the quasi-stationary approach defined by (6)-(7) to the fluxes and source terms of (8)-(10). The continuity equation (8) yields $(\rho u)^+ = (\rho u)^-$. With $m = \rho u$ we receive from momentum and energy equation

$$\left(\frac{m^2}{\rho^+} + p^+\right) - \left(\frac{m^2}{\rho^-} + p^-\right) = -\Delta x \rho g \tag{11}$$

$$\left(E^+ + p^+\right)\frac{m}{\rho^+} - \left(E^- + p^-\right)\frac{m}{\rho^-} = -\Delta x m g\,. \tag{12}$$

We introduce δ_ρ, $\delta_E \in (-1, 1)$ and define

$$\begin{array}{rclcl} \rho^\pm & = & \rho \pm \tilde{\delta}_\rho & = & \rho(1 \pm \delta_\rho) \\ E^\pm & = & E \pm \tilde{\delta}_E & = & E(1 \pm \delta_E)\,. \end{array}$$

Incorporating these definitions and $p^\pm = (\gamma - 1)(E - m^2/2\rho^\pm)$ into equations (11) and (12) gives the fourth order polynoms

$$\frac{m^2(\gamma-3)}{\rho^2}\delta_\rho + \left[\frac{2(\gamma-1)E}{\rho}\delta_E + \Delta x g\right](1 - \delta_\rho^2) = 0$$

$$\frac{2m^2}{\rho^2}(\gamma-1)\delta_\rho + \left[\frac{2\gamma E}{\rho}(\delta_E - \delta_\rho) + (1-\delta_\rho^2)\Delta x g\right](1 - \delta_\rho^2) = 0\,.$$

From these equations the following second-order accurate approximations to δ_ρ and δ_E can be derived:

$$\begin{array}{rcl} \delta_\rho & = & \dfrac{g}{(\gamma-1)(m^2\Gamma/\rho^2 - 2E\gamma/\rho)}\Delta x + O(\Delta x^3) \\ \delta_E & = & \dfrac{-g\rho}{2E(\gamma-1)}\left[1 - \dfrac{m^2(3-\gamma)}{(\gamma-1)(m^2\Gamma - 2E\gamma\rho)}\right]\Delta x + O(\Delta x^3) \end{array}$$

Further explanations for the derivation of the jump magnitudes $\delta\rho$ and δE can be found in [6].

4 Implementation of boundary conditions

Physical boundary conditions for the wave propagation algorithm can easily be handled by utilizing two ghost cells with fictious values [5]. An implementation of the quasi-steady extension has to ensure, that these fictious values are set in respect to the indermediate cell values. Otherwise, unphysical waves would emerge from the boundary.

We introduce jump magnitudes δq_i for the ghost cells as well. After each time step, ghost cell values are first of all created from unmodified internal cell values in the usual way. Values of δq_i for the ghost cells are created under consideration to internal jump quantities. Applying all jump magnitudes yields appropriate Riemann problems at the boundary.

As an example, we consider a boundary at the right side of cell M. In case of the equations (8)-(10), a reflective boundary is implemented by mirroring the internal cells into the ghost cells [11]. For the quasi-steady method we set

$$\begin{array}{lllllllll} \rho^-_{M+1} & = & \rho^+_M & E^-_{M+1} & = & E^+_M & m_{M+1} & = & -m_M \\ \rho^+_{M+1} & = & \rho^-_M & E^+_{M+1} & = & E^-_M & & & \\ \rho^-_{M+2} & = & \rho^+_{M-1} & E^-_{M+2} & = & E^+_{M-1} & m_{M+2} & = & -m_{M-1} \\ \rho^+_{M+2} & = & \rho^-_{M-1} & E^+_{M+2} & = & E^-_{M-1}\,. & & & \end{array} \tag{13}$$

For the jump magnitudes of the ghost cells $M+1$ and $M+2$ we receive

$$\begin{array}{llllll} \delta_{\rho,M+1} & = & -\delta_{\rho,M} & \delta_{E,M+1} & = & -\delta_{E,M} \\ \delta_{\rho,M+2} & = & -\delta_{\rho,M-1} & \delta_{E,M+2} & = & -\delta_{E,M-1}\,. \end{array}$$

At a zero order outflow boundary no change in flux should occur [11]. We achieve Riemann problems with zero flux-difference by setting

$$\begin{array}{lllllllll} \rho^-_{M+1} & = & \rho^+_M & E^-_{M+1} & = & E^+_M & m_{M+1} & = & m_M \\ \rho^+_{M+1} & = & \rho^-_M & E^+_{M+1} & = & E^-_M & & & \\ \rho^-_{M+2} & = & \rho^-_M & E^-_{M+2} & = & E^-_M & m_{M+2} & = & m_M \\ \rho^+_{M+2} & = & \rho^+_M & E^+_{M+2} & = & E^+_M\,. & & & \end{array} \tag{14}$$

The jump magnitudes are

$$\begin{array}{llllll} \delta_{\rho,M+1} & = & -\delta_{\rho,M} & \delta_{E,M+1} & = & -\delta_{E,M} \\ \delta_{\rho,M+2} & = & \delta_{\rho,M} & \delta_{E,M+2} & = & \delta_{E,M}\,. \end{array}$$

In the present case, a practical implementation can employ an auxiliary array, which contains the gravitational constant in each cell. Jump magnitudes according to the boundary conditions can be achieved by using negative gravitational constants for the ghost cells.

5 Three-dimensional Euler equations with gravity

We consider the three-dimensional Euler equations with standard gravitational field acting in z-direction

$$\begin{array}{lllllllll} \rho_t & + & (\rho u)_x & + & (\rho v)_y & + & (\rho w)_z & = & 0 \\ (\rho u)_t & + & (\rho u^2+p)_x & + & (\rho uv)_y & + & (\rho uw)_z & = & 0 \\ (\rho v)_t & + & (\rho uv)_x & + & (\rho v^2+p)_y & + & (\rho vw)_z & = & 0 \\ (\rho w)_t & + & (\rho uw)_x & + & (\rho vw)_y & + & (\rho w^2+p)_z & = & -\rho g \\ E_t & + & [u(E+p)]_x & + & [v(E+p)]_y & + & [w(E+p)]_z & = & -\rho w g \end{array} \tag{15}$$

with the equation of state

$$p = \rho\,(\gamma-1)\left[E - \rho\left(\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]\,.$$

The quasi-stationary algorithm, derived in the previous sections for the one-dimensional Euler equations, can easily be extended to three dimensions. Under influence of the standard gravitational field the basic approach of the quasi-stationary method defined in (4) and (5) carries over directly. According to (4) and (5) the quasi-stationary method for (15) is based on

$$h(q)_z = \psi(q) \tag{16}$$

$$q_t + f(q)_x + g(q)_y + h(q)_z = 0\,. \tag{17}$$

The method derived from (16) and (17) modifies just the Riemann problems in z-direction. The Riemann problems in x- and y-direction remain unaltered. The method can easily be implemented using the three-dimensional wave propagation algorithm, because the algorithm calculates the Riemann problems in each coordinate direction in a seperate pass. By solving "transverse" Riemann problems a multidimensional second order accurate method is achieved [3].

We treat the two gases with different adiabatic coefficients γ using the non-conservative transport equation

$$\left(\frac{1}{\gamma-1}\right)_t + u\left(\frac{1}{\gamma-1}\right)_x + v\left(\frac{1}{\gamma-1}\right)_y + w\left(\frac{1}{\gamma-1}\right)_z = 0\,. \tag{18}$$

For the homogenous Euler equations it is proven, that the use of (18) avoids spurious numerical oscillations at moving contact discontinuities [9]. These oscillations are typical for numerical methods based on Riemann problems, if multiple continuity equations are used [8]. Although these theoretical results have not been extended to Euler equations with gravitational influence yet, we utilize the same, unmodified seperation model for our numerical investigations.

6 Computational results

We consider a two-dimensional example from [1] and expand it cylindrical symmetric to three dimensions. Standard gravitation acts in z-direction. In this example, air with density $1.225kg/m^3$ lies above the lighter gas helium with a density of $0.1694kg/m^3$. The gases are initially at rest and the pressure is $1bar$ everywhere. The domain is $2m$ in x- and y-direction and $3m$ in z-direction. The interface between the gases is initially defined by a cylindrical symmetric sine with wavelength $1m$ and amplitude $5cm$. The sine wave smoothly changes to a straight line normal to z at the outer regions. We choose a reflective boundary at the lower side and a constant inflow equal to the initial values at the upper side. In x- and y-direction outflow is assumed. By exploiting the symmetry of the problem the calculation domain is reduced to a quarter.

Two-dimensional reference calculations exploit the cylindrical symmetry of the problem. In this case the system of equations (15) reduces to

$$\begin{array}{lllllll}
\rho_t & + & (\rho u)_r & + & (\rho w)_z & = & -\frac{\rho u}{r} \\
(\rho u)_t & + & (\rho u^2+p)_r & + & (\rho u w)_z & = & -\frac{\rho u^2}{r} \\
(\rho w)_t & + & (\rho u w)_r & + & (\rho w^2+p)_z & = & -\frac{\rho u w}{r} \quad -\rho g \\
E_t & + & \left[u(E+p)\right]_r & + & \left[w(E+p)\right]_z & = & -\frac{u(E+p)}{r} \quad -\rho w g \\
\multicolumn{7}{l}{p = \rho\,(\gamma-1)\left[E - \rho\left(\frac{u^2}{2}+\frac{w^2}{2}\right)\right]\,.}
\end{array} \tag{19}$$

The γ-equation (18) gives

$$\left(\frac{1}{\gamma-1}\right)_t + u\left(\frac{1}{\gamma-1}\right)_r + w\left(\frac{1}{\gamma-1}\right)_z = 0\,.$$

The additional source term in (19) arising from lowering the dimension is numerically treated by Strang splitting.

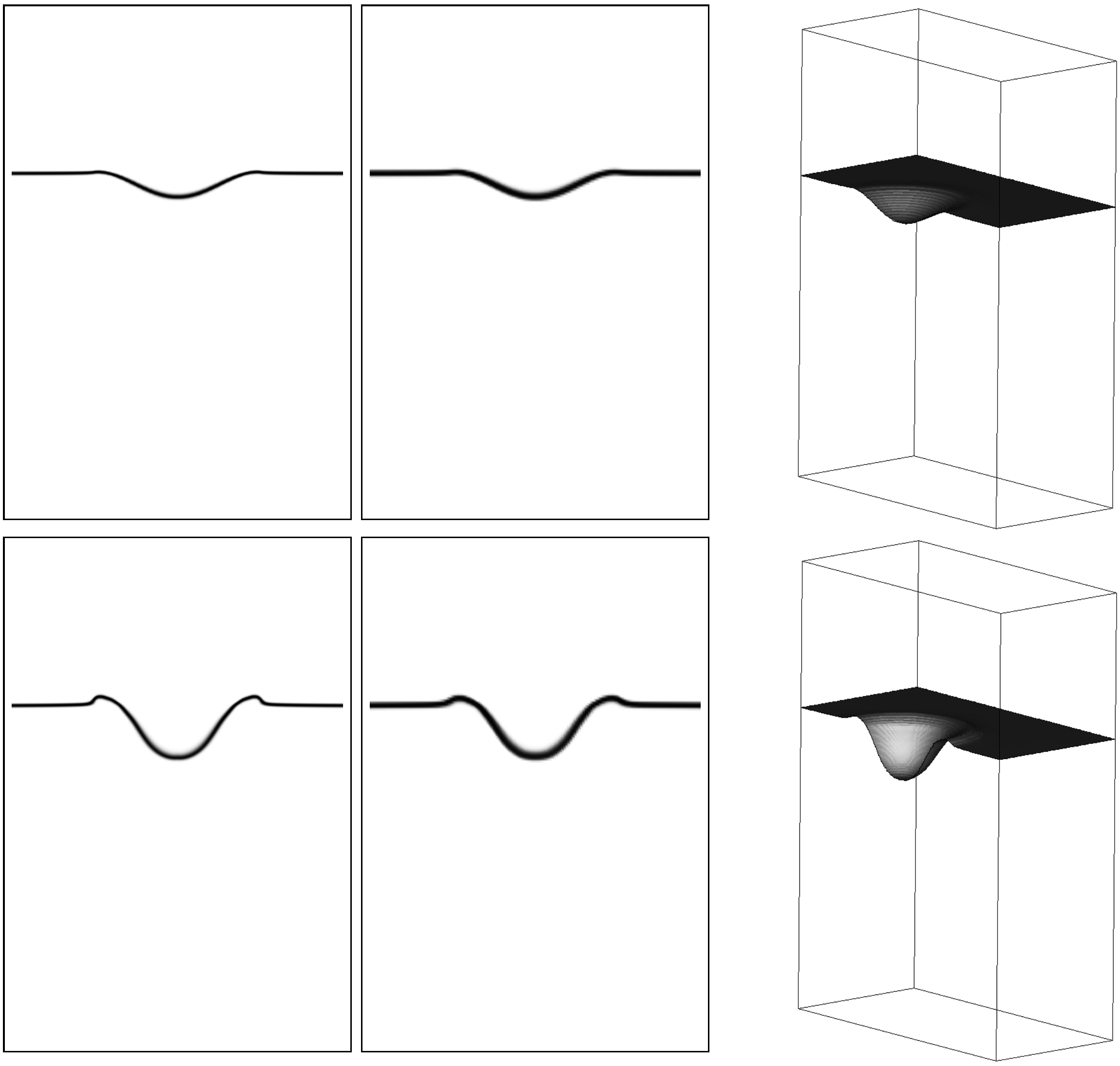

Figure 1: Comparison of 2D (left) and 3D (middle and right) computational results at times $t = 0.0158s$ and $0.0316s$. The accurate 2D computation uses a 240 x 720 grid. The 3D results have been obtained with an adaptive mesh refinement algorithm. The resolution corresponds to a 80 x 80 x 240 grid.

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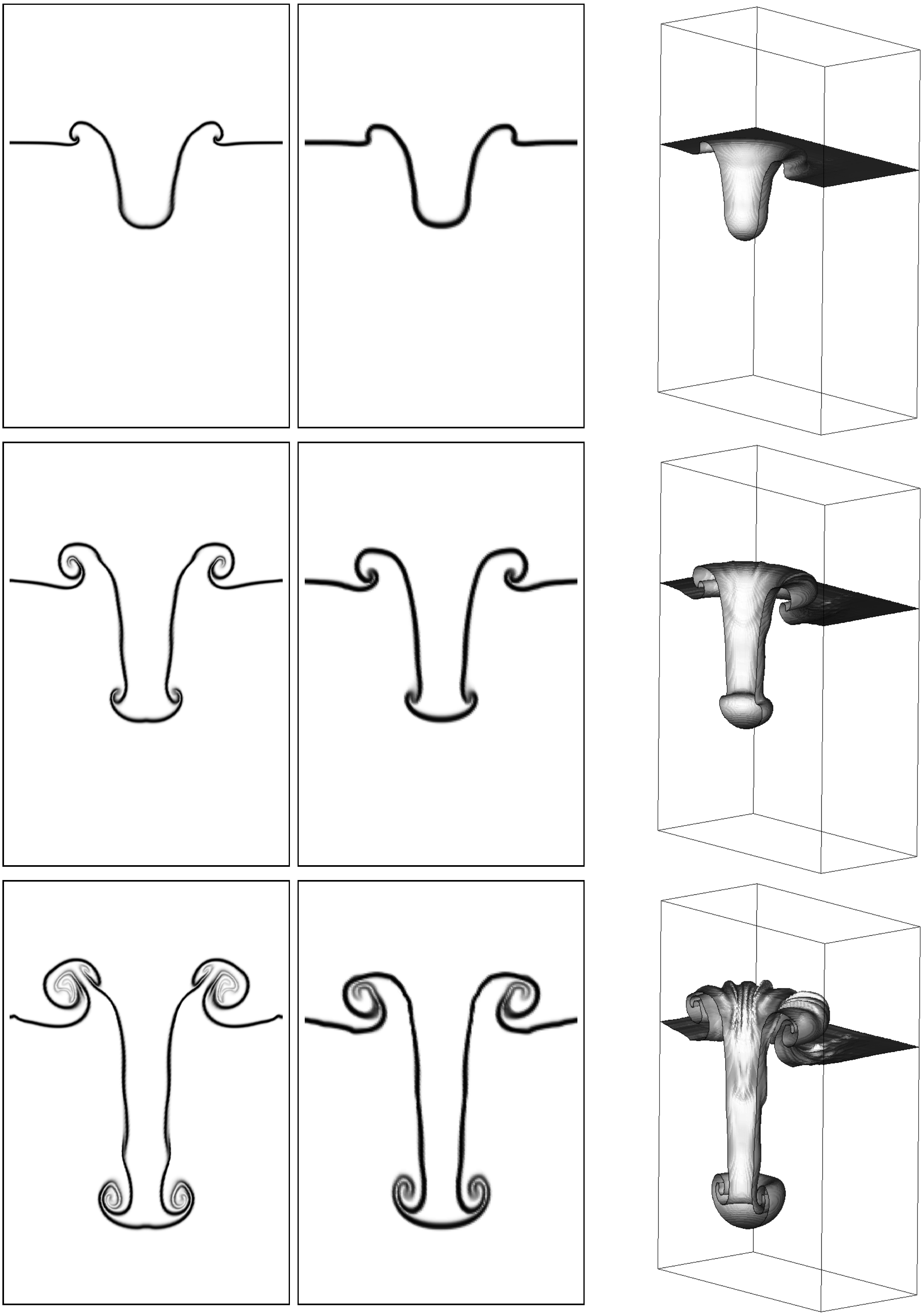

Figure 2: Computational results for the Rayleigh-Taylor-instability at times $t = 0.0474s$, $0.0632s$, $0.0791s$.