Fluid-mixture type models & methods for compressible multicomponent flow

I: Linear equation of state

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Compressible flow model: Single-phase case

Assume continuum mechanics modelling of fluid motion, basic physical principles for pure phase are

1. Mass balance:
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$
2. Momentum balance:
$$\frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) = \nabla \cdot \overline{\overline{T}}$$
3. Energy balance:
$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho E \vec{u}) = \nabla \cdot \left(\overline{\overline{T}} \vec{u} \right) - \nabla \cdot \vec{q}$$
4. Entropy balance:
$$\frac{\partial (\rho s)}{\partial t} + \nabla \cdot (\rho s \vec{u}) = -\nabla \cdot \vec{q}_s + \Delta_s$$

Assume Newtonian fluid & Fourier's, we have

ρ : density, $\vec{u}$: flow velocity

E : specific total energy

$$E = e + \frac{1}{2}\vec{u}\cdot\vec{u}, \quad e : \text{specific internal energy}$$

$\overline{\overline{T}}$: stress tensor

$$\overline{\overline{T}} = -p\overline{\overline{I}} + \tau, \quad p\text{: pressure}, \quad \tau\text{: dissipative stress tensor}$$

$$\tau = \mu\left(\nabla\vec{u} + \nabla^T\vec{u} - \frac{2}{3}\left(\nabla\cdot\vec{u}\right)\overline{\overline{I}}\right), \quad \mu\text{: viscosity}$$

$\vec{q}$: heat flux

$$\vec{q} = -\kappa\nabla T, \quad \kappa\text{: thermal conductivity}, \ T\text{: temperature}$$

s : specific entropy

$\vec{q}_s$: entropy flux, $\vec{q}_s = \dfrac{\vec{q}}{T}$

Δ_s : entropy source, $\Delta_s = \kappa\dfrac{\nabla T\cdot\nabla T}{T^2} + \mu\dfrac{\nabla\vec{u} : \nabla\vec{u}}{T}$

Thermodynamic laws

Second law of thermodynamics:

$$ds = \frac{dQ}{T}, \quad Q\text{: heat transfer}, \quad T\text{: temperature}$$

First law of thermodynamics:

$$dQ = de + pdV, \quad V = 1/\rho\text{: specific volume}$$

This leads to

$$Tds = de + pdV \quad \Longrightarrow \quad de = Tds - pdV$$

yielding definiton of p & T, *i.e.*,

$$p = -\left(\frac{\partial e}{\partial V}\right)_s, \quad T = \left(\frac{\partial e}{\partial s}\right)_V$$

when expression for $e(V, s)$ is known a priori

Equation of state

In compressible fluid flow theory, equation of state such as

$$p = p(\rho, e), \quad p = p(\rho, T), \quad \text{or} \quad p = p(\rho, s)$$

is commonly used to characterize thermodynamic behavior of underlying medium

If equation of state depends on density only, $p = p(\rho)$, it is callled isentropic (or barotropic) equation

Here with fixed entropy s, equation of state is assumed to be monotonically nondecreasing & convex, *i.e.*,

$$\left(\frac{\partial p}{\partial \rho}\right)_s \geq 0, \quad \left(\frac{\partial^2 p}{\partial \rho^2}\right)_s \geq 0$$

Define speed of sound, denoted by $c \in \mathbf{R}$, as

$$c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s \geq 0; \quad c^2 = 0 \quad \text{only if } \rho = 0 \text{ (vacuum)}$$

Equation of state: Ideal gas

Gas medium is assumed to be ideal gas, if it satisfies laws of Boyle & Gay-Lussac as expressed by equation of state

$$pV = RT$$

$R = nR_0$ (n: number of gas moles & R_0: univ. gas constant)

In ideal gas, internal energy e is function of temperature T only, see Courant-Friedrichs p.8-9

If gas is polytropic, we have

$$e(T) = C_V T, \quad C_V\text{: specific heat at constant volume}$$

$$p(\rho, e) = (\gamma - 1)\rho e, \quad \gamma\text{: ratio of specific heats}$$

$$p(\rho, s) = (\gamma - 1)\exp\left(\frac{s - s_0}{C_V}\right)\rho^\gamma$$

$$e(\rho, s) = \exp\left(\frac{s - s_0}{C_V}\right)\rho^{(\gamma-1)}$$

Balance equations: Remark

When balance equations are closed, entropy balance equation & energy balance equation are equivalent

In this case, entropy balance equation can be written as

$$\rho C_p \frac{DT}{Dt} = \nabla \cdot (\kappa \nabla T) + \kappa_T T \frac{Dp}{Dt} + \tau : \nabla \vec{u}$$

where C_p & κ_T denotes specific heat at constant pressure & coefficient of thermal expansion defined by

$$C_p = \frac{T}{(\partial T/\partial s)_p} \quad \& \quad \kappa_T = -\rho \left(\frac{\partial s}{\partial p}\right)_T = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p$$

Recall double dot product of two tensors $\overline{\overline{U}}$ & $\overline{\overline{V}}$ is defined by

$$\overline{\overline{U}} : \overline{\overline{V}} = \sum_i \sum_j U_{ij} V_{ji}$$

D/Dt denotes material derivative

Compressible flow: Model summary

System of balance equations for compressible flow is

1. Mass balance:
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$
2. Momentum balance:
$$\frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla \left(p \overline{\overline{I}} \right) = \nabla \cdot \tau$$
3. Energy balance*:
$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot \left(\rho E \vec{u} + p \overline{\overline{I}} \vec{u} \right) = \nabla \cdot (\tau \vec{u}) + \nabla \cdot (\kappa \nabla T)$$
4. Entropy balance*:
$$\rho C_p \frac{dT}{dt} = \nabla \cdot (\kappa \nabla T) + \kappa_T T \frac{dp}{dt} + \tau : \nabla \vec{u}$$

Take only one equation from $*$ & model closes with EOS

Inviscid compressible flow: Riemann problem

For compressible Euler equations in 1D, Riemann problem is Cauchy problem that consists of

$$\frac{\partial w}{\partial t} + \frac{\partial f(w)}{\partial x} = 0, \quad x \in \mathbf{R}, \quad t > 0$$

with

$$w = \begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix}, \qquad f(w) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho E u + p u \end{bmatrix}$$

as for model equations, & piece-wise constant data

$$w(x, 0) = \begin{cases} w_L & \text{if} \quad x < 0 \\ w_R & \text{if} \quad x > 0 \end{cases}$$

as for initial condition

Riemann problem: Hyperbolicity

To close model & Riemann problem, assume ideal gas law

$$p = (\gamma - 1)\rho e$$

Jacobian matrix of $f(w)$, denoted by A, is

$$A = \frac{\partial f(w)}{\partial w} = \begin{bmatrix} 0 & 1 & 0 \\ (\gamma - 3)u^2/2 & -(\gamma - 1)u & \gamma - 1 \\ (\gamma - 1)u^3/2 - Hu & H - (\gamma - 1)u^2 & \gamma u \end{bmatrix}$$

Its eigen-decomposition $AR = R\Lambda$, is with

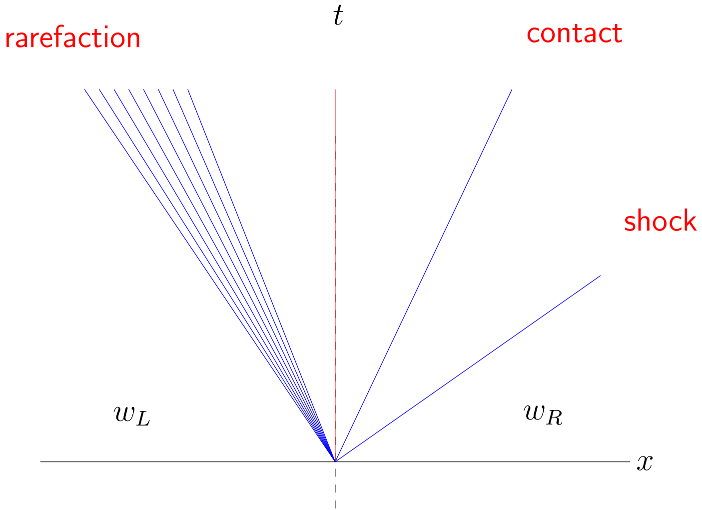
$$\Lambda = \text{diag}(u - c,\ u,\ u + c)$$

$$R = \begin{bmatrix} 1 & 1 & 1 \\ u - c & u & u + c \\ H - uc & \frac{1}{2}u^2 & H + uc \end{bmatrix}$$

$c = \sqrt{\gamma p/\rho} > 0$ is speed of sound & $H = (e + p)/\rho$ is specific enthalpy

Riemann problem: Basic solution structure

Elementary waves of Riemann problem in x-t plane



Riemann problem: Remarks

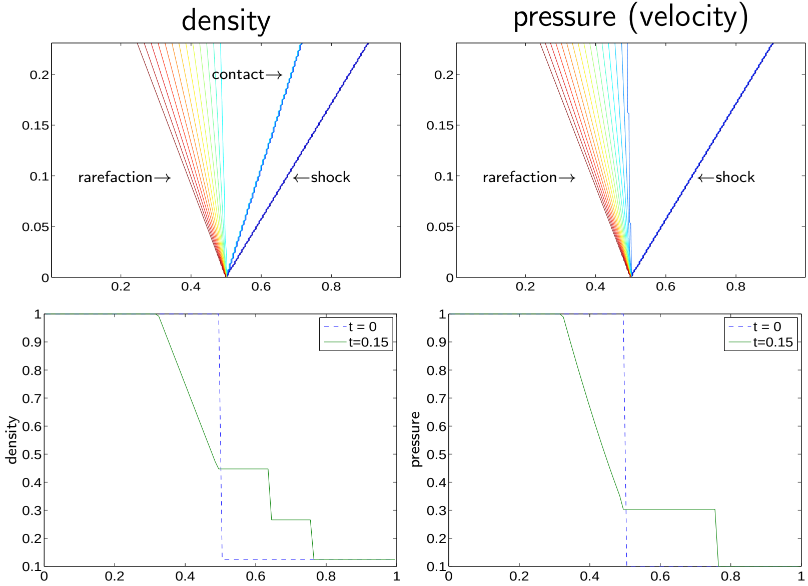
Basic properties of elementary waves are

1. Shock wave
   - Genuinely nonlinear wave
   - Solution is discontinuous across wave that follows Rankine-Hugoniot jump condition

$$\sigma[w] = [f(w)], \quad \sigma\text{: shock speed } \& \ [w] = w_R - w_L$$

2. Contact discontinuity
   - Linearly degenerate wave
   - Solution is in mechanical equilibrium across wave, *i.e.*, $[u] = 0$, $[p] = 0$, while typically $[\rho] \neq 0$, $[T] \neq 0$, $[s] \neq 0$
3. Rarefaction wave
   - Genuinely nonlinear wave
   - Riemann invariant is constant across wave

Sod Riemann problem: Exact solution



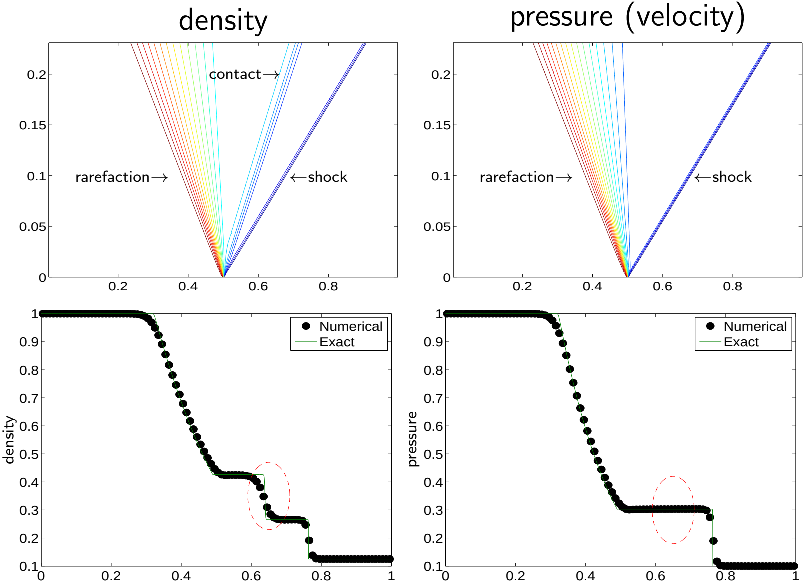
Fluid-mixture type methods

Basic elements:

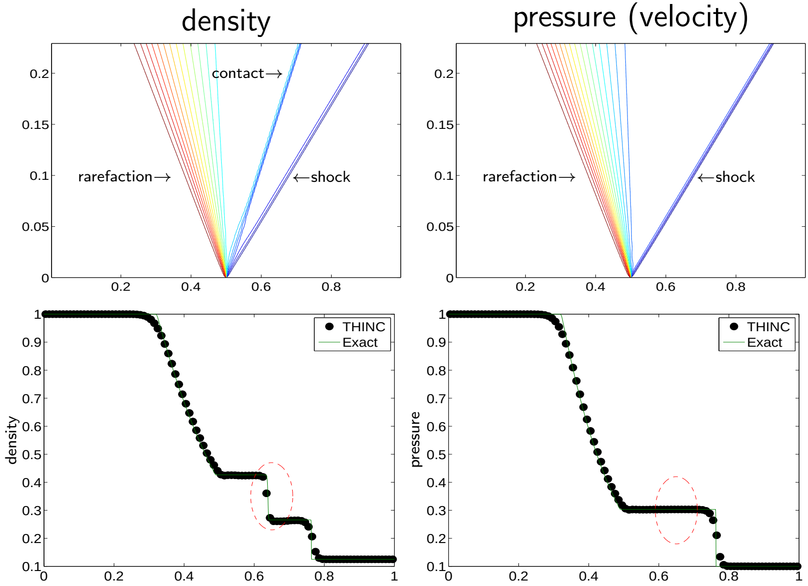
1. Use diffuse interface model of fluid-mixture type
2. Employ state-of-the-art finite-volume method to capture discontinuities (shocks & contacts) implicitly
3. Underlying grid may be either static & uniform or time-dependent & nonuniform

Focus on fluid-mixture model first, numerical discretization of model will be discussed later (when time permits)

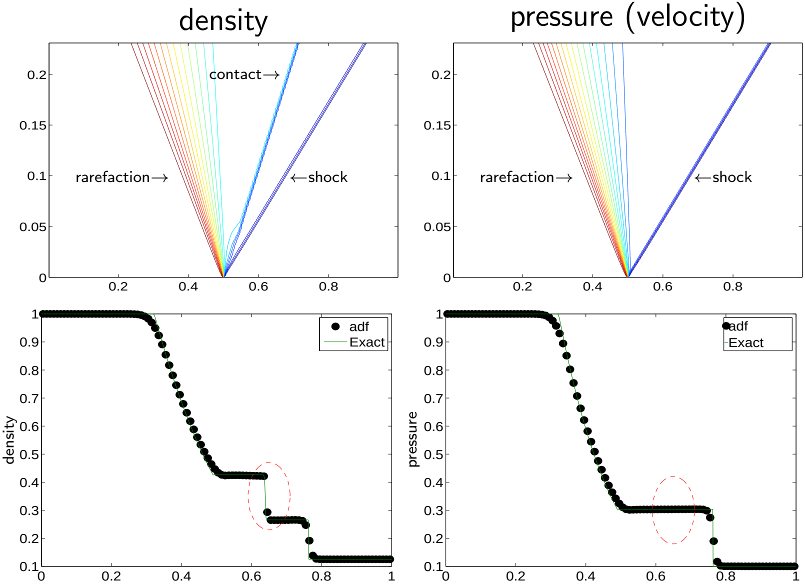
Sod Riemann problem: High-resolution result



Sod Riemann problem: THINC result



Sod Riemann problem: Anti-diffusion result



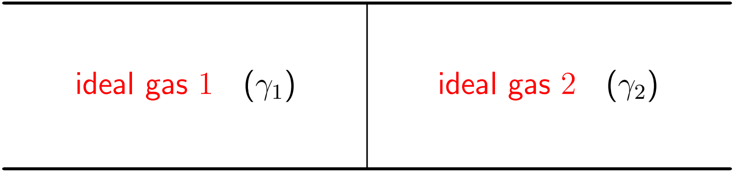
Extension to two-fluid flow: Model problem

Consider shock-tube problem with immiscible membrane separating two different ideal gases, say, air & He

Assume mechanical equilibrium condition for states across interface, *i.e.*,

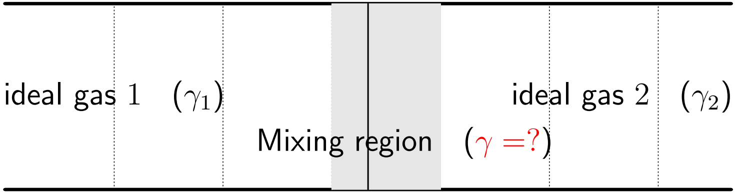
$$\text{kinematic: } [u] = 0 \quad \& \quad \text{dynamic: } [p] = 0$$

Breaking of membrane would result in shock/rarafaction waves separated by moving interface



Fluid-mixture methods: Numerical issues

1. On continuous level:
   - Equations of motions & equation of state for fluid mixtures ?
2. On discrete level:
   - Consistent approximation of model system ?



Benchmark test: 2-fluid interface only

- Initial Condition

$$\begin{pmatrix} \rho \\ u \\ p \\ \gamma \end{pmatrix}_L = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1.4 \end{pmatrix} \qquad \& \qquad \begin{pmatrix} \rho \\ u \\ p \\ \gamma \end{pmatrix}_R = \begin{pmatrix} 0.125 \\ 1 \\ 1 \\ 1.2 \end{pmatrix}$$

- Exact solution

$$\begin{pmatrix} \rho \\ u \\ p \\ \gamma \end{pmatrix}(x,t) = \begin{pmatrix} \rho_0(x-t) \\ 1 \\ 1 \\ \gamma_0(x-t) \end{pmatrix}$$

Model equations ?

1. Basic conservation laws for ρ, ρu, & ρE (fluid mixtures)

2. Pressure computed from

   (a) Equation of state $p = (\gamma - 1)[\rho E - (\rho u)^2/(2\rho)]$ with

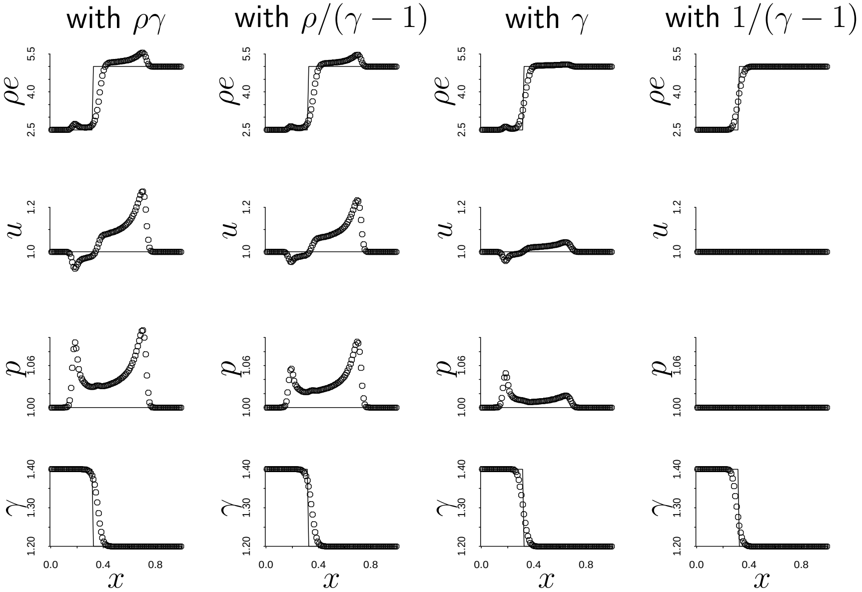
   $$(i) \quad \frac{\partial \gamma}{\partial t} + u \, \frac{\partial \gamma}{\partial x} = 0$$

   $$(ii) \quad \frac{\partial}{\partial t}\left(\frac{1}{\gamma - 1}\right) + u \, \frac{\partial}{\partial x}\left(\frac{1}{\gamma - 1}\right) = 0 \quad \text{(or others)}$$

   (b) Pressure evolution equation directly (Karni 1996)

   $$\frac{\partial p}{\partial t} + u \, \frac{\partial p}{\partial x} + \gamma p \frac{\partial u}{\partial x} = 0$$

Interface only problem: fluid-mixture results



Fluid-mixture model: Ideal gas

Abgrall (1996): Single-density version in multi-D

1. Model (quasi-conservative) system

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \\
&\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} + p \overline{\overline{I}}\right) = 0 \\
&\frac{\partial}{\partial t}(\rho E) + \nabla \cdot \left(\rho E \vec{u} + p \overline{\overline{I}} \vec{u}\right) = 0 \\
&\frac{\partial}{\partial t}\left(\frac{1}{\gamma - 1}\right) + \vec{u} \cdot \nabla \left(\frac{1}{\gamma - 1}\right) = 0
\end{aligned}$$

2. Equation of state

$$p(\rho, e, \gamma) = (\gamma - 1)\rho e$$

Transport equation for $1/(\gamma - 1)$ plays role near interfaces only

Fluid-mixture model: Mapped grid version

1. Model system

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{1}{J}\nabla_\xi \cdot \left(\rho \vec{U}\right) = 0 \\
&\frac{\partial}{\partial t}\left(\rho \vec{u}\right) + \frac{1}{J}\nabla_\xi \cdot \left(\rho \vec{u} \otimes \vec{U} + p\overline{\overline{IJ}}\right) = 0 \\
&\frac{\partial}{\partial t}(\rho E) + \frac{1}{J}\nabla_\xi \cdot \left(\rho E \vec{U} + p\overline{\overline{I}}\vec{U}\right) = 0 \\
&\frac{\partial}{\partial t}\left(\frac{1}{\gamma - 1}\right) + \frac{1}{J}\vec{U} \cdot \nabla_\xi \left(\frac{1}{\gamma - 1}\right) = 0
\end{aligned}
$$

2. Equation of state

$$
p(\rho, e, \gamma) = (\gamma - 1)\,\rho e
$$

$U_j = \sum_{i=1}^{N} u_i \partial_{x_i} \xi_j$: contravariant velocity in ξ_j-direction

Mapped grid model: Grid metrics

Basic coordinate mapping relations in $N = 3$ are

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \partial_{x_1}\xi_1 & \partial_{x_2}\xi_1 & \partial_{x_3}\xi_1 \\ 0 & \partial_{x_1}\xi_2 & \partial_{x_2}\xi_2 & \partial_{x_3}\xi_2 \\ 0 & \partial_{x_1}\xi_3 & \partial_{x_2}\xi_3 & \partial_{x_3}\xi_3 \end{pmatrix} = \frac{1}{J}\begin{pmatrix} J & 0 & 0 & 0 \\ 0 & J_{11} & J_{21} & J_{31} \\ 0 & J_{12} & J_{22} & J_{32} \\ 0 & J_{13} & J_{23} & J_{33} \end{pmatrix}$$

where $J = |\partial(x_1, x_2, x_3)/\partial(\xi_1, \xi_2, \xi_3)| =$ det $(\partial(x_1, x_2, x_3)/\partial(\xi_1, \xi_2, \xi_3))$,

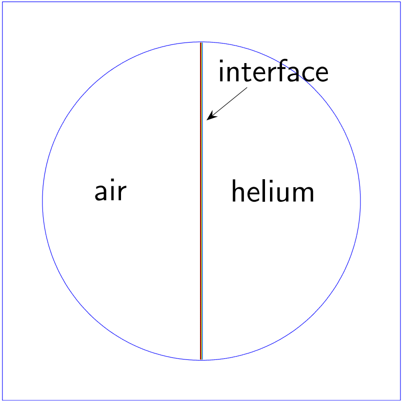
$$J_{11} = \left|\frac{\partial(x_2, x_3)}{\partial(\xi_2, \xi_3)}\right|, \quad J_{21} = \left|\frac{\partial(x_1, x_3)}{\partial(\xi_3, \xi_2)}\right|, \quad J_{31} = \left|\frac{\partial(x_1, x_2)}{\partial(\xi_2, \xi_3)}\right|,$$

$$J_{12} = \left|\frac{\partial(x_2, x_3)}{\partial(\xi_3, \xi_1)}\right|, \quad J_{22} = \left|\frac{\partial(x_1, x_3)}{\partial(\xi_1, \xi_3)}\right|, \quad J_{32} = \left|\frac{\partial(x_1, x_2)}{\partial(\xi_3, \xi_1)}\right|,$$

$$J_{13} = \left|\frac{\partial(x_2, x_3)}{\partial(\xi_1, \xi_2)}\right|, \quad J_{23} = \left|\frac{\partial(x_1, x_3)}{\partial(\xi_2, \xi_1)}\right|, \quad J_{33} = \left|\frac{\partial(x_1, x_2)}{\partial(\xi_1, \xi_2)}\right|.$$

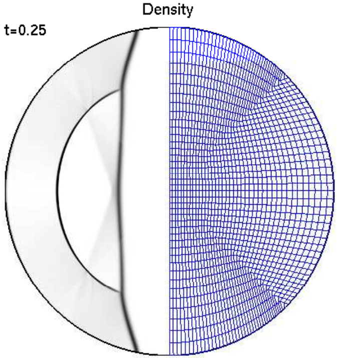
Moving cylindrical vessel

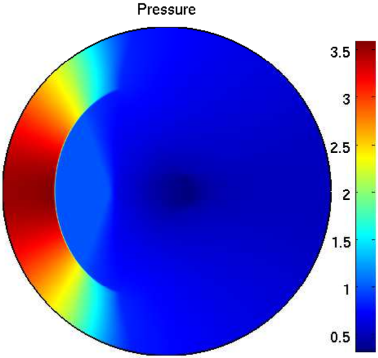
Impose uniform flow velocity $(u_1, u_2) = (-1, 0)$ (*i.e.*, in the frame of vessel moving with speed one in x_1-direction)



Moving cylindrical vessel

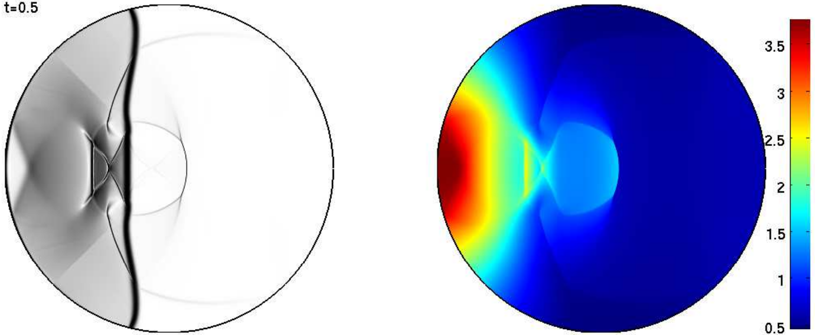
- Solution at time $t = 0.25$





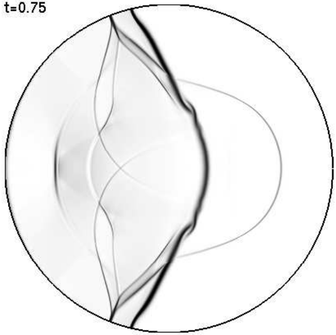
Moving cylindrical vessel

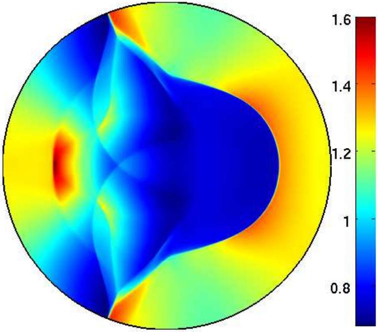
- Solution at time $t = 0.5$



Moving cylindrical vessel

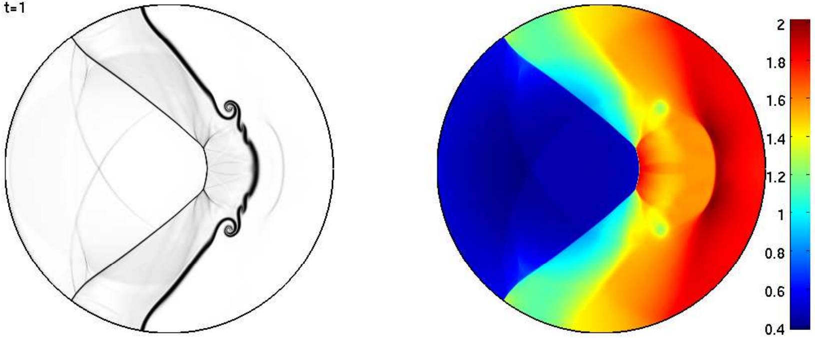
- Solution at time $t = 0.75$





Moving cylindrical vessel

- Solution at time $t = 1$



Extension to stiffened gas

One simple equation of state that models materials not only gases, but also compressible liquids & solids is stiffened gas

$$p(\rho, e) = (\gamma - 1)\,\rho e + (\rho - \rho_0)\,\mathcal{B}$$

In this case, with basic conservation laws, diffuse interface model includes additional transport equations as

$$\begin{aligned}
\frac{\partial}{\partial t}\left(\frac{1}{\gamma - 1}\right) + \vec{u} \cdot \nabla \left(\frac{1}{\gamma - 1}\right) &= 0 \\
\frac{\partial}{\partial t}\left(\frac{\rho_0 \mathcal{B}}{\gamma - 1}\right) + \vec{u} \cdot \nabla \left(\frac{\rho_0 \mathcal{B}}{\gamma - 1}\right) &= 0 \\
\frac{\partial}{\partial t}\left(\frac{\rho \mathcal{B}}{\gamma - 1}\right) + \nabla \cdot \left(\frac{\rho \mathcal{B}}{\gamma - 1}\vec{u}\right) &= 0
\end{aligned}$$

Transport equations for interfaces

Assume equilibrium pressure p & velocity $\vec{u}$, motion of interface (contact discontinuity) is governed by

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho &= 0 \\ \vec{u} \left(\frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho \right) &= 0 \\ \frac{\vec{u} \cdot \vec{u}}{2} \left(\frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho \right) + \left[\frac{\partial}{\partial t} (\rho e) + \vec{u} \cdot \nabla (\rho e) \right] &= 0 \end{aligned}$$

This is,

$$\frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho = 0$$

$$\frac{\partial}{\partial t} (\rho e) + \vec{u} \cdot \nabla (\rho e) = 0$$

Effective transport equations: Stiffened gas

With stiffened gas EOS, tranport equation for ρe of interface

$$\frac{\partial}{\partial t}(\rho e) + \vec{u} \cdot \nabla (\rho e) = 0$$

takes form

$$\frac{\partial}{\partial t}\left(\frac{p}{\gamma - 1} - \frac{\rho - \rho_0}{\gamma - 1}\mathcal{B}\right) + \vec{u} \cdot \nabla \left(\frac{p}{\gamma - 1} - \frac{\rho - \rho_0}{\gamma - 1}\mathcal{B}\right) = 0$$

To ensure pressure in equilibrium, split equation into two parts

$$\frac{\partial}{\partial t}\left(\frac{p}{\gamma - 1}\right) + \vec{u} \cdot \nabla \left(\frac{p}{\gamma - 1}\right) = 0$$

$$\frac{\partial}{\partial t}\left(\frac{\rho - \rho_0}{\gamma - 1}\mathcal{B}\right) + \vec{u} \cdot \nabla \left(\frac{\rho - \rho_0}{\gamma - 1}\mathcal{B}\right) = 0$$

That is, to retain pressure equilibrium across interface, we must have

$$\frac{\partial}{\partial t}\left(\frac{1}{\gamma-1}\right)+\vec{u}\cdot\nabla\left(\frac{1}{\gamma-1}\right)=0$$
$$\frac{\partial}{\partial t}\left(\frac{\rho-\rho_0}{\gamma-1}\mathcal{B}\right)+\vec{u}\cdot\nabla\left(\frac{\rho-\rho_0}{\gamma-1}\mathcal{B}\right)=0$$

However, to ensure conservation of mass in region away from interface, latter equation needs to split further & rewrite as

$$\frac{\partial}{\partial t}\left(\frac{\rho_0\mathcal{B}}{\gamma-1}\right)+\vec{u}\cdot\nabla\left(\frac{\rho_0\mathcal{B}}{\gamma-1}\right)=0$$
$$\frac{\partial}{\partial t}\left(\frac{\rho\mathcal{B}}{\gamma-1}\right)+\nabla\cdot\left(\frac{\rho\mathcal{B}}{\gamma-1}\vec{u}\right)=0$$

Note that from

$$\frac{\partial}{\partial t}\left(\frac{\rho\mathcal{B}}{\gamma-1}\right)+\vec{u}\cdot\nabla\left(\frac{\rho\mathcal{B}}{\gamma-1}\right)=0$$

& by employing chain rule with respect to ρ, we have

$$\begin{aligned}
\frac{\partial}{\partial t}\left(\frac{\rho\mathcal{B}}{\gamma-1}\right)+\vec{u}\cdot\nabla\left(\frac{\rho\mathcal{B}}{\gamma-1}\right) &= \frac{\mathcal{B}}{\gamma-1}\frac{\partial\rho}{\partial t}+\frac{\mathcal{B}}{\gamma-1}\vec{u}\cdot\nabla\rho \\
&= \frac{\mathcal{B}}{\gamma-1}\left(\frac{\partial\rho}{\partial t}+\vec{u}\cdot\nabla\rho\right) \\
&= \frac{\mathcal{B}}{\gamma-1}\left(\frac{\partial\rho}{\partial t}+\vec{u}\cdot\nabla\rho\right) \\
&= -\frac{\rho\mathcal{B}}{\gamma-1}\nabla\vec{u}
\end{aligned}$$

yielding

$$\frac{\partial}{\partial t}\left(\frac{\rho\mathcal{B}}{\gamma-1}\right)+\nabla\cdot\left(\frac{\rho\mathcal{B}}{\gamma-1}\vec{u}\right)=0$$

Fluid-mixture model: Stiffened gas

Saurel, Abgrall (SISC 1999), Shyue (JCP 1998, 1999)

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \\
&\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} + p \overline{\overline{I}}\right) = 0 \\
&\frac{\partial}{\partial t}(\rho E) + \nabla \cdot \left(\rho E \vec{u} + p \overline{\overline{I}} \vec{u}\right) = 0 \\
&\frac{\partial}{\partial t}\left(\frac{1}{\gamma - 1}\right) + \vec{u} \cdot \nabla \left(\frac{1}{\gamma - 1}\right) = 0 \\
&\frac{\partial}{\partial t}\left(\frac{\rho_0 \mathcal{B}}{\gamma - 1}\right) + \vec{u} \cdot \nabla \left(\frac{\rho_0 \mathcal{B}}{\gamma - 1}\right) = 0 \\
&\frac{\partial}{\partial t}\left(\frac{\rho \mathcal{B}}{\gamma - 1}\right) + \nabla \cdot \left(\frac{\rho \mathcal{B}}{\gamma - 1} \vec{u}\right) = 0 \\
&p(\rho, e, \gamma, \mathcal{B}) = (\gamma - 1)\, \rho e + (\rho - \rho_0)\, \mathcal{B}
\end{aligned}
$$

Fluid-mixture model: Volume-fraction version I

Suppose there exists $M_f \geq 1$ different immiscible phases initially where each of them occupies distinct portion with volume fraction $\alpha_k \in [0, 1]$, $k = 1, 2, \ldots, M_f$, $\sum_{k=1}^{M_f} \alpha_k = 1$

Define mixture states for ρ & ρe as

$$\rho = \sum_{k=1}^{M_f} \alpha_k \rho_k, \qquad \rho e = \sum_{k=1}^{M_f} \alpha_k \rho_k e_k$$

Suppose pressure p is in equilibrium & constitutive law for each fluid phase is characterized by stiffened gas, we then have

$$\rho e = \sum_{k=1}^{M_f} \alpha_k \left(\frac{p}{\gamma_k - 1} - \frac{\rho_k - \rho_{0,k}}{\gamma_k - 1} \mathcal{B}_k \right) = \frac{p}{\gamma - 1} - \frac{\rho - \rho_0}{\gamma - 1} \mathcal{B}$$

It follows

$$\frac{1}{\gamma - 1} = \sum_{k=1}^{M_f} \alpha_k \left(\frac{1}{\gamma_k - 1} \right)$$

$$\frac{\rho_0 \mathcal{B}}{\gamma - 1} = \sum_{k=1}^{M_f} \alpha_k \left(\frac{\rho_{0,k} \mathcal{B}_k}{\gamma_k - 1} \right)$$

$$\frac{\rho \mathcal{B}}{\gamma - 1} = \sum_{k=1}^{M_f} \alpha_k \left(\frac{\rho_k \mathcal{B}_k}{\gamma_k - 1} \right)$$

Note that rather than using $1/(\gamma - 1)$ & $\rho_0 \mathcal{B}/(\gamma - 1)$ as state variables in our model system, instead we may use α_k as

$$\frac{\partial \alpha_k}{\partial t} + \vec{u} \cdot \nabla \alpha_k = 0, \quad k = 1, 2, \ldots, M_f$$

This leads to volume-fraction based model of form

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \\
&\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} + p\overline{\overline{I}} \right) = 0 \\
&\frac{\partial}{\partial t}(\rho E) + \nabla \cdot \left(\rho E \vec{u} + p\overline{\overline{I}}\vec{u} \right) = 0 \\
&\frac{\partial}{\partial t}\left(\frac{\rho \mathcal{B}}{\gamma - 1} \right) + \nabla \cdot \left(\frac{\rho \mathcal{B}}{\gamma - 1} \vec{u} \right) = 0 \\
&\frac{\partial \alpha_k}{\partial t} + \vec{u} \cdot \nabla \alpha_k = 0, \quad k = 1, 2, \ldots, M_f
\end{aligned}$$

If partial density $\alpha_k \rho_k$ is used as state variables, rather than mixture density ρ, this leads to so called 5-equation transport model (Allaire *et al.* , JCP 2002), if $M_f = 2$, that is,

Fluid-mixture model: Volume-fraction version II

$$
\begin{aligned}
&\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \vec{u}) = 0, \quad k = 1, 2, \ldots, M_f \\
&\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} + p \overline{\overline{I}} \right) = 0 \\
&\frac{\partial}{\partial t}(\rho E) + \nabla \cdot \left(\rho E \vec{u} + p \overline{\overline{I}} \vec{u} \right) = 0 \\
&\frac{\partial \alpha_k}{\partial t} + \vec{u} \cdot \nabla \alpha_k = 0, \quad k = 1, 2, \ldots, M_f
\end{aligned}
$$

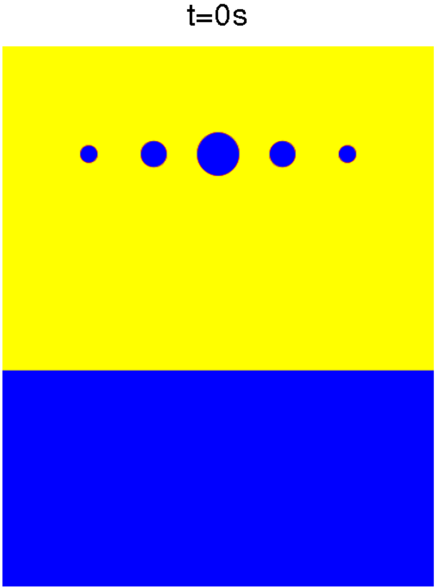
This gives $2M_f + 2$ equations in total for M_f-fluid problem

Pressure is computed directly by solving

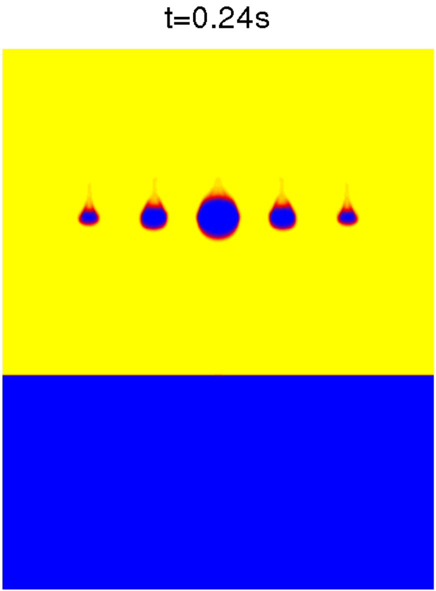
$$
\rho e = \sum_{k=1}^{M_f} \alpha_k \rho_k e_k(\rho_k, p)
$$

which is easy to do if EOS can be written in Mie-Grüneisen form (see next lecture)

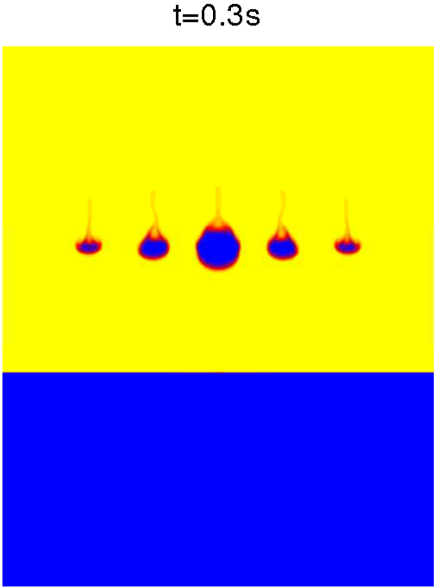
Liquid-falling problem



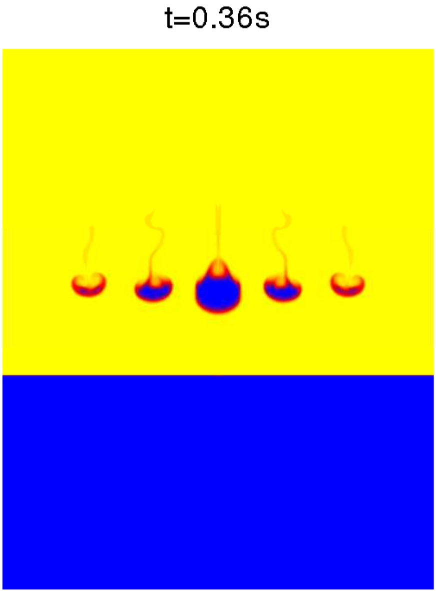
Liquid-falling problem



Liquid-falling problem

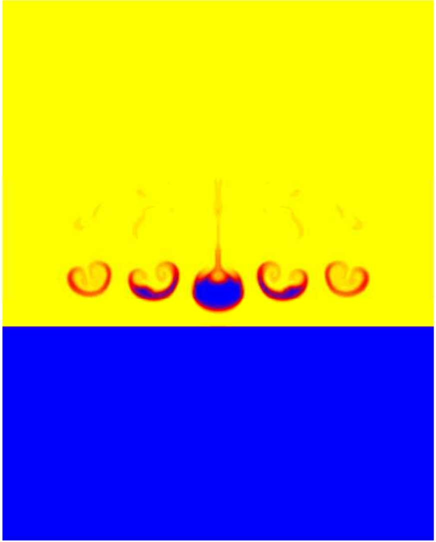


Liquid-falling problem

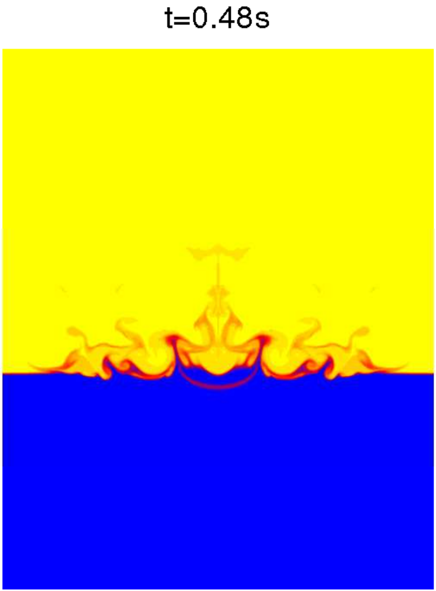


Liquid-falling problem

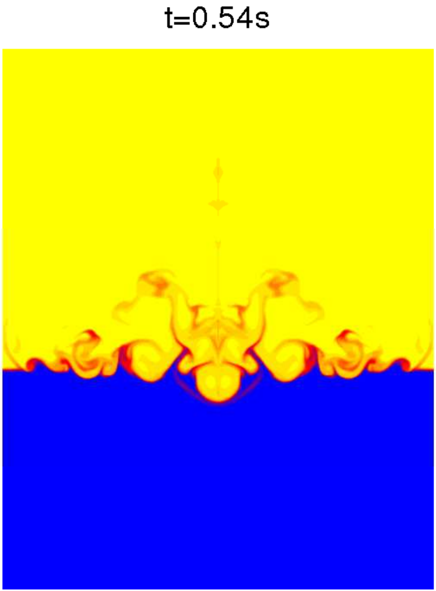
t=0.42s



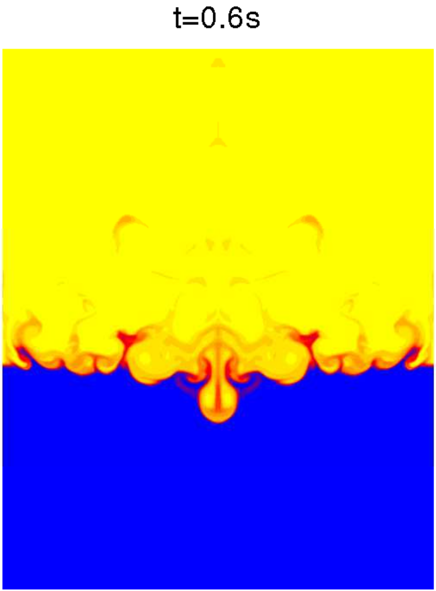
Liquid-falling problem



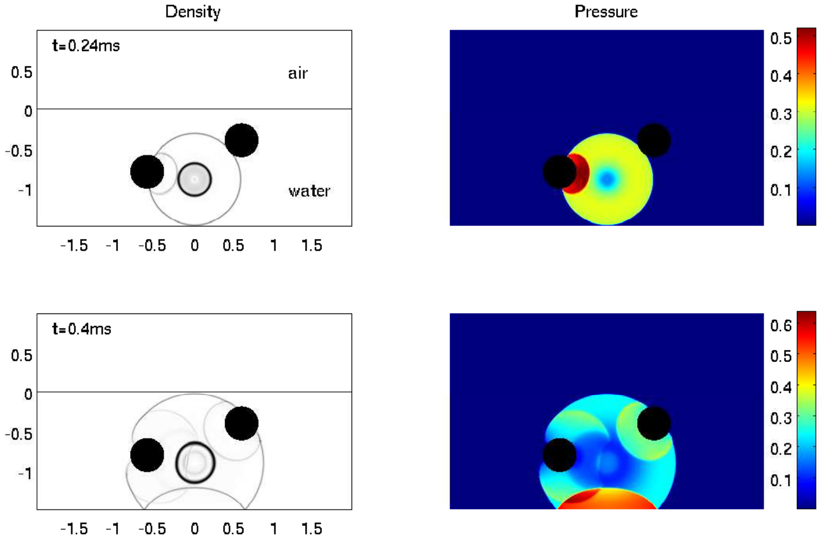
Liquid-falling problem



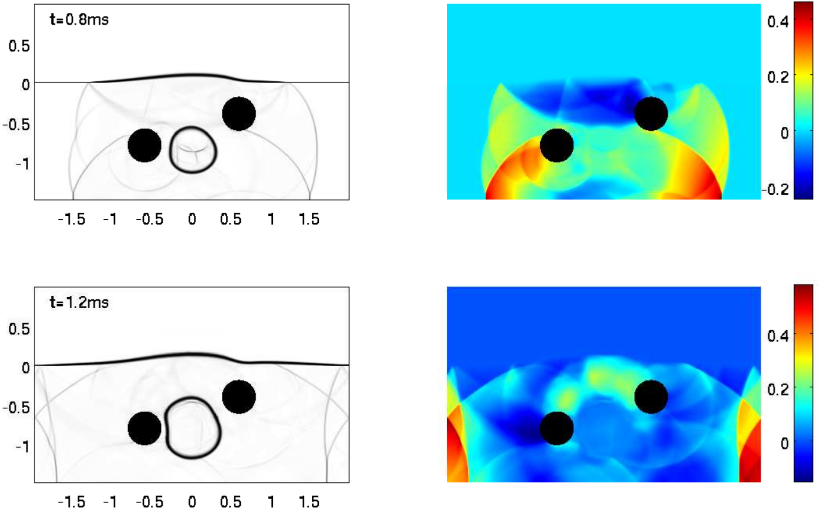
Liquid-falling problem



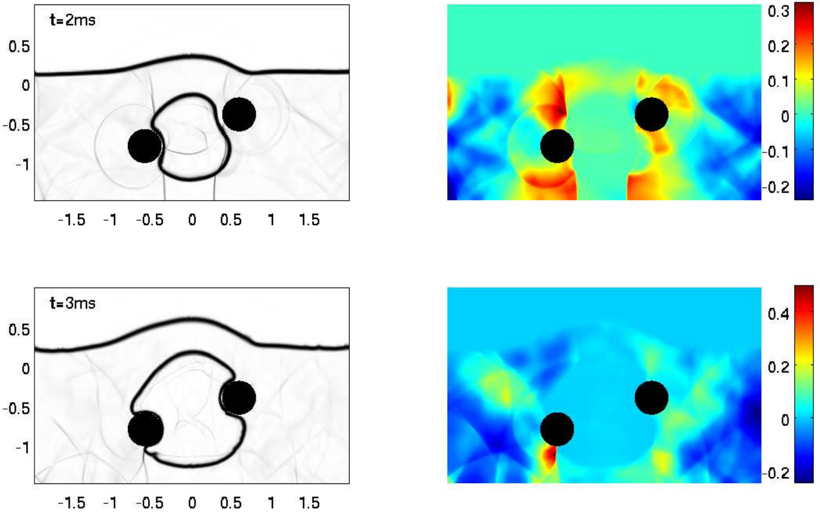
Underwater explosion with two circular obstacles



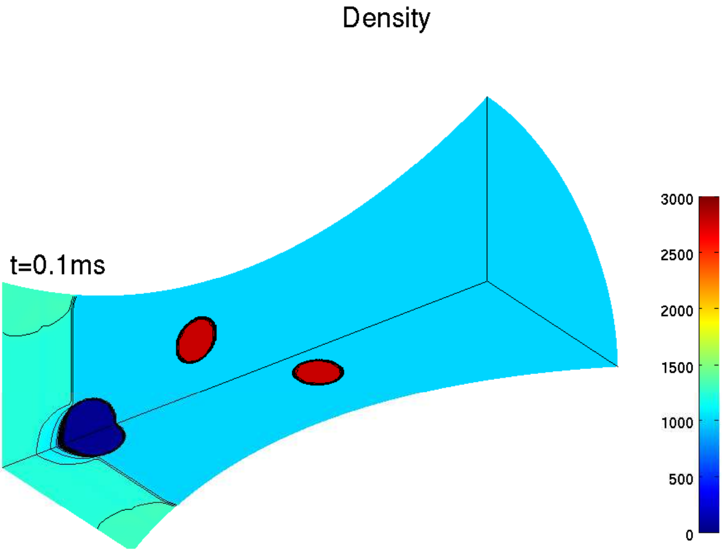
Underwater explosion with two circular obstacles



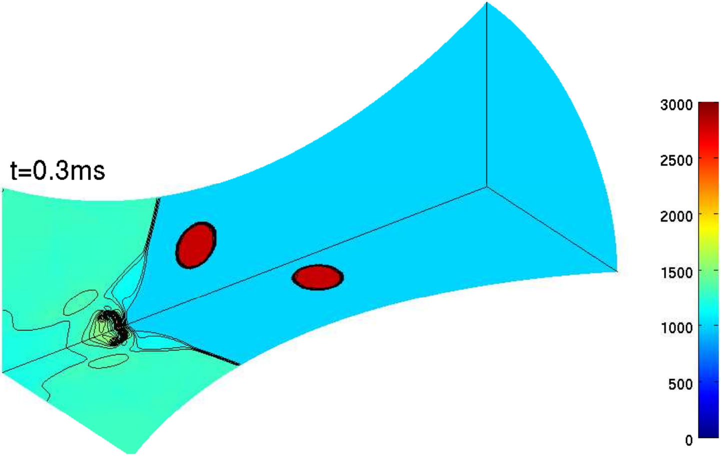
Underwater explosion with two circular obstacles



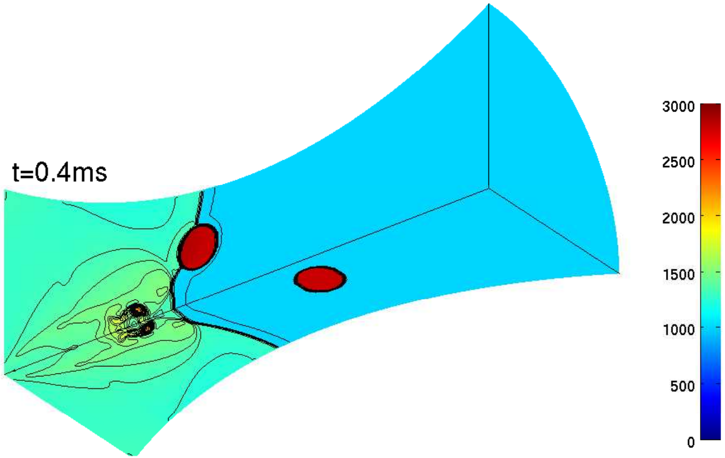
Shock in water over dispersed gas/solid in cylindrical nozzle



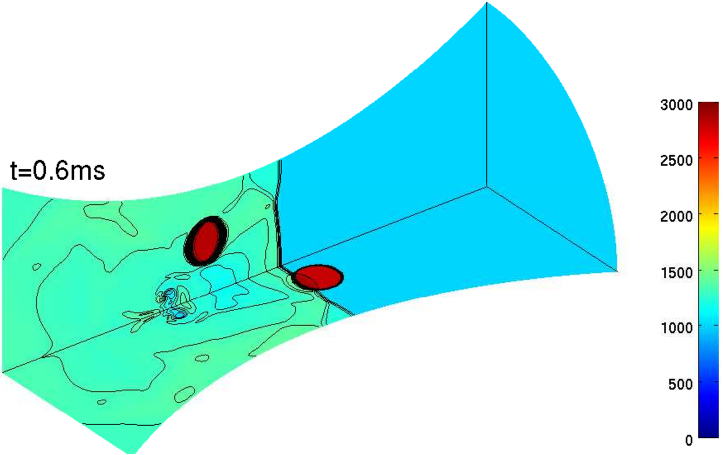
Shock in water over dispersed gas/solid in cylindrical nozzle



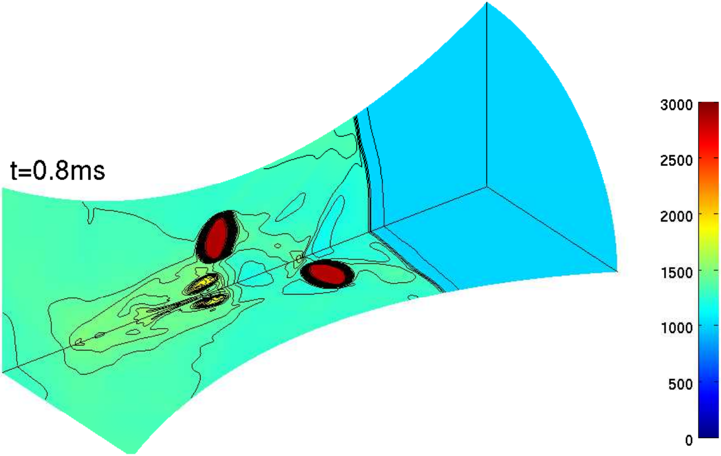
Shock in water over dispersed gas/solid in cylindrical nozzle



Shock in water over dispersed gas/solid in cylindrical nozzle



Shock in water over dispersed gas/solid in cylindrical nozzle



Shock in water over dispersed gas/solid in cylindrical nozzle