Numerical methods for weakly compressible two-phase flow

Recent advances

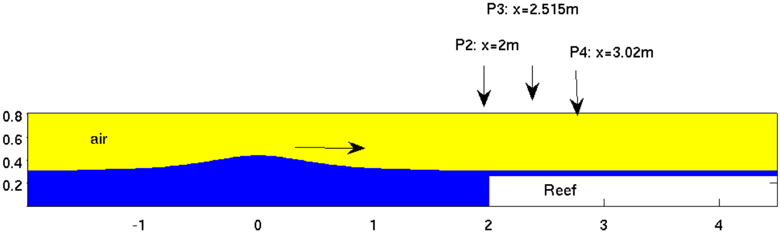
Keh-Ming Shyue

Institute of Applied Mathematical Sciences
National Taiwan University

Scientific example 1: Wave-breaking problem

Problem setup

- Rightward-going solitary water wave travels towards a step-like reef on right



Wave-breaking problem: Schlieren-type image

$t = 1.20$s

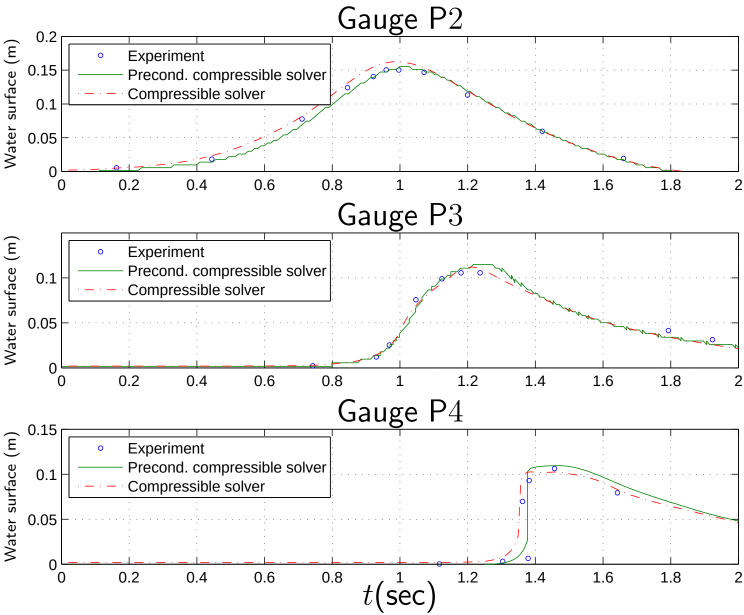
1.35s

Wave-breaking problem: Schlieren-type image

$t = 1.60\text{s}$

$t = 1.80\text{s}$

Wave-breaking problem: Gauge diagnosis



Wave-breaking problem: CPU time Diagnosis

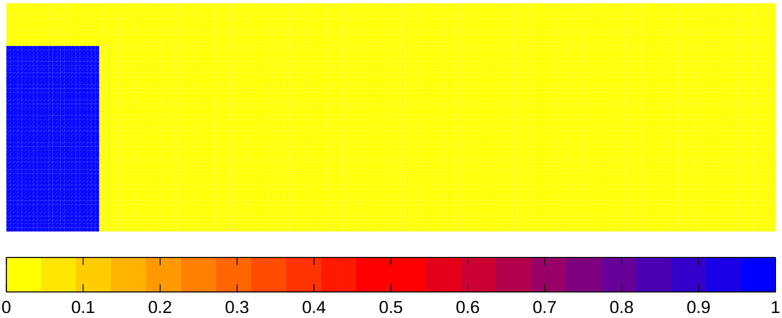
Method	Mesh	CPU time	CPU type
Compressible 1	400×50	6756	AMD
	800×100	55253	Opteron 2220
	1600×200	476429	2.8GHz
Compressible 2	1500×200	172800	Alpha 666 MHz
Pre compressible	1500×200	146400	Intel Xeon 3.0GHz
Incompressible	1200×200	273600	Itanium 1.4GHz

Scientific example 2: Water column collapse

Problem setup

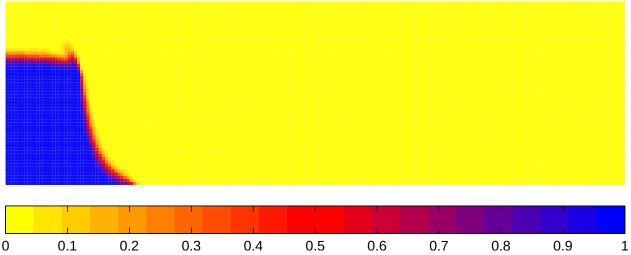
- Water column dimension: $a \times 2a$ ($a = 0.06$m)
- Gravity is directed downward

Results shown below are run with 200×60 grid

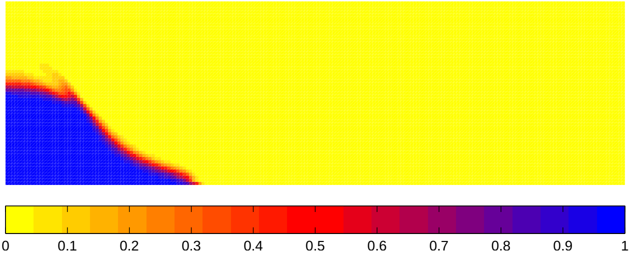


Water column collapse: Pseudo-color plot

$t = 0.066$s

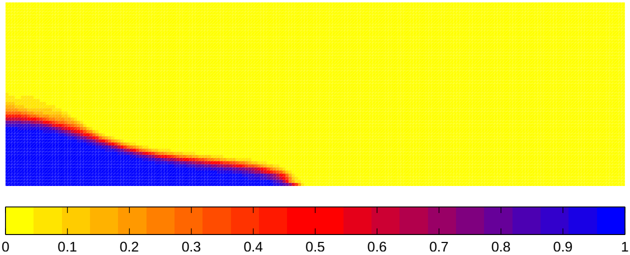


$t = 0.109$s

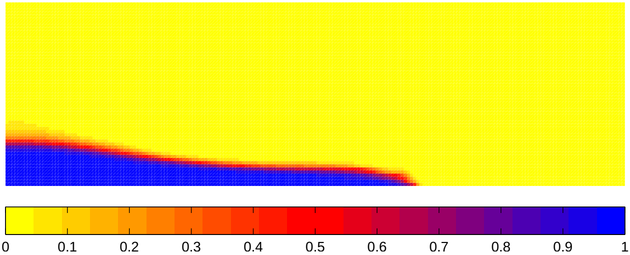


Water column collapse: Pseudo-color plot

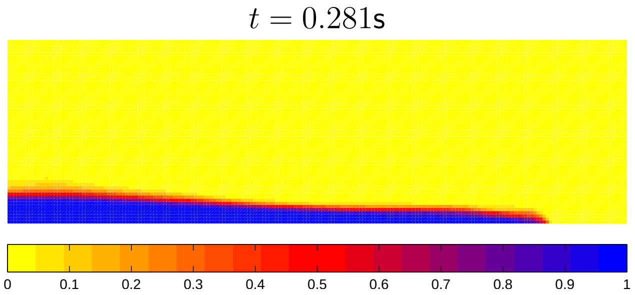
$t = 0.164\text{s}$

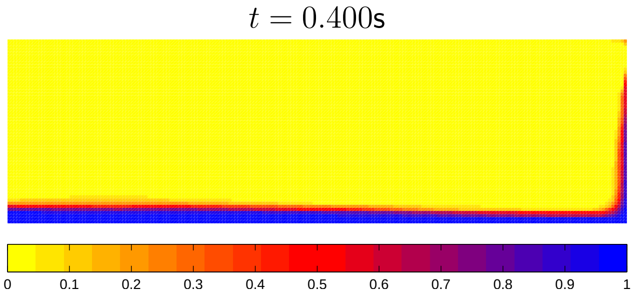


$t = 0.222\text{s}$

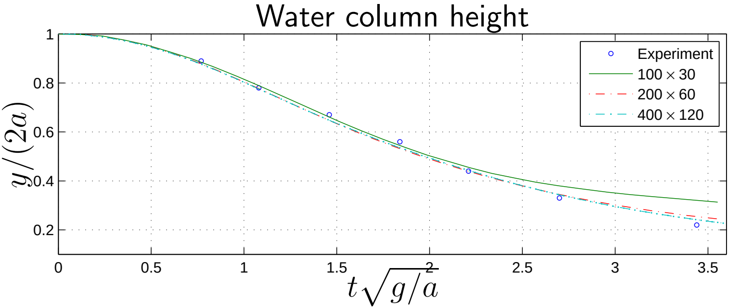


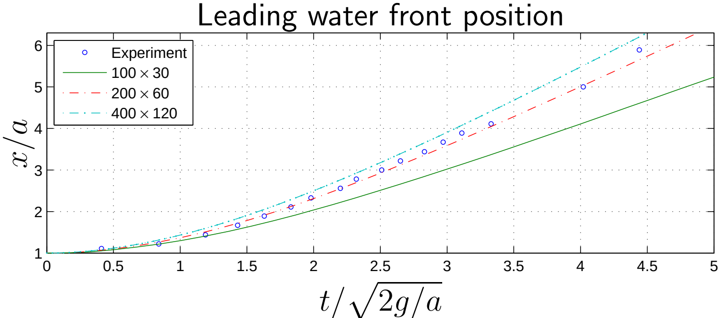
Water column collapse: Pseudo-color plot



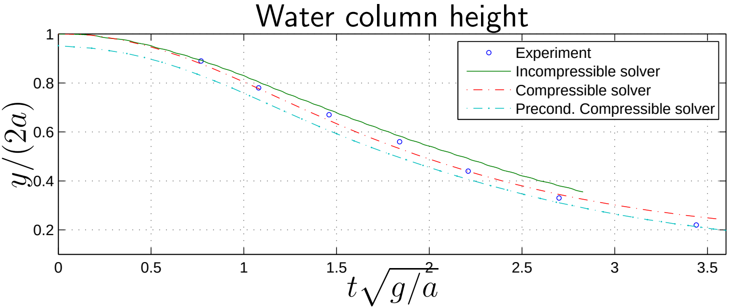


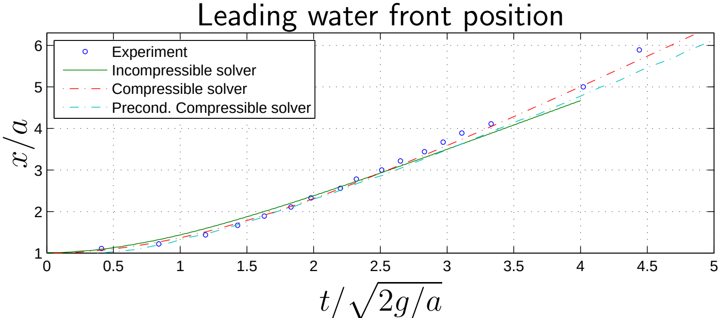
Column collapse: Wave front diagnosis (Meshes)





Column collapse: Wave front diagnosis (Methods)



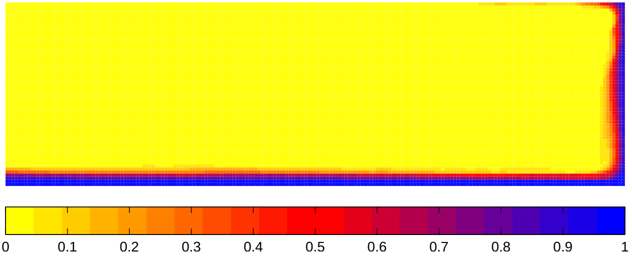


Column collapse: CPU timing diagnosis

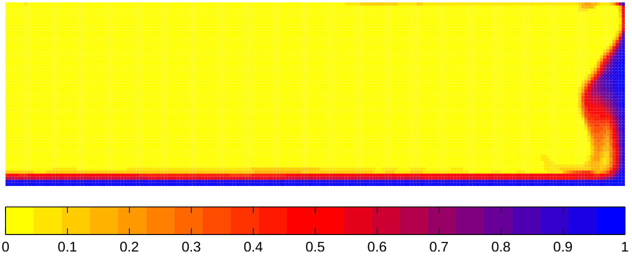
Method	Mesh	CPU time	CPU type
Compressible solver	100×30	492	AMD
	200×60	3782	Opteron 2220
	400×120	31783	2.8GHz
Precond. compressible	100×30	352	Intel Core 2
	200×60	2453	Duo 3.0GHz
	400×120	21780	
Incompressible solver	200×60	9804	Intel Pentium 4 3.4GHz
Mach-uniform solver	200×60	129	Intel Core i7 2.2GHz

Water column collapse: Large time solution

$t = 0.5$s

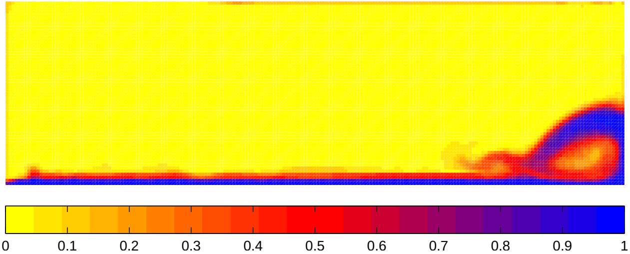


$t = 0.6$s

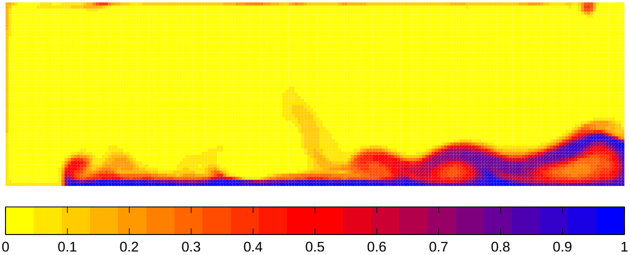


Water column collapse: Large time solution

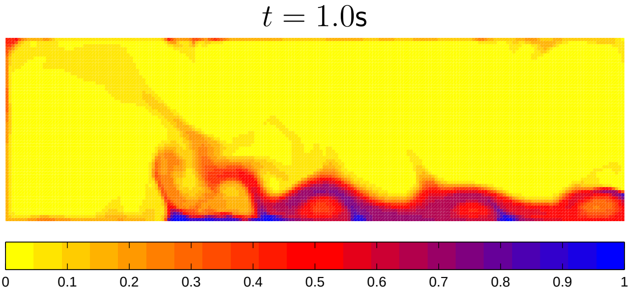
$t = 0.7\text{s}$



$t = 0.8\text{s}$



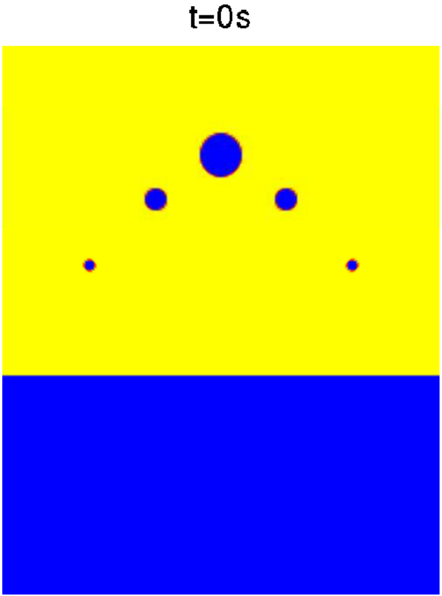
Water column collapse: Large time solution



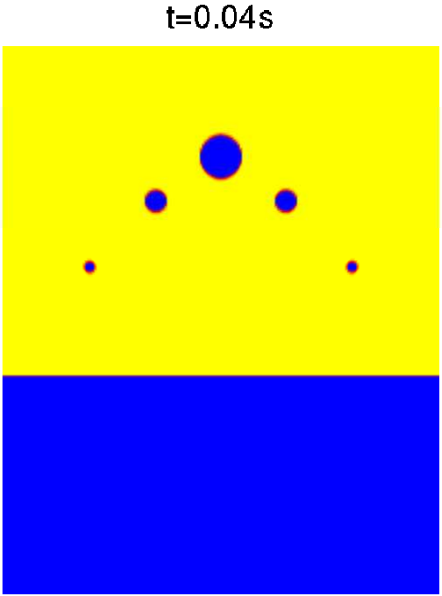
Computed solutions becomes chaotic at later time

Is this physically correct or simply numerical artifact ? (Issues to be resolved as compared with laboratory experiments, for example, for numerical validation)

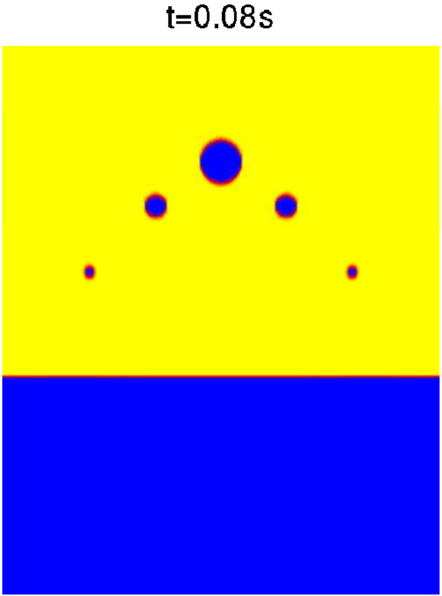
Liquid-falling problem



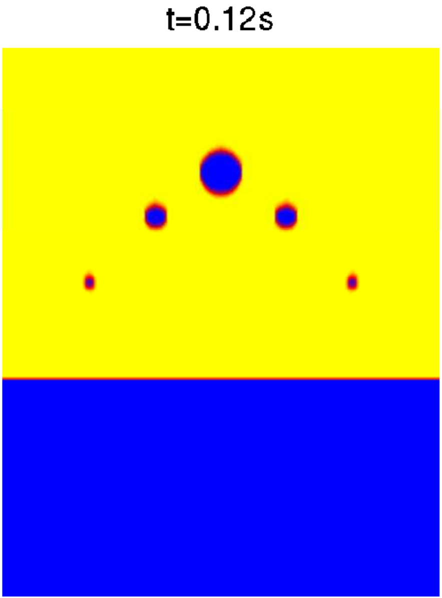
Liquid-falling problem



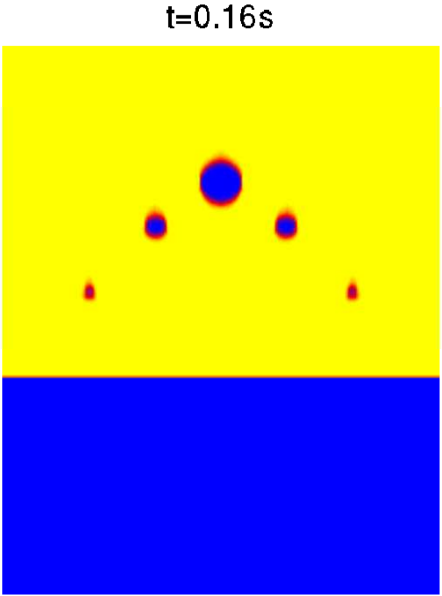
Liquid-falling problem



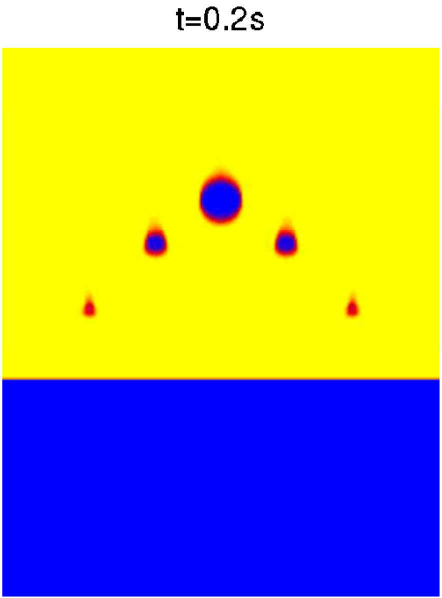
Liquid-falling problem



Liquid-falling problem



Liquid-falling problem



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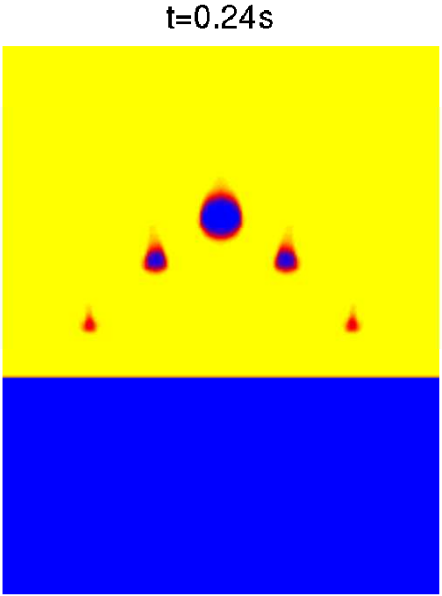

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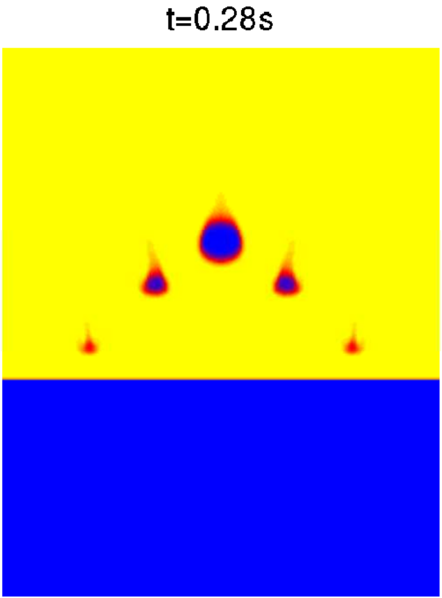

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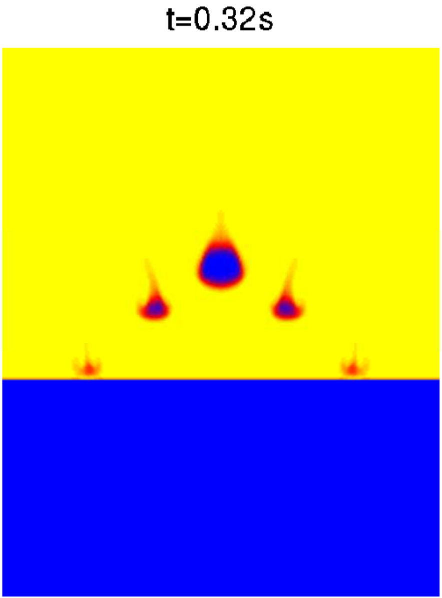

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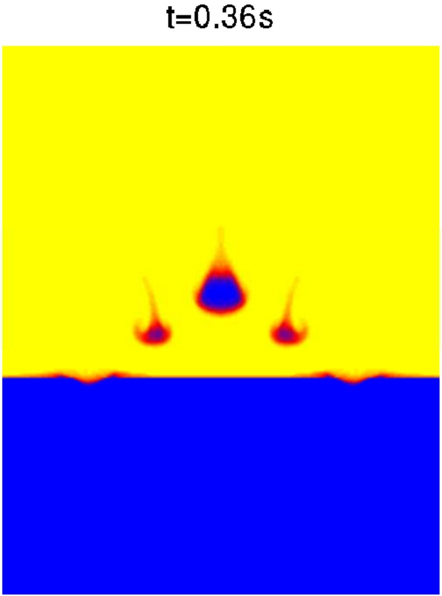

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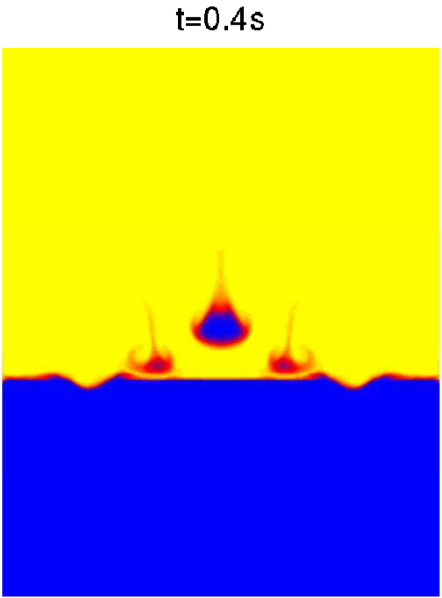

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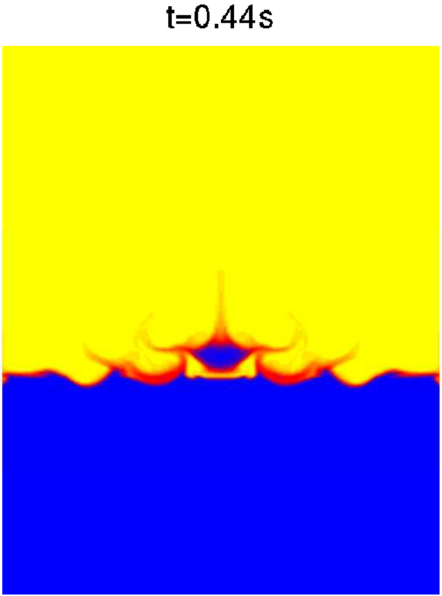

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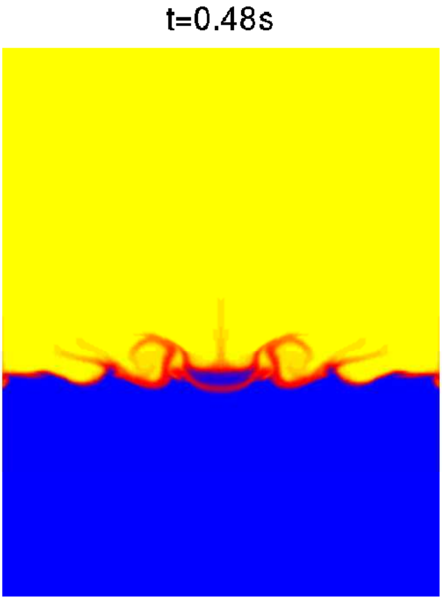

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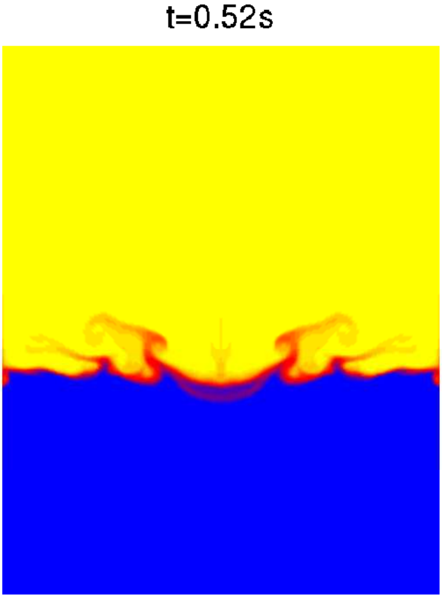

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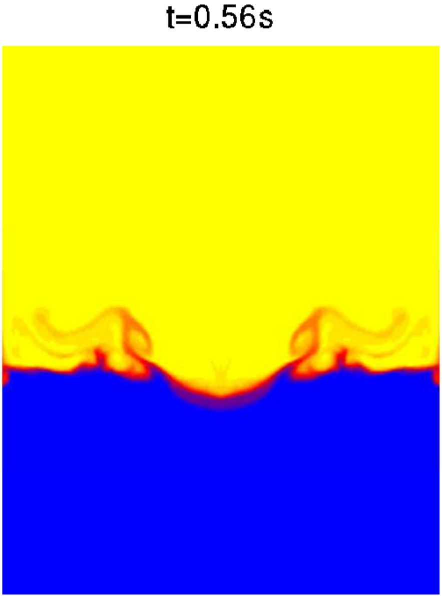
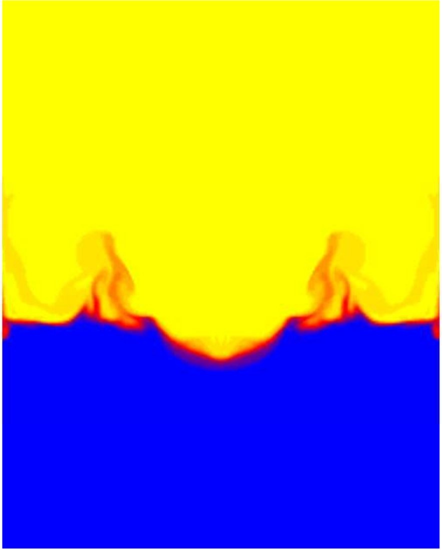


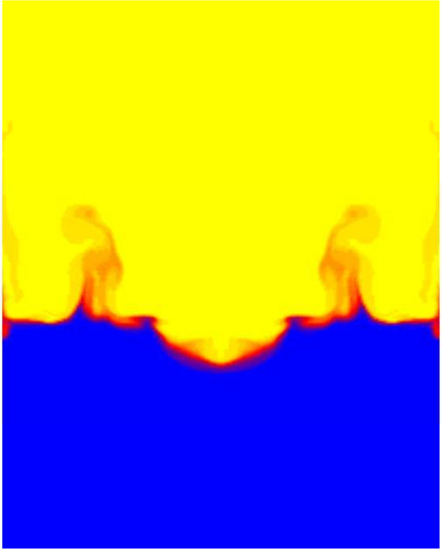
Liquid-falling problem

t=0.6s



Liquid-falling problem

t=0.64s



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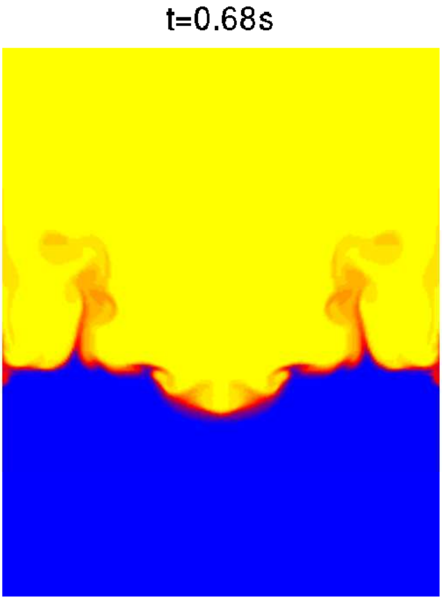

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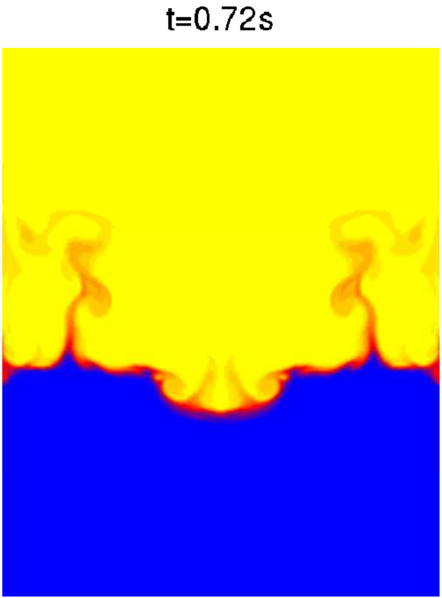
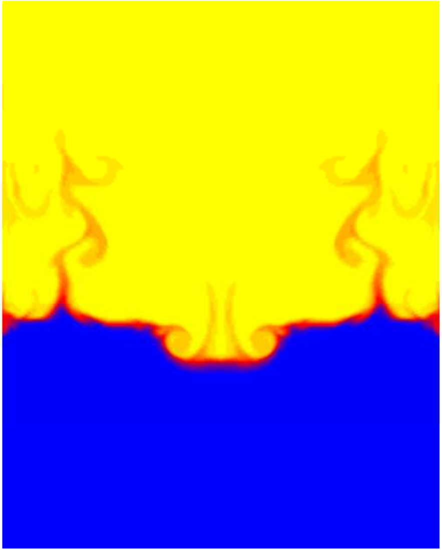


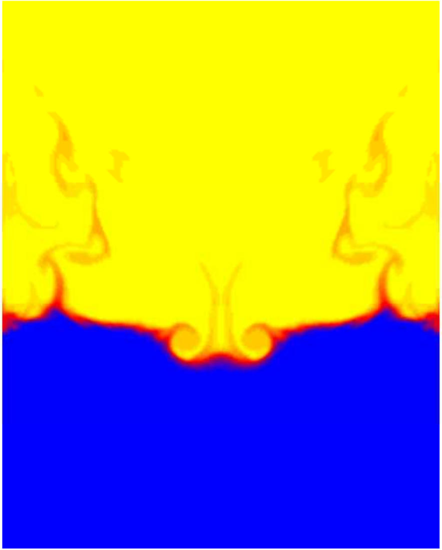
Liquid-falling problem

t=0.76s



Liquid-falling problem

t=0.8s



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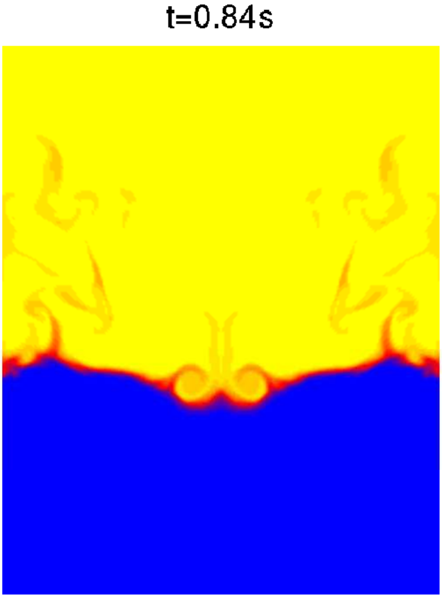
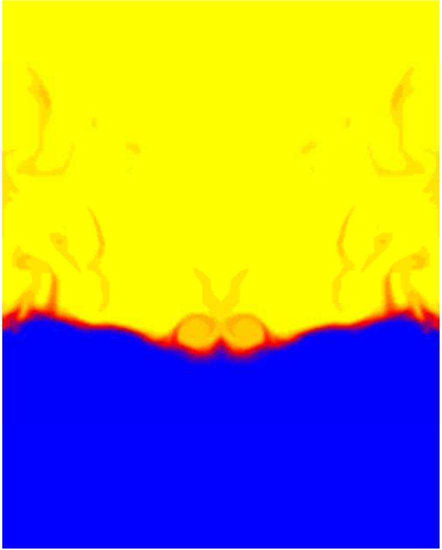


Liquid-falling problem

t=0.88s



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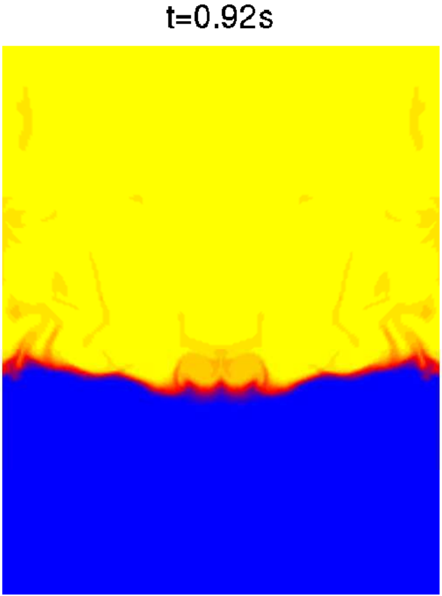

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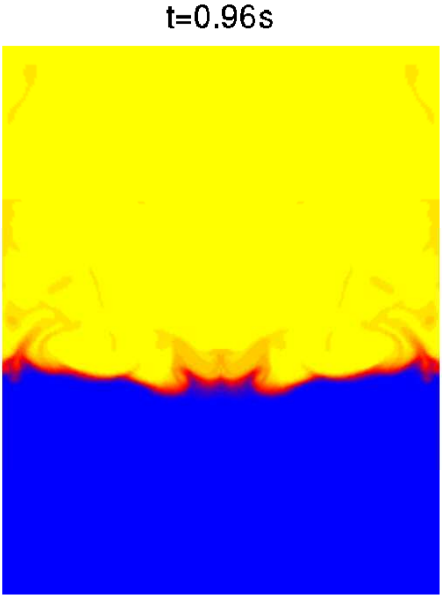

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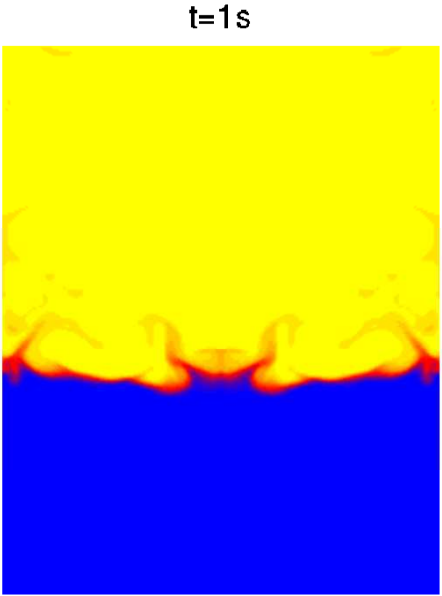
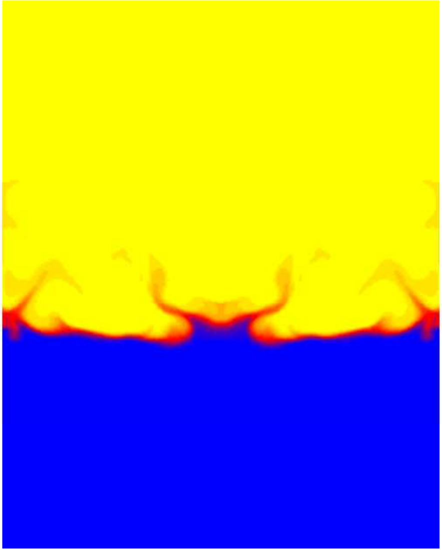


Liquid-falling problem

t=1.04s



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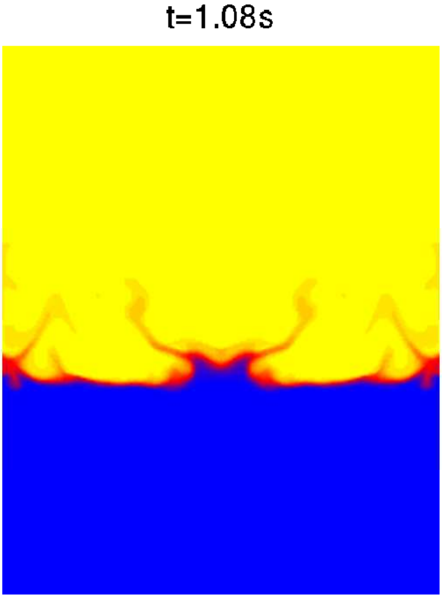

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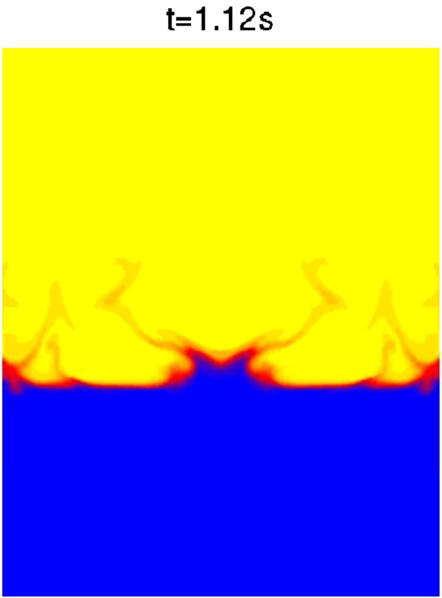

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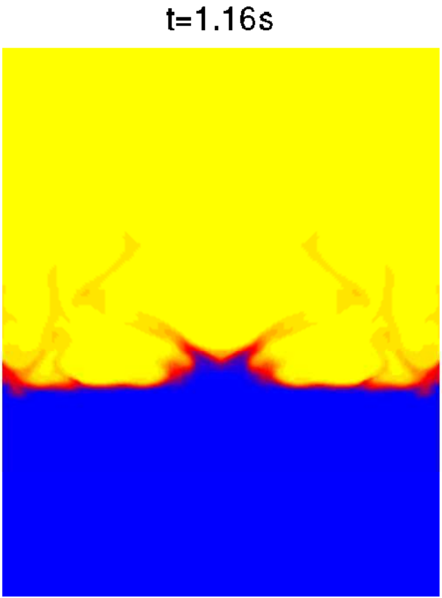

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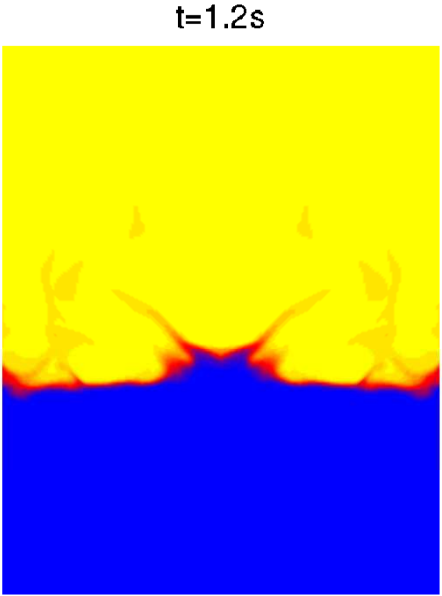

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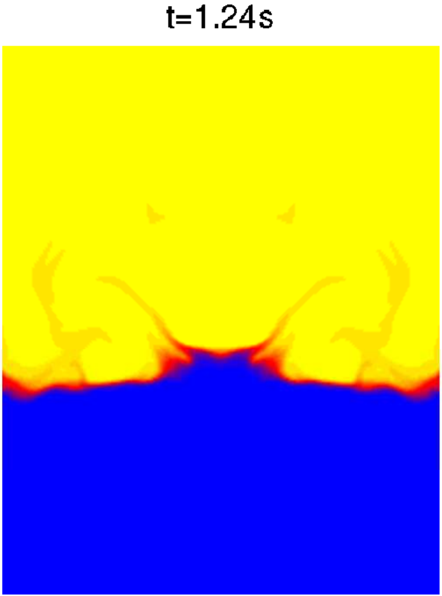

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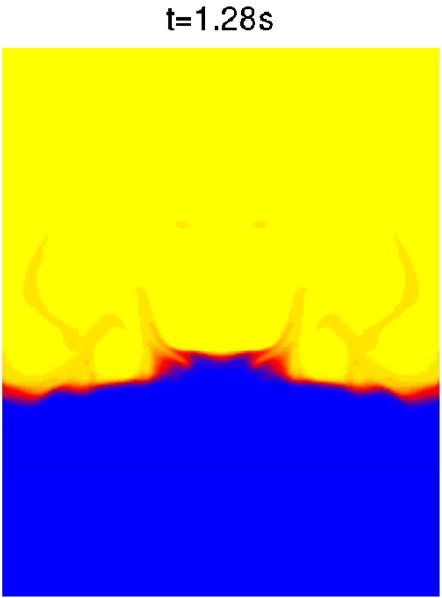

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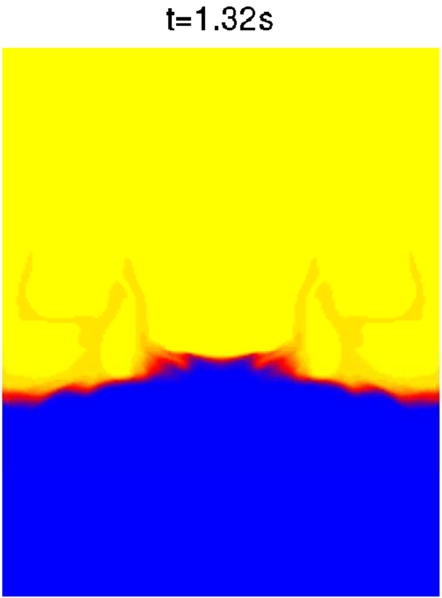

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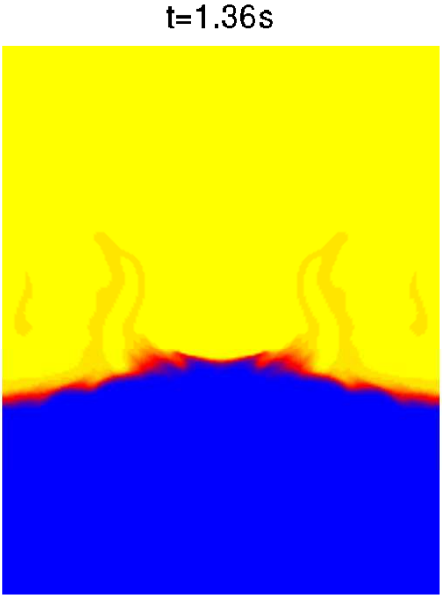

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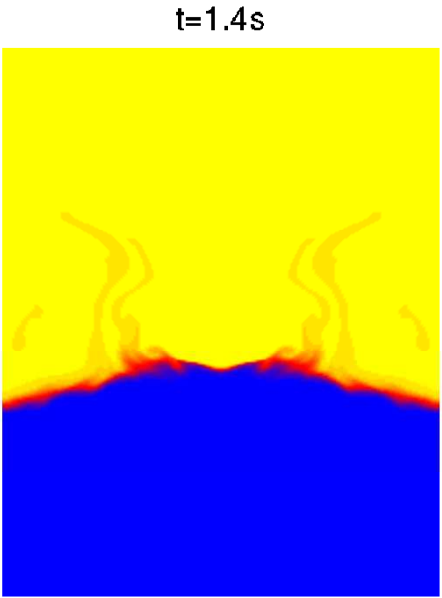

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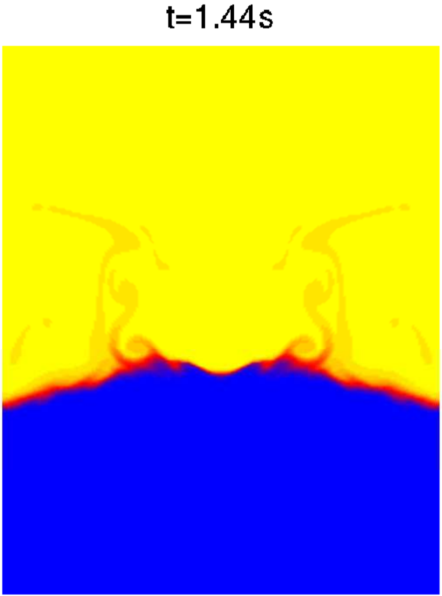

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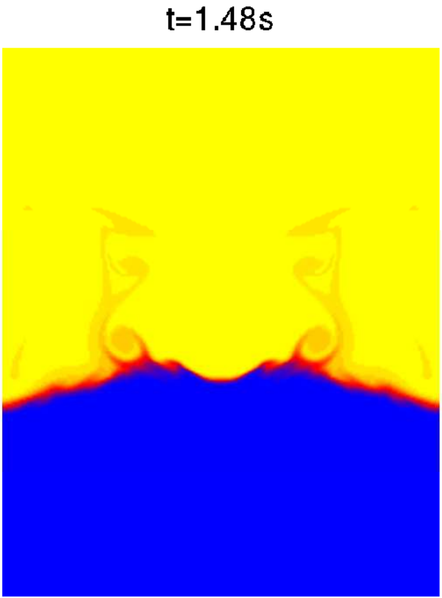

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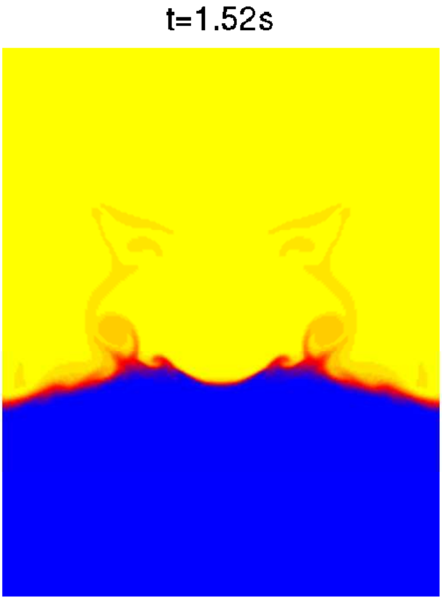

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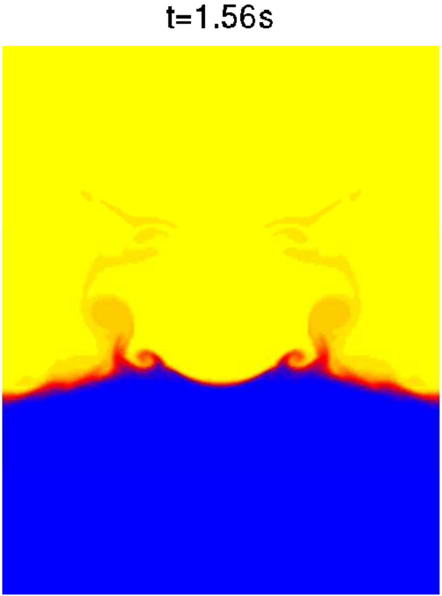
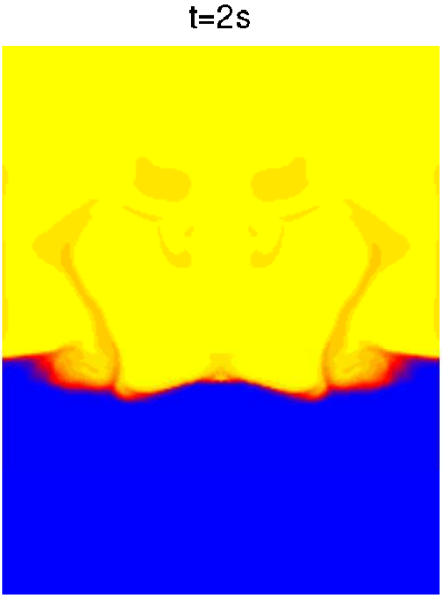


Liquid-falling problem: Large time



Weakly compressible 2-phase flow: Overview

Challenges for classical compressible flow solver

- Accuracy (due to incorrect pressure fluctuations)
- Efficiency (due to small time step)

Existing methods for modeling low Mach flow

1. Density-based approach
   - low Mach preconditioning for accuracy
   - Dual-time or implicit for efficiency
2. Pressure-based approach
   - Pressure Poisson solver for accuracy
   - Particle-velocity based advection for efficiency
3. Multiscale asymptotic-based approximations

Talk outline

1. Compressible 1-phase flow: Overview
   - Model
     - Euler's equations
   - Numerics
     - Density-based method
     - Pressure-based method
2. Compressible 2-phase flow
   - Model
     - Homogeneous relaxation models
   - Numerics
     - Density-based method
     - Pressure-based method
3. Future perspectives

Compressible gas dynamics: 1 phase

Compressible Euler's equations in conservation form is

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho \vec{u}) &= 0 \\ \partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p &= 0 \\ \partial_t (\rho E) + \nabla \cdot (\rho E \vec{u} + p \vec{u}) &= 0 \end{aligned} \tag{1}$$

Assume fluid constitutive law satisfies stiffened gas EOS

$$p(\rho, e) = (\gamma - 1) \rho e - \gamma p_\infty \tag{2}$$

- For air $\gamma = 1.4$, $p_\infty = 0$
- For water $\gamma = 4.4$, $p_\infty = 6.0 \times 10^8$Pa
- For stone $\gamma = 1.66$, $p_\infty = 1.12 \times 10^{10}$Pa

Model is hyperbolic with information propagating at speeds $\vec{u}$, $\vec{u} - c$ & $\vec{u} + c$; c is sound speed

Low Mach number flow: Explicit method

For low speed flows, when effect of sound waves is unimportant to overall solution, numerical simulation based on (1) with explicit time-discretization [1] is inefficient

This is because for stability explicit method is subject to CFL (Courant-Friedrichs-Lewy) time step constraint

$$\Delta t \le \min\left(\frac{\Delta x}{|u| + c}\right) = \min\left(\frac{\Delta x}{c(M+1)}\right), \qquad M = \frac{|u|}{c}$$

For very low Mach number flow, $M \ll 1$, this is

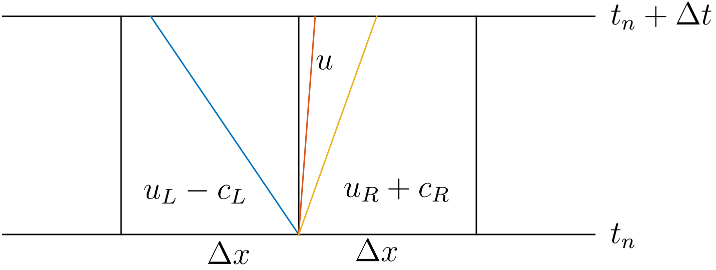
$$\Delta t \sim \frac{\Delta x}{c} \quad \Longrightarrow \quad \Delta x \sim |u| \frac{c}{|u|} \Delta t = \frac{1}{M} |u| \Delta t$$

i.e., $1/M$ timesteps for interface to move one mesh zone

[1] *i.e.*, new state is expressed solely in terms of present state

Low Mach number flow: Explicit method

$M \ll 1$, severe time step restriction for explicit method



Desirable to reformulate (1) to filter out sound waves, while retaining compressibility effects, yielding timestep constraint

$$\Delta t \leq \min\left(\frac{\Delta x}{|u|}\right)$$

Alternatively, employ implicit time-discretization to allow larger time step for stability

Low Mach number approximations: Overview

Approaches for low Mach number approximations

1. Incompressible hydrodynamics
   Formally $M \to 0$ limit of Navier-Stokes equations; velocity satisfies

$$\nabla \cdot \vec{u} = 0 \qquad \Longrightarrow \qquad \frac{D\rho}{Dt} = 0$$

   No compressibility effects modeled in this approximation

2. Anelastic hydrodynamics (used in atmospheric sciences)
   Velocity & density satisfy constraint equation

$$\nabla \cdot (\rho_0 \vec{u}) = 0 \qquad (\rho_0 \text{ variant hydrostatic density})$$

   - Gatti-Bono & Colella (JCP 2006): An anelastic allspeed projection method for gravitationally stratified flows

Low Mach number approximations: Overview

3. Pseudo-incompressibility hydrodynamics
   Velocity satisfies constraint equation

$$\nabla \cdot (\alpha \vec{u}) = \beta$$

   for some α & β depending on class of problems

   - Almgren, Bell, Rendleman & Zingale (APJ 2006): Low Mach number modeling of type Ia supernovae. I. Hydrodynamics

4. Low Mach number preconditioning

   - Guillard & Murrone (CAF 2004): On the behavior of upwind schemes in the low Mach number limit: II. Godunov type schemes
   - LeMartelot, Nkonga, & Saurel (JCP 2013): Liquid and liquidgas flows at all speeds

Compressible gas dynamics: Scaling analysis

Define material derivative as

$$\frac{D}{Dt} = \partial_t + \vec{u} \cdot \nabla$$

Write (1) in primitive form with respect to ρ, $\vec{u}$, & p as

$$\begin{aligned} \frac{D\rho}{Dt} + \rho \, \nabla \cdot \vec{u} = 0 \\ \frac{D\vec{u}}{Dt} + \frac{1}{\rho} \, \nabla p = 0 \\ \frac{Dp}{Dt} + \rho c^2 \, \nabla \cdot \vec{u} = 0 \end{aligned} \tag{3}$$

Introduce dimensionless variables

$$\tilde{\rho} = \frac{\rho}{\rho_0}, \quad \tilde{\vec{u}} = \frac{\vec{u}}{u_0}, \quad \tilde{p} = \frac{p}{\rho_0 c_0^2}, \quad \tilde{\vec{x}} = \frac{\vec{x}}{x_0}, \quad \tilde{t} = \frac{u_0 t}{x_0}$$

Compressible gas dynamics: Scaling analysis

With that, dimensionless form of (3) is

$$\begin{aligned} \frac{D\tilde{\rho}}{D\tilde{t}} + \tilde{\rho}\,\tilde{\nabla}\cdot\tilde{\vec{u}} &= 0 \\ \frac{D\tilde{\vec{u}}}{D\tilde{t}} + \frac{1}{M^2\tilde{\rho}}\,\tilde{\nabla}\tilde{p} &= 0 \\ \frac{D\tilde{p}}{D\tilde{t}} + \tilde{\rho}\tilde{c}^2\,\tilde{\nabla}\cdot\tilde{\vec{u}} &= 0 \end{aligned} \tag{4}$$

where scaling material derivative is defined as

$$\frac{D}{D\tilde{t}} = \partial_{\tilde{t}} + \tilde{\vec{u}}\cdot\tilde{\nabla}$$

$M = u_0/c_0$ is reference Mach number

Drop ˜ in (4) below for simplicity

Compressible gas dynamics: Incompressible scaling

Assume formal asymptotic expansion of state z of form

$$z = z_0 + M z_1 + M^2 z_2 + \cdots \qquad \text{as} \quad M \to 0^+$$

Substituting above into (4), we get

- Order $1/M^2$:

$$\nabla p_0 = 0$$

- Order $1/M$:

$$\nabla p_1 = 0$$

- Order 1:

$$\partial_t \rho_0 + \vec{u}_0 \cdot \nabla \rho_0 + \rho_0 \nabla \cdot \vec{u}_0 = 0$$

$$\partial_t \vec{u}_0 + \vec{u}_0 \cdot \nabla \vec{u}_0 + \frac{1}{\rho_0} \nabla p_2 = 0$$

$$\partial_t p_0 + \rho_0 c_0^2 \, \nabla \cdot \vec{u}_0 = 0$$

Compressible gas dynamics: Incompressible scaling

Under condition

$$\partial_t p_0 = 0 \tag{5}$$

limit system at leading order tends formally to

$$\begin{aligned}
\partial_t p_0 + \rho_0 c_0^2\, \nabla \cdot \vec{u}_0 = 0 \quad &\Longrightarrow \quad \nabla \cdot \vec{u}_0 = 0 \\
\partial_t \rho_0 + \vec{u}_0 \cdot \nabla \rho_0 + \rho_0 \nabla \cdot \vec{u}_0 = 0 \quad &\Longrightarrow \quad \partial_t \rho_0 + \vec{u}_0 \cdot \nabla \rho_0 = 0 \\
\partial_t \vec{u}_0 + \vec{u}_0 \cdot \nabla \vec{u}_0 + \frac{1}{\rho_0}\, \nabla p_2 = 0 \quad &
\end{aligned}$$

Simple asymptotic analysis: Compressible Euler contains

Incompressible + Acoustic

How these different phenomena organize ? No general answer

Compressible gas dynamics: Preconditioned system

To enforce (5), Turkel (JCP 1987) introduces penalization

$$\frac{1}{M^2}\partial_t p_0 + \rho_0 c_0^2 \, \nabla \cdot \vec{u}_0 = 0$$

to ensure formal convergence to incompressible solutions of limit system, yielding leading order system (ignore subscript)

$$\partial_t \rho + \vec{u} \cdot \nabla \rho + \rho \nabla \cdot \vec{u} = 0$$

$$\partial_t \vec{u} + \vec{u} \cdot \nabla \vec{u} + \frac{1}{\rho} \, \nabla p = 0$$

$$\partial_t p + M^2 \vec{u} \cdot \nabla p + M^2 \rho c^2 \, \nabla \cdot \vec{u} = 0$$

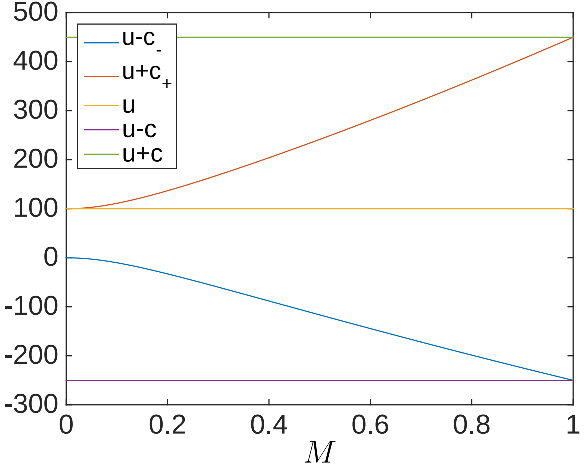
System is hyperbolic with wave speeds $\vec{u}$, $\vec{u} - \tilde{c}_-$, & $\vec{u} + \tilde{c}_+$;

$$\tilde{c}_- = \frac{(1 - M^2) u_i + \sqrt{(M^2 - 1)^2 u_i^2 + 4 M^2 c^2}}{2}$$

$$\tilde{c}_+ = \frac{(M^2 - 1) u_i + \sqrt{(M^2 - 1)^2 u_i^2 + 4 M^2 c^2}}{2}$$

Preconditioned system: Wave speeds

Wave speed is scaled with respect to Mach number



Now let us go to numerical schemes

Density-based implicit scheme: Conservation laws

Consider 1D hyperbolic conservation laws of form

$$\partial_t q + \partial_x f(q) = 0, \quad x \in [a, b], \quad t > 0 \tag{6}$$

with suitable initial & boundary conditions

q: vector of conservative variables & f: flux vector

Hyperbolicity of (6) means existence of real eigenvalues of flux Jacobian $\partial_q f(q)$ for all q

Denote Q_i^n as numerical cell-average of q at cell i & time t_n

$$Q_i^n := \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x, t_n)\, dx$$

$\Delta x_i = \Delta x$: mesh size, Δt: time step

Density-based implicit scheme: Conservation laws

Discretize (6) conservatively with backward Euler in time

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}\left(F_{i+1/2}^{n+1} - F_{i-1/2}^{n+1}\right) \tag{7}$$

with numerical flux

$$F_{i+1/2} = \frac{1}{2}\left[f(Q_i) + f(Q_{i+1}) - D_{i+1/2}(Q_{i+1} - Q_i)\right] \tag{8}$$

$D_{i+1/2}$ is so-called diffusion matrix &, *e.g.*, assumes

1. $D_{i+1/2} = \dfrac{\Delta x}{\Delta t} I$ (Lax-Friedrichs)
2. $D_{i+1/2} = a_{i+1/2} I$ (Rusanov)

   $$a_{i+1/2} = \max\left(|f'(Q_i)|, |f'(Q_{i+1})|\right)$$
3. $D_{i+1/2} = |\hat{A}_{i+1/2}|$ (Upwind)

   $$\hat{A}_{i+1/2} = (\partial_q f)_{i+1/2} \quad \text{(average matrix)}$$

Implicit conservative method: Matrix equations

Denote variation of Q_i in time

$$\Delta Q_i = Q_i^{n+1} - Q_i^n$$

To approximate $F_{i\pm 1/2}^{n+1}$, one may linearize $F_{i\pm 1/2}^{n+1}$ via Taylor series expansions as

$$\begin{aligned}
F_{i+1/2}^{n+1} &= F\left(Q_i^{n+1}, Q_{i+1}^{n+1}\right) \\
&= F_{i+1/2}^{n} + \left(\frac{\partial F_{i+1/2}}{\partial Q_i}\right)^n \Delta Q_i + \left(\frac{\partial F_{i+1/2}}{\partial Q_{i+1}}\right)^n \Delta Q_{i+1} \\
F_{i-1/2}^{n+1} &= F\left(Q_{i-1}^{n+1}, Q_{i}^{n+1}\right) \\
&= F_{i-1/2}^{n} + \left(\frac{\partial F_{i-1/2}}{\partial Q_{i-1}}\right)^n \Delta Q_{i-1} + \left(\frac{\partial F_{i-1/2}}{\partial Q_{i}}\right)^n \Delta Q_{i}
\end{aligned}$$

Implicit conservative method: Matrix equations

With that, it follows (7) satisfies block tridiagonal linear system of equations for ΔQ as

$$B_{-1}\Delta Q_{i-1} + B_0\Delta Q_i + B_1\Delta Q_{i+1} = \\ -\frac{\Delta t}{\Delta x}\left(F^n_{i+1/2} - F^n_{i-1/2}\right) \tag{9a}$$

block matrices B_{-1}, B_0, & B_1 are

$$B_{-1} = -\frac{\Delta t}{\Delta x}\left(\frac{\partial F_{i-1/2}}{\partial Q_{i-1}}\right)^n \tag{9b}$$

$$B_0 = I - \frac{\Delta t}{\Delta x}\left(\frac{\partial F_{i-1/2}}{\partial Q_i}\right)^n + \frac{\Delta t}{\Delta x}\left(\frac{\partial F_{i+1/2}}{\partial Q_i}\right)^n \tag{9c}$$

$$B_1 = \frac{\Delta t}{\Delta x}\left(\frac{\partial F_{i+1/2}}{\partial Q_{i+1}}\right)^n \tag{9d}$$

Implicit conservative method: Matrix equations

Approaches for determining numerical fluxes $F_{i\pm1/2}$ & various flux derivatives in (9) include

1. Use (8) as basis & take derivatives, yielding

$$B_{-1} = -\frac{\Delta t}{2\Delta x}\left(A_{i-1}^n + D_{i-1/2}^n\right)$$
$$B_0 = I - \frac{\Delta t}{2\Delta x}\left(A_i^n - D_{i-1/2}^n\right) + \frac{\Delta t}{2\Delta x}\left(A_i^n + D_{i+1/2}^n\right)$$
$$B_1 = \frac{\Delta t}{2\Delta x}\left(A_{i+1}^n - D_{i+1/2}^n\right)$$

2. Take derivatives to general wave-propagation-based flux

$$F_{i+1/2} = \frac{1}{2}\left[f(Q_i) + f(Q_{i+1}) - \sum_{m=1}^{M_w} \left|\lambda_{i+1/2}^m\right| \mathcal{W}_{i+1/2}^m\right] \tag{10}$$

Implicit conservative method: Matrix equations

Suppose $\lambda^m_{i+1/2}$ & $\mathcal{W}^m_{i+1/2}$, $m = 1, 2, \ldots, M_w$ are defined via solution of Riemann problem at each cell edge (see below)

With that, in determining B_{-1}, for instance, we perform

$$\frac{\partial F_{i-1/2}}{\partial Q_{i-1}} = \frac{\partial}{\partial Q_{i-1}} \left(\frac{1}{2} \left[f(Q_{i-1}) + f(Q_i) - \sum_{m=1}^{M_w} \left| \lambda^m_{i-1/2} \right| \mathcal{W}^m_{i-1/2} \right] \right)$$

$$= \frac{1}{2} A_{i-1} - \frac{1}{2} \sum_{m=1}^{M_w} \left[\mathcal{W}^m_{i-1/2} \left(\nabla_{Q_{i-1}} |\lambda^m_{i-1/2}| \right) + |\lambda^m_{i-1/2}| \left(\frac{\partial \mathcal{W}^m_{i-1/2}}{\partial Q_{i-1}} \right) \right]$$

yielding need to compute terms such as

$$\nabla_{Q_{i-1}} |\lambda^m_{i-1/2}| \quad \& \quad \frac{\partial \mathcal{W}^m_{i-1/2}}{\partial Q_{i-1}}, \quad m = 1, 2, \ldots, M_w$$

Riemann problem: Gas dynamics

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

$$\partial_t q + \partial_x f(q) = 0, \quad x \in \mathbf{R}, \quad t > 0 \tag{11a}$$

with

$$q = \begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix}, \qquad f(q) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho E u + p u \end{bmatrix} \tag{11b}$$

as for model equations, & piece-wise constant data

$$q(x,0) = \begin{cases} q_L & \text{if} \quad x < 0 \\ q_R & \text{if} \quad x > 0 \end{cases} \tag{11c}$$

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 in (11), denoted by A, is

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

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

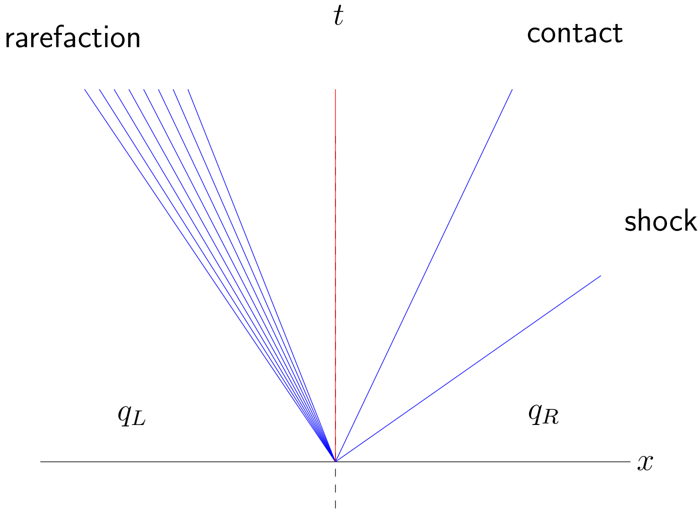
$$\Lambda = \mathsf{diag}(u - c,\ u,\ u + c)$$

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

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

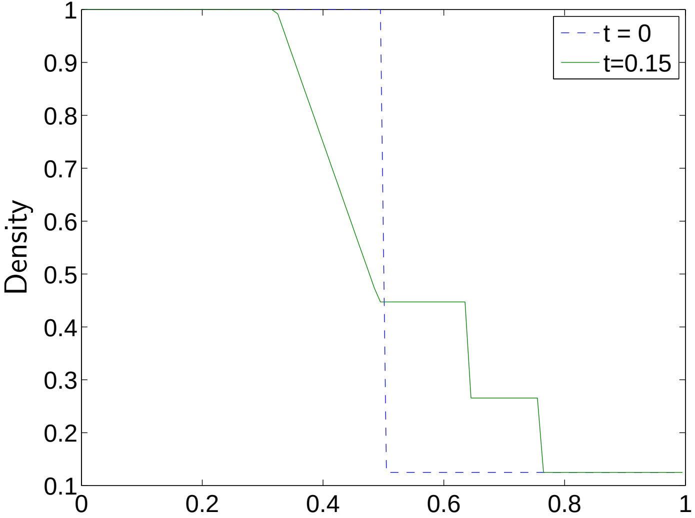
Riemann problem: Basic solution structure

Elementary waves for Riemann problem in x-t plane



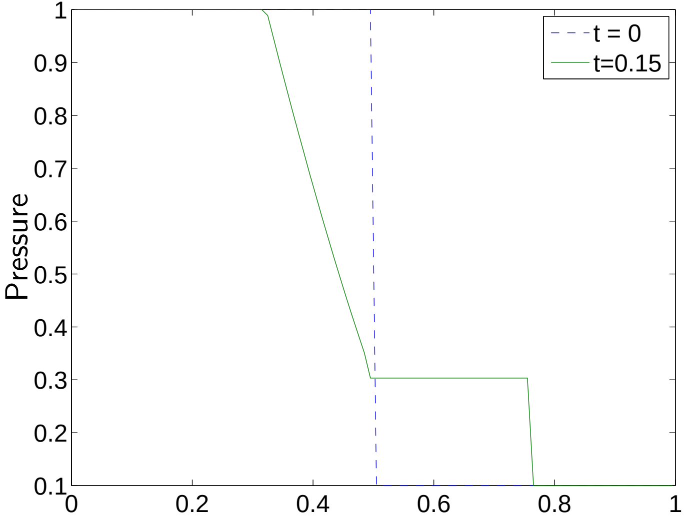
Riemann problem: Basic solution structure

Snap shot of density for Sod Riemann problem



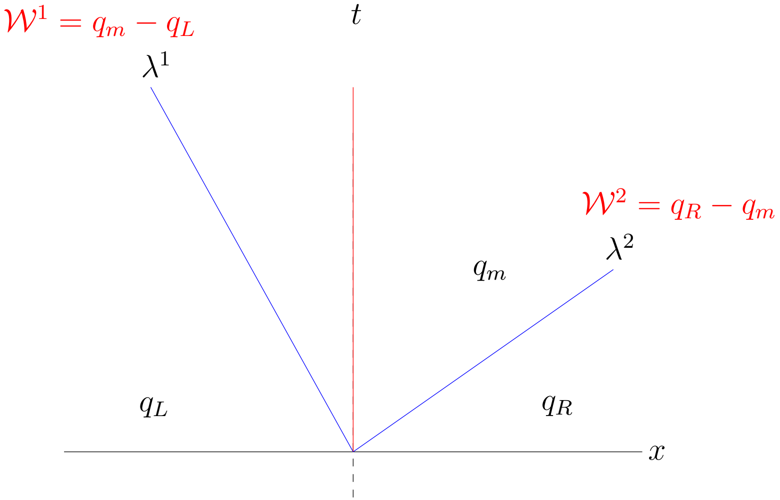
Riemann problem: Basic solution structure

Snap shot of pressure for Sod Riemann problem



Approximate Riemann solver: HLL

Harten-van Leer-Lax (HLL) approximate Riemann solver assumes 2-wave structure of solution



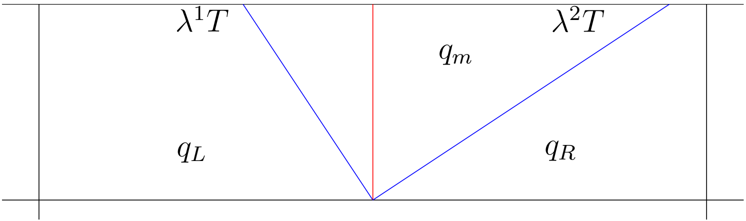
Approximate Riemann solver: HLL

In HLL solver for Euler equations, left- & right-most speeds λ^1 & λ^2 can be chosen, *e.g.*, from estimate proposed by Davis,

$$\begin{aligned} \lambda^1 &= \min\left(u_R - c_R, u_L - c_L\right) \\ \lambda^2 &= \max\left(u_R + c_R, u_L + c_L\right) \end{aligned} \tag{12}$$

Define q_m as average of solution over $[\lambda^1 T,\ \lambda^2 T]$ at time T,

$$q_m = \frac{1}{(\lambda^2 - \lambda^1)T} \int_{\lambda^1 T}^{\lambda^2 T} q(x, T)\, dx$$



Approximate Riemann solver: HLL

Using integral form of conservation laws over $[\lambda^1 T,\ \lambda^2 T] \times [0, T]$, it follows

$$q_m = \frac{\lambda^2 q_R - \lambda^1 q_L - f(q_R) + f(q_L)}{\lambda^2 - \lambda^1}$$

$f(q_\iota)$ is flux evaluated at state q_ι for $\iota = L,\ R$, yielding

$$\mathcal{W}^1 = q_m - q_L$$
$$\mathcal{W}^2 = q_R - q_m$$

Now return to computing B_k, $k = -1, 0, 1$

Since definition of λ^1 & λ^2 in (12), it leads to assuming

$$\nabla_{q_\iota} \lambda^1 = \nabla_{q_\iota} \lambda^2 = 0 \quad \text{for} \quad \iota = L, R$$

Matrix equations: HLL-based solver

As to derivatives of $\mathcal{W}^1$, there are

$$
\begin{aligned}
\frac{\partial \mathcal{W}^1}{\partial q_L} &= \frac{\partial}{\partial q_L}\left(q_m - q_L\right) \\
&= \frac{\partial}{\partial q_L}\left(\frac{\lambda^2 q_R - \lambda^1 q_L - f(q_R) + f(q_L)}{\lambda^2 - \lambda^1}\right) - 1 \\
&= \left(-\lambda^2 I + \frac{\partial f(q_L)}{\partial q_L}\right) \Big/ \left(\lambda^2 - \lambda^1\right) \\
\frac{\partial \mathcal{W}^1}{\partial q_R} &= \frac{\partial}{\partial q_R}\left(q_m - q_L\right) \\
&= \frac{\partial}{\partial q_R}\left(\frac{\lambda^2 q_R - \lambda^1 q_L - f(q_R) + f(q_L)}{\lambda^2 - \lambda^1}\right) \\
&= \left(\lambda^2 I - \frac{\partial f(q_R)}{\partial q_R}\right) \Big/ \left(\lambda^2 - \lambda^1\right)
\end{aligned}
$$

Matrix equations: HLL-based solver

Now to derivaives of $\mathcal{W}^2$, there are

$$\begin{aligned}
\frac{\partial \mathcal{W}^2}{\partial q_L} &= \frac{\partial}{\partial q_L}\left(q_R - q_m\right) \\
&= -\frac{\partial}{\partial q_L}\left(\frac{\lambda^2 q_R - \lambda^1 q_L - f(q_R) + f(q_L)}{\lambda^2 - \lambda^1}\right) \\
&= -\left(-\lambda^1 I + \frac{\partial f(q_L)}{\partial q_L}\right) \bigg/ \left(\lambda^2 - \lambda^1\right) \\
\frac{\partial \mathcal{W}^2}{\partial q_R} &= \frac{\partial}{\partial q_R}\left(q_R - q_m\right) \\
&= 1 - \frac{\partial}{\partial q_R}\left(\frac{\lambda^2 q_R - \lambda^1 q_L - f(q_R) + f(q_L)}{\lambda^2 - \lambda^1}\right) \\
&= \left(-\lambda^1 I + \frac{\partial f(q_R)}{\partial q_R}\right) \bigg/ \left(\lambda^2 - \lambda^1\right)
\end{aligned}$$

Matrix equations: HLL-based solver

Recall
$$B_{-1} = -\frac{\Delta t}{\Delta x}\left(\frac{\partial F_{i-1/2}}{\partial Q_{i-1}}\right)^n$$
$$B_0 = I - \frac{\Delta t}{\Delta x}\left(\frac{\partial F_{i-1/2}}{\partial Q_i}\right)^n + \frac{\Delta t}{\Delta x}\left(\frac{\partial F_{i+1/2}}{\partial Q_i}\right)^n$$
$$B_1 = \frac{\Delta t}{\Delta x}\left(\frac{\partial F_{i+1/2}}{\partial Q_{i+1}}\right)^n$$

Denote $F_{i-1/2} = F_{LR}$, $Q_{i-1} = q_L$, & $Q_i = q_R$. We have

$$\frac{\partial F_{LR}}{\partial q_L} = \frac{1}{2}A_L - \frac{1}{2}\left(|\lambda^1|\frac{\partial \mathcal{W}^1}{\partial q_L} + |\lambda^2|\frac{\partial \mathcal{W}^2}{\partial q_L}\right)$$
$$= \frac{1}{2}A_L - \frac{1}{2}\left[\frac{|\lambda^1|}{\lambda^2 - \lambda^1}\left(-\lambda^2 I + A_L\right) + \frac{|\lambda^2|}{\lambda^2 - \lambda^1}\left(\lambda^1 I - A_L\right)\right]$$

Matrix equations: HLL-based solver

In addition,

$$\frac{\partial F_{LR}}{\partial q_R} = \frac{1}{2}A_R - \frac{1}{2}\left[\frac{|\lambda^1|}{\lambda^2-\lambda^1}\left(\lambda^2 I - A_R\right) + \frac{|\lambda^2|}{\lambda^2-\lambda^1}\left(-\lambda^1 I + A_R\right)\right]$$

It is easy to show if $\lambda^1_{i+1/2} = -\lambda^2_{i+1/2}$ for all i, we recoover

$$B_\iota^{\mathsf{HLL}} = B_\iota^{\mathsf{LLF}}, \qquad \iota = -,\ 0,\ +$$

Using general wave-propagation form numerical fluxes (10), we may relax dependence on characteristic decomposition of model equations; difficult to do in some instances

Implicit conservative scheme as $M \to 0$

Recall that asymptotic analysis show that when $M \to 0$, solution of pressure is of form

$$p(\vec{x}, t) = p_0(t) + M p_1(t) + M^2 p_2(\vec{x}, t) + \cdots \qquad (13)$$

In discrete case, as $M \to 0$, it is known that (cf. Guillard & Viozat CAF 1999) computed pressure obtained using above implicit scheme with Roe solver would behave like

$$p(\vec{x}, t) = p_0(t) + M p_1(\vec{x}, t)$$

this is clearly different from (13)

Preconditioned system & scheme

To obtain desire asymptotic behavior of computed pressure in form (13), preconditioned dissipation is proposed, *i.e.*,

$$F_{i+1/2} = \frac{1}{2}\left[f(Q_i) + f(Q_{i+1}) - P^{-1}_{i+1/2}|P_{i+1/2}A_{i+1/2}|(Q_{i+1} - Q_i)\right]$$

Here P is a chosen preconditioned matrix which scales sound speed as seen before

In essence, original conservation law (6) is modified by

$$\partial_t q + P\partial_x f(q) = 0$$

Preconditioned system & scheme

To obtain desire asymptotic behavior of computed pressure in form (13), preconditioned dissipation is proposed, *i.e.*,

$$F_{i+1/2} = \frac{1}{2}\left[f(Q_i) + f(Q_{i+1}) - P^{-1}_{i+1/2}|P_{i+1/2}A_{i+1/2}|(Q_{i+1} - Q_i)\right]$$

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In essence, original conservation law (6) is modified by

$$\partial_t q + P\partial_x f(q) = 0$$

This is work ongoing; we next discuss pressure-based scheme

Pressure-based method: Primitive case

Non-conservative formulation: Yabe & coworkers

- Write Euler's equations in non-conservative form

$$\partial_t q + \vec{u} \cdot \nabla q = \psi(q)$$
$$q = \begin{bmatrix} \rho, & \vec{u}, & p \end{bmatrix}^T$$
$$\psi = \begin{bmatrix} -\rho \nabla \cdot \vec{u}, & -\frac{1}{\rho} \nabla p, & -\rho c^2 \nabla \cdot \vec{u} \end{bmatrix}^T$$

- Perform non-advection step first to solve

$$\partial_t q = \psi(q)$$

- Perform advection step next to solve

$$\partial_t q + \vec{u} \cdot \nabla q = 0$$

Pressure-based method: Primitive case

In non-advection step, say in 2D, we assume $\Delta\rho$ & Δe can be well-approximated by

$$\Delta\rho = \rho^{n+1} - \rho^n = -\rho^n \Delta t \left(D_x u^{n+1} + D_y v^{n+1} \right)$$
$$\Delta e = e^{n+1} - e^n = -\frac{p^n}{\rho^n} \Delta t \left(D_x u^{n+1} + D_y v^{n+1} \right)$$

Substituting them into basic thermodynamic relation

$$\Delta p = p^{n+1} - p^n = \left(\frac{\partial p}{\partial \rho} \right)_e^n \Delta\rho + \left(\frac{\partial p}{\partial e} \right)_\rho^n \Delta e, \quad \text{yielding}$$

$$\Delta p = -\left(\rho c^2 \right)^n \Delta t \left(D_x u^{n+1} + D_y v^{n+1} \right)$$

Pressure-based method: Primitive case

From

$$\Delta u = u^{n+1} - u^n = -\frac{D_x p^{n+1}}{\rho^n} \Delta t$$

$$\Delta v = v^{n+1} - v^n = -\frac{D_y p^{n+1}}{\rho^n} \Delta t$$

Substituting u^{n+1} & v^{n+1} into

$$\Delta p = -\left(\rho c^2\right)^n \Delta t \left(D_x u^{n+1} + D_y v^{n+1}\right),$$

yielding Helmholtz equation for p^{n+1} as

$$D_x \left(\frac{D_x p^{n+1}}{\rho^n}\right) + D_y \left(\frac{D_y p^{n+1}}{\rho^n}\right) = \frac{p^{n+1} - p^n}{(\rho c^2)^n (\Delta t)^2} + \frac{1}{\Delta t} \left(D_x u^n + D_y v^n\right)$$

Pressure-based method: Conservaive form

Conservative formulation: Xiao, Sussman, Fedwik, $\cdots$

- Use Euler's equations in conservation form

$$
\begin{aligned}
&\partial_t q + \nabla \cdot f(q) = \psi(q) \\
&q = \left[\rho, \quad \rho\vec{u}, \quad \rho E\right]^T \\
&f(q) = \left[\rho\vec{u}, \quad \rho\vec{u} \otimes \vec{u}, \quad \rho E\vec{u}\right]^T \\
&\psi = \left[0, \quad -\nabla p, \quad -\nabla \cdot (p\vec{u})\right]^T
\end{aligned}
$$

- Perform colorred advection step first to solve

$$\partial_t q + \nabla \cdot f(q) = 0$$

- Perform non-advection step next to solve

$$\partial_t q = \psi(q)$$

Pressure-based method: Conservaive form

First, update advection terms of conserved variables

$$
\begin{aligned}
\rho^{n+1} &= \rho^n - \Delta t \nabla \cdot (\rho \vec{u})^n \\
(\rho \vec{u})^{n+1} &= (\rho \vec{u})^n - \Delta t \nabla \cdot (\rho \vec{u} \otimes \vec{u})^n - \Delta t \nabla p^{n+1} \\
E^{n+1} &= E^n - \Delta t \nabla \cdot (E \vec{u})^n - \Delta t \nabla \cdot (p \vec{u})^{n+1}
\end{aligned}
$$

Non-advection momentum & energy updates are

$$
\begin{aligned}
(\rho \vec{u})^{n+1} &= (\rho \vec{u})^* - \Delta t \nabla p^{n+1} \\
E^{n+1} &= E^* - \Delta t \nabla \cdot (p \vec{u})^{n+1}, \quad \text{yielding also} \\
\nabla \cdot \vec{u}^{n+1} &= \nabla \cdot \vec{u^*} - \Delta t \nabla \cdot \left(\frac{\nabla p^{n+1}}{\rho^{n+1}} \right)
\end{aligned}
$$

Pressure-based method: Conservaive form

$\nabla \cdot \vec{u}^{n+1} = 0$ in case of incompressible flow, here it follows

$$(p_t + \vec{u} \cdot \nabla p)^n \approx -\left(\rho c^2\right)^n \nabla \cdot \vec{u}^{n+1}$$

approximately or

$$\frac{p^{n+1} - p^n}{\Delta t} + (\vec{u} \cdot \nabla p)^n \approx -\left(\rho c^2\right)^n \nabla \cdot \vec{u}^{n+1}$$

This leads to Helmholtz equation for pressure

$$p^{n+1} - (\rho c^2)^n \Delta t^2 \nabla \cdot \left(\frac{\nabla p^{n+1}}{\rho^{n+1}} \right) = p^a - (\rho c^2)^n \Delta t \nabla \cdot \vec{u^*}, \quad \text{where}$$

$$p^a = p^n + \Delta t \left(\vec{u}^n \cdot \nabla p^n \right)$$

Pressure-based method: Conservaive form

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$$p^a = p^n + \Delta t \left(\vec{u}^n \cdot \nabla p^n\right)$$

We next move to 2-phase flow case

Compressible 2-phase flow: Mathematical Models

In this talk, our interest is on following class of model for compressible 2-phase flow

1. 7-equation model (Baer-Nunziato type)
2. Reduced 5-equation model (Kapila type)
3. Homogeneous 6-equation model
   - Saurel *et al.* (JCP 2009), Pelanti & Shyue (JCP 2014)

Homogeneous 2-phase flow model: Barotropic case

One simple homogeneous (1 velocity, 1 pressure) model for barotropic 2-phase flow is

$$\begin{aligned} \partial_t (\alpha_1 \rho_1) + \nabla \cdot (\alpha_1 \rho_1 \vec{u}) &= 0 \\ \partial_t (\alpha_2 \rho_2) + \nabla \cdot (\alpha_2 \rho_2 \vec{u}) &= 0 \\ \partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p &= 0 \end{aligned}$$

Assume constitutive law for each fluid phase satisfies

$$p_k (\rho_k) = \mathcal{A}_k \left(\frac{\rho_k}{\rho_{0k}} \right)^{\gamma} - \mathcal{B}_k \qquad \text{(Tait equation of state)}$$

Equilibrium pressure $p = p_1 = p_2$ follows saturation relation

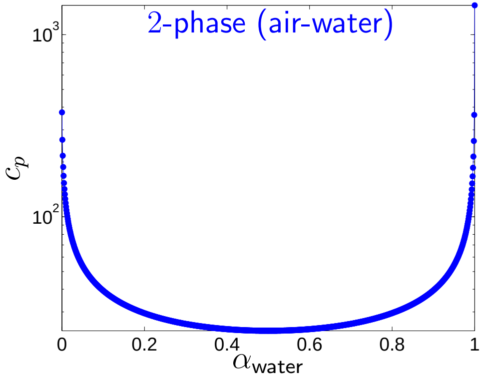
$$\alpha_1 + \alpha_2 = \frac{\alpha_1 \rho_1}{\rho_1(p)} + \frac{\alpha_2 \rho_2}{\rho_2(p)} = 1$$

yielding nonlinear algebraic equation to be solved

Homogeneous 2-phase flow model: Sound speed

Model is hyperbolic with equilibrium sound speed c_p:

$$\frac{1}{\rho c_p^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2}$$



Non-monotonic c_p leads to stiffness in equations & difficulties in numerical solver, *e.g.*, positivity-preserving in volume fraction & pressure

Homogeneous relaxation model: Barotropic case

Numerically, it is more stable to consider relaxation model

$$\begin{aligned}
\partial_t \left(\alpha_1 \rho_1\right) + \nabla \cdot \left(\alpha_1 \rho_1 \vec{u}\right) &= 0 \\
\partial_t \left(\alpha_2 \rho_2\right) + \nabla \cdot \left(\alpha_2 \rho_2 \vec{u}\right) &= 0 \\
\partial_t \left(\rho \vec{u}\right) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u}\right) + \nabla \left(\alpha_1 p_1 + \alpha_2 p_2\right) &= 0 \\
\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 &= \mu \left(p_1 - p_2\right)
\end{aligned}$$

Write model in compact form as

$$\partial_t q + \nabla \cdot f(q) + w(q, \nabla q) = \psi_\mu(q)$$

Compute approximate solution based on fractional step:

1. Homogeneous hyperbolic step

$$\partial_t q + \nabla \cdot f(q) + w(q, \nabla q) = 0$$

2. Source-term relaxation step as parameter $\mu \to \infty$

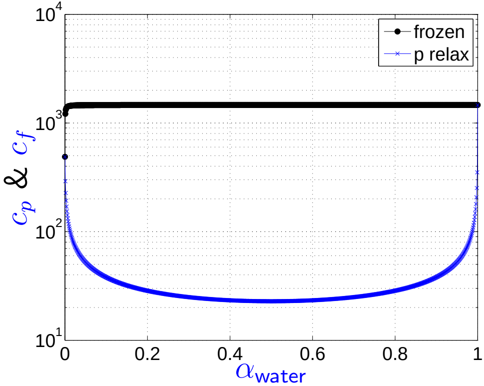
$$\partial_t q = \psi_\mu(q) \qquad \Longrightarrow \quad p_1 \left(\frac{\alpha_1 \rho_1}{\alpha_1}\right) - p_2 \left(\frac{\alpha_2 \rho_2}{1 - \alpha_1}\right) = 0$$

Homogeneous relaxation model: Hyperbolic step

Sound speed in hyperbolic step, denoted by c_f, is

$$\rho c_f^2 = \sum_{k=1}^{2} \alpha_k \rho_k c_k^2 \qquad \text{(frozen speed)}$$

which satisfies sub-characteristic condition $c_p \leq c_f$



Monotonic c_f gives better conditioning of hyperbolic step, but is less efficient due to CFL time-step constraint

Homogeneous relaxation model: Frozen sound speed

$$
\begin{aligned}
c_f^2 &= \partial_\rho \left(\sum_{k=1}^{2} \alpha_k p_k \right)_{Y_k, \alpha_k, s_k} = \sum_{k=1}^{2} \alpha_k \partial_\rho p_k \\
&= \sum_{k=1}^{2} \alpha_k \left(\partial_{\rho_k} p_k \right) \left(\partial_\rho \rho_k \right) = \sum_{k=1}^{2} \alpha_k c_k^2 \left(\partial_\rho \rho_k \right) \\
&= \sum_{k=1}^{2} Y_k c_k^2 \\
dY_k &= d \left(\frac{\alpha_k \rho_k}{\rho} \right) = \frac{\rho \alpha_k d\rho_k - \alpha_k \rho_k d\rho}{\rho^2} \\
&= \frac{\alpha_k}{\rho} \left(d\rho_k - \frac{\rho_k}{\rho} d\rho \right) = 0 \quad \implies \quad \frac{d\rho_k}{d\rho} = \frac{\rho_k}{\rho}
\end{aligned}
$$

Homogeneous relaxation model: Asymptotics

Take formal asymptotic expansion ansatz of solution

$$q = q^0 + \varepsilon q^1 + \cdots$$

Derive equilibrium equation for q^0 as $\mu = 1/\varepsilon \to \infty$ $(\varepsilon \to 0^+)$

Recall material derivative as

$$\frac{D}{Dt} = \partial_t + \vec{u} \cdot \nabla$$

We find

$$\frac{D\alpha_1}{Dt} = \frac{1}{\varepsilon}(p_1 - p_2)$$

$$\frac{Dp_k}{Dt} = \frac{\partial p_k}{\partial \rho_k}\frac{D\rho_k}{Dt} = c_k^2 \frac{D\rho_k}{Dt} = -\frac{c_k^2}{\alpha_k}\left(\rho_k \frac{D\alpha_k}{Dt} + \alpha_k \rho_k \nabla \cdot \vec{u}\right)$$

$$\Longrightarrow \quad \frac{Dp_k}{Dt} + \rho_k c_k^2 \nabla \cdot \vec{u} = -\frac{\rho_k c_k^2}{\alpha_k}\frac{D\alpha_k}{Dt}$$

Homogeneous relaxation model: Asymptotics

Substituting asymptotic expansions to equations, we get

$$\frac{D}{Dt}\left(\alpha_1^0 + \varepsilon\alpha_1^1 + \cdots\right) = \frac{1}{\varepsilon}\left[\left(p_1^0 - p_2^0\right) + \varepsilon\left(p_1^1 - p_2^1\right) + \cdots\right]$$

$$\frac{D}{Dt}\left(p_k^0 + \varepsilon p_k^1 + \cdots\right) + \left(\rho_k^0 c_k^{0^2} + \varepsilon\rho_k^1 c_k^{1^2} + \cdots\right)\nabla\cdot\vec{u} =$$

$$-\left(\frac{\rho_k^0 c_k^{0^2} + \varepsilon\rho_k^1 c_k^{1^2} + \cdots}{\alpha_k^0 + \varepsilon\alpha_k^1 + \cdots}\right)\frac{D}{Dt}\left(\alpha_k^0 + \varepsilon\alpha_k^1 + \cdots\right)$$

Collecting equal power of ε, we have

$$O(1/\varepsilon) \qquad p_1^0 = p_2^0 \equiv p^0$$

$$O(1) \qquad \frac{Dp_k^0}{Dt} + \rho_k^0 c_k^{0^2}\nabla\cdot\vec{u} = -\left(\frac{\rho_k^0 c_k^{0^2}}{\alpha_k^0}\right)\frac{D\alpha_k^0}{Dt}$$

Homogeneous relaxation model: Asymptotics

$$\Longrightarrow \qquad \frac{Dp_1^0}{Dt} + \rho_1^0 c_1^{0^2} \nabla \cdot \vec{u} = -\left(\frac{\rho_1^0 c_1^{0^2}}{\alpha_1^0}\right)\left(p_1^1 - p_2^1\right)$$

$$\frac{Dp_2^0}{Dt} + \rho_2^0 c_2^{0^2} \nabla \cdot \vec{u} = -\left(\frac{\rho_2^0 c_2^{0^2}}{\alpha_2^0}\right)\left(p_2^1 - p_1^1\right)$$

Subtracting former two equations & with $p_1^0 = p_2^0$, we find

$$\left(\rho_1^0 c_1^{0^2} - \rho_2^0 c_2^{0^2}\right) \nabla \cdot \vec{u} = \left(\frac{\rho_1^0 c_1^{0^2}}{\alpha_1^0} + \frac{\rho_2^0 c_2^{0^2}}{\alpha_2^0}\right)\left(p_2^1 - p_1^1\right)$$

i.e.,

$$\frac{D\alpha_1^0}{Dt} = p_1^1 - p_2^1 = \left(\frac{\rho_2^0 c_2^{0^2} - \rho_1^0 c_1^{0^2}}{\rho_1^0 c_1^{0^2}/\alpha_1^0 + \rho_2^0 c_2^{0^2}/\alpha_2^0}\right) \nabla \cdot \vec{u}$$

Homogeneous equilibrium model

Ignore superscript 0 to simplify notation

In summary, as $\mu \to \infty$ leading order approximation of homogeneous relaxation model (HRM) gives so-called homogeneous equilibrium model (HEM) & takes

$$
\begin{aligned}
&\partial_t (\alpha_1 \rho_1) + \nabla \cdot (\alpha_1 \rho_1 \vec{u}) = 0 \\
&\partial_t (\alpha_2 \rho_2) + \nabla \cdot (\alpha_2 \rho_2 \vec{u}) = 0 \\
&\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p = 0 \\
&\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \left(\frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\rho_1 c_1^2/\alpha_1 + \rho_2 c_2^2/\alpha_2} \right) \nabla \cdot \vec{u},
\end{aligned}
$$

Mixture pressure $p = \alpha_1 p_1 + \alpha_2 p_2$

$p_1 \to p_2$ means p approaches towards mechanical equilibrium

Homogeneous equilibrium model: Volume fraction

Volume-fraction equation is differential form of pressure equilibrium condition $p_1(\rho_1) = p_2(\rho_2)$

Denote $K = (\rho_2 c_2^2 - \rho_1 c_1^2) / (\rho_1 c_1^2/\alpha_1 + \rho_2 c_2^2/\alpha_2)$.

Assume $K < 0$, *i.e.*, $\rho_2 c_2^2 < \rho_1 c_1^2$ (phase 1 less compressible)

1. Compaction effect $(K\ \nabla \cdot \vec{u} > 0)$
   α_1 increases when $\nabla \cdot \vec{u} < 0$ (compression or shock waves)

2. Relaxation effect $(K\ \nabla \cdot \vec{u} < 0)$
   α_1 decreases when $\nabla \cdot \vec{u} > 0$ (expansion waves)

3. No effect
   α_1 remains unchanged when $\nabla \cdot \vec{u} = 0$ (contacts)

Homogeneous equilibrium model: Sound speed

Sound speed in HEM can be derived easily as

$$\frac{Dp}{Dt} = c_1^2 \frac{D\rho_1}{Dt} = c_1^2 \frac{\rho_1}{\alpha_1} \frac{D\alpha_1}{Dt} - \rho_1 c_1^2 \nabla \cdot \vec{u}$$

$$\Longrightarrow \quad \frac{\alpha_1}{\rho_1 c_1^2} \frac{Dp}{Dt} = \frac{D\alpha_1}{Dt} - \alpha_1 \nabla \cdot \vec{u}$$

Analogously, we have

$$\frac{\alpha_2}{\rho_2 c_2^2} \frac{Dp}{Dt} = \frac{D\alpha_2}{Dt} - \alpha_2 \nabla \cdot \vec{u}$$

Adding together leads to

$$\left(\frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2} \right) \frac{Dp}{Dt} = \frac{D}{Dt} (\alpha_1 + \alpha_2) - (\alpha_1 + \alpha_2) \nabla \cdot \vec{u}$$

$$\Longrightarrow \quad \frac{Dp}{Dt} = -\rho c^2 \nabla \cdot \vec{u}, \qquad \frac{1}{\rho c^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2} = \frac{1}{\rho c_p^2}$$

Pressure correction scheme: Primitive HRM

Begin with Mach-uniform approach for HRM in primitive form

$$\partial_t\left(\alpha_1\rho_1\right)+\vec{u}\cdot\nabla\left(\alpha_1\rho_1\right)=-\alpha_1\rho_1\nabla\cdot\vec{u}$$
$$\partial_t\left(\alpha_2\rho_2\right)+\vec{u}\cdot\nabla\left(\alpha_2\rho_2\right)=-\alpha_2\rho_2\nabla\cdot\vec{u}$$
$$\partial_t\vec{u}+\vec{u}\cdot\nabla\vec{u}=-\frac{1}{\rho}\nabla p+\vec{g}$$
$$\partial_t\alpha_1+\vec{u}\cdot\nabla\alpha_1=\mu\left(p_1-p_2\right)$$

Split model into advection part & non-advection part

advection part	non-advection part
$\partial_t\left(\alpha_1\rho_1\right)+\vec{u}\cdot\nabla\left(\alpha_1\rho_1\right)=0$	$\partial_t\left(\alpha_1\rho_1\right)=-\alpha_1\rho_1\nabla\cdot\vec{u}$
$\partial_t\left(\alpha_2\rho_2\right)+\vec{u}\cdot\nabla\left(\alpha_2\rho_2\right)=0$	$\partial_t\left(\alpha_2\rho_2\right)=-\alpha_2\rho_2\nabla\cdot\vec{u}$
$\partial_t\vec{u}+\vec{u}\cdot\nabla\vec{u}=0$	$\partial_t\vec{u}=-\nabla p/\rho+\vec{g}$
$\partial_t\alpha_1+\vec{u}\cdot\nabla\alpha_1=0$	$\partial_t\alpha_1=\mu\left(p_1-p_2\right)$

Pressure correction scheme: Primitive HRM

1. Hyperbolic predictor step
   Solve advection-part equations with fluid-velocity CFL
   $$\nu = \frac{\max_i |u_i| \Delta t}{\Delta x} \le 1$$
   yielding intermediate state, denoted by $*$ (easy)
2. Helmholtz corrector step
   Discretize non-advection part equations semi-implicitly
   $$\begin{aligned}(\alpha_1\rho_1)^{n+1} &= (\alpha_1\rho_1)^* - \Delta t\ (\alpha_1\rho_1)^* \nabla\cdot\vec{u}^{n+1}\\ (\alpha_2\rho_2)^{n+1} &= (\alpha_2\rho_2)^* - \Delta t\ (\alpha_2\rho_2)^* \nabla\cdot\vec{u}^{n+1}\\ \vec{u}^{n+1} &= \vec{u}^* - \Delta t\ \nabla p^{n+1}/\rho^* + \Delta t\vec{g}\end{aligned}$$
3. Relaxation step
   Solve for α_1^{n+1} as $\mu \to \infty$, *i.e.*, root-finding
   $$p_1\left[(\alpha_1\rho_1)^{n+1}/\alpha_1^{n+1}\right] - p_2\left[(\alpha_2\rho_2)^{n+1}/(1-\alpha_1^{n+1})\right] = 0$$

Pressure correction: Helmholtz corrector step

In step 2, to derive Helmholtz equation for pressure p, we begin

$$\partial_t p = (\partial_\rho p)(\partial_t \rho) = c^2 (\partial_t \rho)$$

Consistent with semi-discretized scheme for density, propose

$$p^{n+1} = p^* - \Delta t \left(\rho c^2\right)^* \nabla \cdot \vec{u}^{n+1}$$

Substituting $\nabla \cdot \vec{u}$ in above with

$$\nabla \cdot \vec{u}^{n+1} = \nabla \cdot \vec{u}^* - \Delta t \nabla \cdot \left(\frac{\nabla p^{n+1}}{\rho^*}\right)$$

obtained by applying divergence to momentum equation gives

$$\nabla \cdot \vec{u}^* - \Delta t \nabla \cdot \left(\frac{\nabla p^{n+1}}{\rho^*}\right) = -\frac{1}{\Delta t \left(\rho c^2\right)^*} \left(p^{n+1} - p^*\right)$$

equation of Helmholtz-type for pressure p^{n+1}

Pressure correction: Helmholtz corrector step

Discretization of Helmholtz equation

$$\nabla \cdot \left(\frac{\nabla p^{n+1}}{\rho^*} \right) - \frac{p^{n+1}}{(\Delta t)^2 (\rho c^2)^*} = \frac{\nabla \cdot \vec{u}^*}{\Delta t} - \frac{p^*}{(\Delta t)^2 \left(\rho c^2\right)^*}$$

- Suppose, in step 1, finite-volume method is being used, yielding cell-average data for Helmholtz equation
- Suppose pressure p is defined as point-wise value at cell-edge (staggered grid approach)
- Employ standard 2nd or 4th order finite-difference approximation to Helmholtz equation, yielding (sparse) linear system to be solved for pressure

Pressure correction: Helmholtz corrector step

After Helmholtz solve, continue

- Phasic density update

$$(\alpha_k \rho_k)^{n+1} = (\alpha_k \rho_k)^* \cdot \exp\left(-\Delta t \nabla \cdot \vec{u}^{n+1}\right)$$

where divergence of velocity field is

$$\nabla \cdot \vec{u}^{n+1} = -\frac{1}{\Delta t (\rho c^2)^*}\left(p^{n+1} - p^*\right)$$

- Velocity update

$$\vec{u}^{n+1} = \vec{u}^* - \Delta t \frac{\nabla p^{n+1}}{\rho^{n+1}}$$

where $\rho^{n+1} = (\alpha_1 \rho_1)^{n+1} + (\alpha_2 \rho_2)^{n+1}$

Pressure correction scheme: Conservative HRM

PC-based scheme in conservative formulation assumes

advection part	non-advection part
$\partial_t(\alpha_1\rho_1) + \nabla\cdot(\alpha_1\rho_1\vec{u}) = 0$	$\partial_t(\alpha_1\rho_1) = 0$
$\partial_t(\alpha_2\rho_2) + \nabla\cdot(\alpha_2\rho_2\vec{u}) = 0$	$\partial_t(\alpha_2\rho_2) = 0$
$\partial_t(\rho\vec{u}) + \nabla\cdot(\vec{u}\otimes\vec{u}) = 0$	$\partial_t(\rho\vec{u}) = -\nabla p + \rho\vec{g}$
$\partial_t\alpha_1 + \vec{u}\cdot\nabla\alpha_1 = 0$	$\partial_t\alpha_1 = \mu(p_1 - p_2)$

- Apply fractional step method as usual
- Take attentions to ensure method conservative in each step

Future perspectives

6-equation single-velocity 2-phase model with stiff mechanical, thermal, & chemical relaxations reads

$$
\begin{aligned}
&\partial_t\left(\alpha_1\rho_1\right)+\nabla\cdot\left(\alpha_1\rho_1\vec{u}\right)=\dot{m}\\
&\partial_t\left(\alpha_2\rho_2\right)+\nabla\cdot\left(\alpha_2\rho_2\vec{u}\right)=-\dot{m}\\
&\partial_t(\rho\vec{u})+\nabla\cdot(\rho\vec{u}\otimes\vec{u})+\nabla\left(\alpha_1p_1+\alpha_2p_2\right)=0\\
&\partial_t\left(\alpha_1E_1\right)+\nabla\cdot\left(\alpha_1E_1\vec{u}+\alpha_1p_1\vec{u}\right)+\mathcal{B}\left(q,\nabla q\right)=\\
&\qquad\qquad\mu p_I\left(p_2-p_1\right)+\mathcal{Q}+e_I\dot{m}\\
&\partial_t\left(\alpha_2E_2\right)+\nabla\cdot\left(\alpha_2E_2\vec{u}+\alpha_2p_2\vec{u}\right)-\mathcal{B}\left(q,\nabla q\right)=\\
&\qquad\qquad\mu p_I\left(p_1-p_2\right)-\mathcal{Q}-e_I\dot{m}\\
&\partial_t\alpha_1+\vec{u}\cdot\nabla\alpha_1=\mu\left(p_1-p_2\right)+\frac{\mathcal{Q}}{q_I}+\frac{\dot{m}}{\rho_I}
\end{aligned}
$$

$\mathcal{B}\left(q,\nabla q\right)$ is non-conservative product (q: state vector)

$$\mathcal{B}=\vec{u}\cdot\left[Y_1\nabla\left(\alpha_2p_2\right)-Y_2\nabla\left(\alpha_1p_1\right)\right]$$

Phase transition model: 6-equation

$\mu, \theta, \nu \to \infty$: instantaneous exchanges (relaxation effects)

1. Volume transfer via pressure relaxation: $\mu\,(p_1 - p_2)$
   - μ expresses rate toward mechanical equilibrium $p_1 \to p_2$, & is nonzero in all flow regimes of interest
2. Heat transfer via temperature relaxation: $\theta\,(T_2 - T_1)$
   - θ expresses rate towards thermal equilibrium $T_1 \to T_2$,
3. Mass transfer via thermo-chemical relaxation: $\nu\,(g_2 - g_1)$
   - ν expresses rate towards diffusive equilibrium $g_1 \to g_2$, & is nonzero only at 2-phase mixture & metastable state $T_{\text{liquid}} > T_{\text{sat}}$

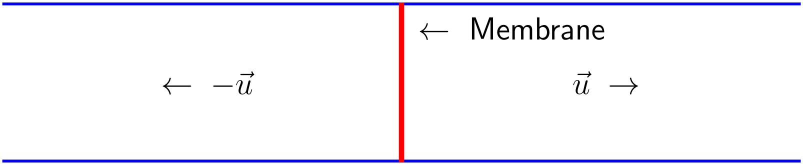
Expansion wave problem: Cavitation test

Saurel *et al.* (JFM 2008) & Zein *et al.* (JCP 2010):

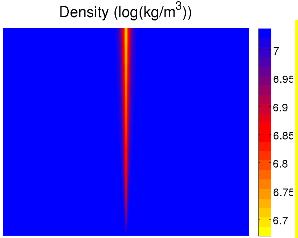
- Liquid-vapor mixture ($\alpha_{\mathrm{vapor}} = 10^{-2}$) for water with

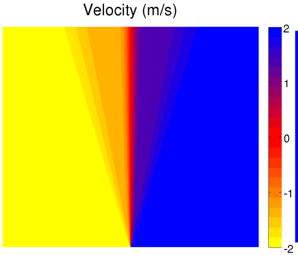
$$p_{\text{liquid}} = p_{\text{vapor}} = 1\text{bar}$$
$$T_{\text{liquid}} = T_{\text{vapor}} = 354.7284\text{K} < T^{\text{sat}}$$
$$\rho_{\text{vapor}} = 0.63\text{kg/m}^3 > \rho^{\text{sat}}_{\text{vapor}}, \quad \rho_{\text{liquid}} = 1150\text{kg/m}^3 > \rho^{\text{sat}}_{\text{liquid}}$$
$$g^{\text{sat}} > g_{\text{vapor}} > g_{\text{liquid}}$$

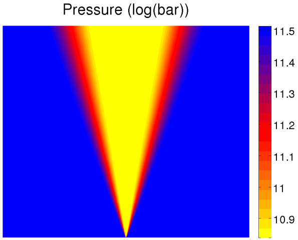
- Outgoing velocity $u = 2\text{m/s}$

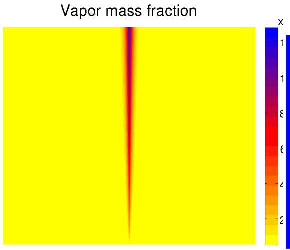


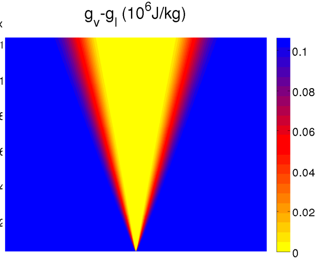
Expansion wave problem: Sample solution





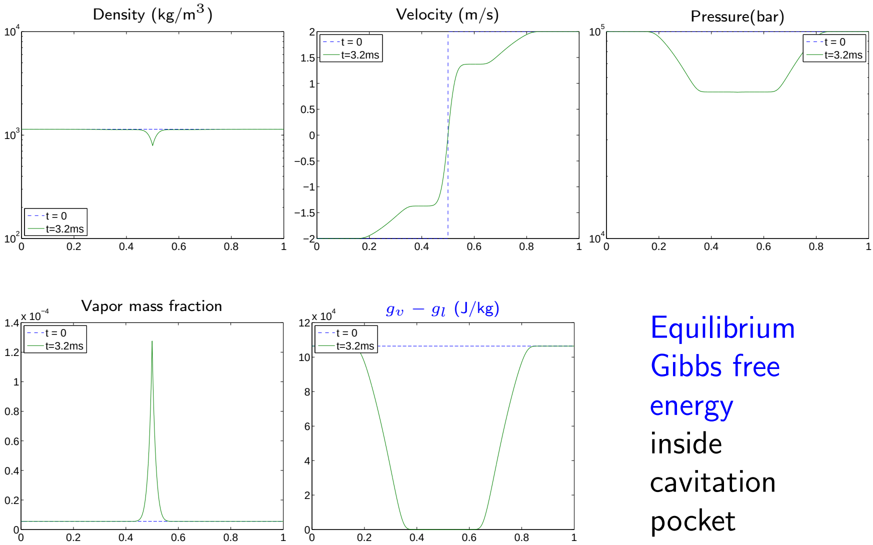






Cavitation pocket formation & mass transfer

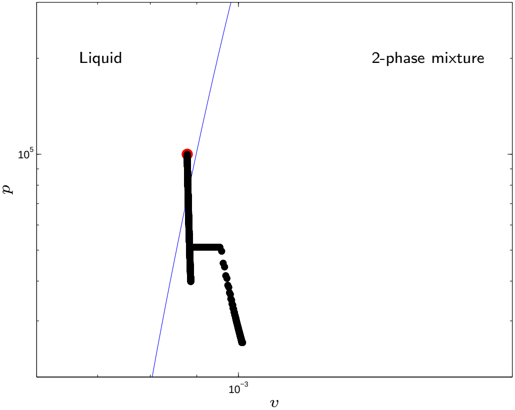
Expansion wave problem: Sample solution



Equilibrium Gibbs free energy inside cavitation pocket

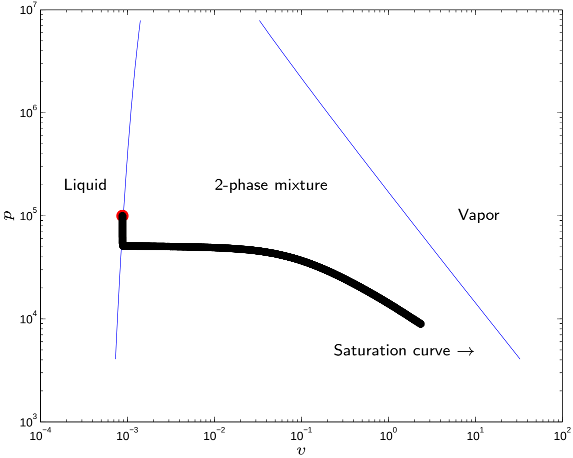
Expansion wave problem: Phase diagram

Solution remains in 2-phase mixture; phase separation has not reached

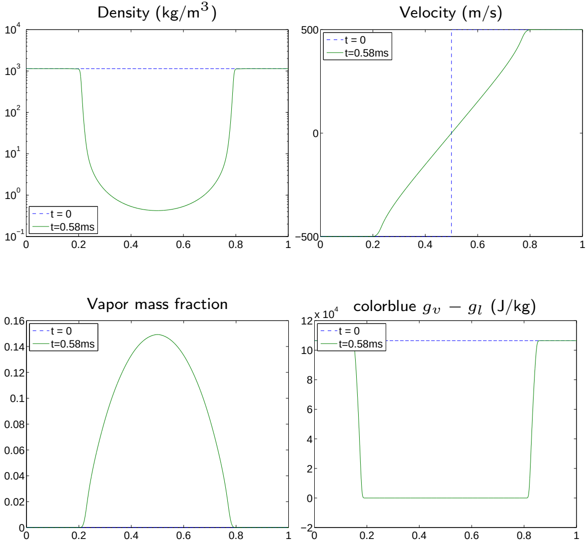


Expansion wave $\vec{u} = 500\text{m/s}$: Phase diagram

With faster $\vec{u} = 500\text{m/s}$, phase separation becomes more evident



Expansion wave $\vec{u} = 500\mathrm{m/s}$: Sample solution



Equilibrium Gibbs free energy inside cavitation pocket

Dodecane 2-phase Riemann problem

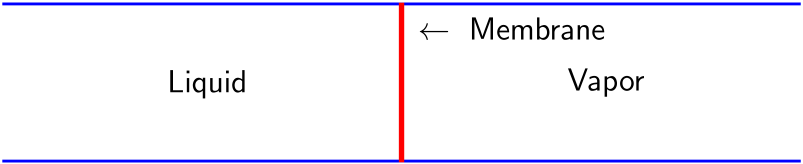
Saurel *et al.* (JFM 2008) & Zein *et al.* (JCP 2010):

- Liquid phase: Left-hand side ($0 \le x \le 0.75$m)

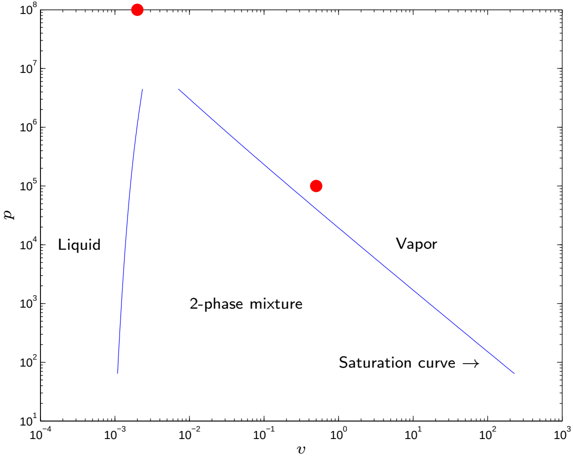
$$(\rho_v, \rho_l, u, p, \alpha_v)_L = \left(2\text{kg/m}^3,\ 500\text{kg/m}^3,\ 0,\ 10^8\text{Pa},\ 10^{-8}\right)$$

- Vapor phase: Right-hand side (0.75m $< x \le 1$m)

$$(\rho_v, \rho_l, u, p, \alpha_v)_R = \left(2\text{kg/m}^3,\ 500\text{kg/m}^3,\ 0,\ 10^5\text{Pa},\ 1 - 10^{-8}\right)$$

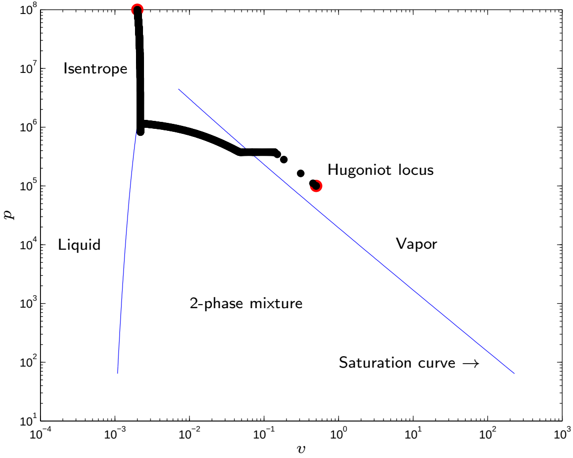


Dodecane 2-phase problem: Phase diagram

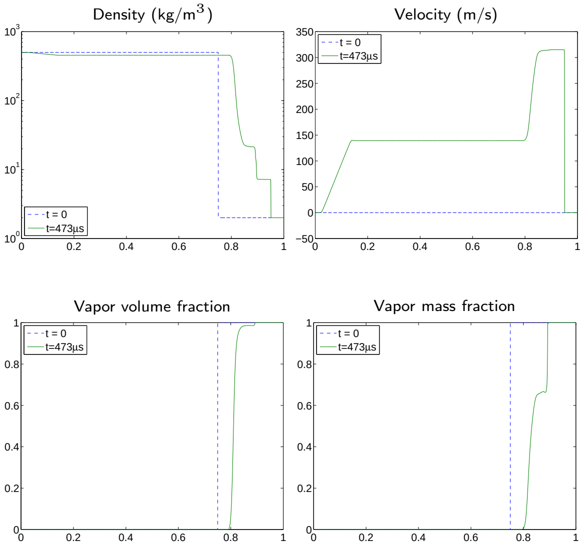


Dodecane 2-phase problem: Phase diagram

Wave path in p-v phase diagram

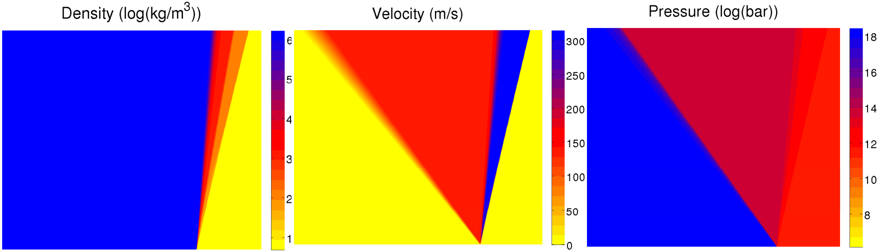


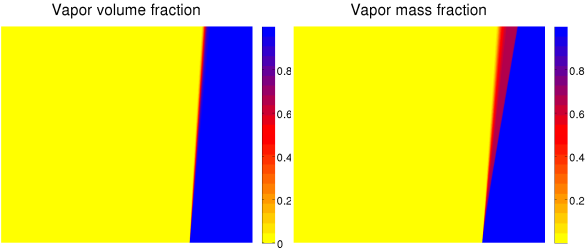
Dodecane 2-phase problem: Sample solution



4-wave structure: Rarefaction, phase, contact, & shock

Dodecane 2-phase problem: Sample solution

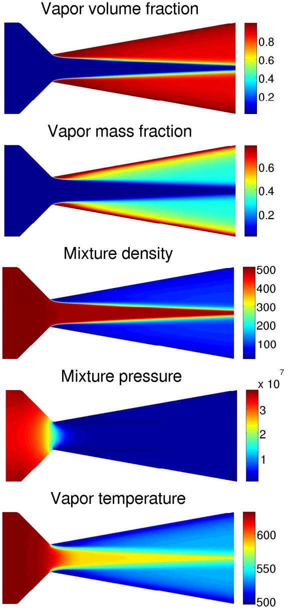




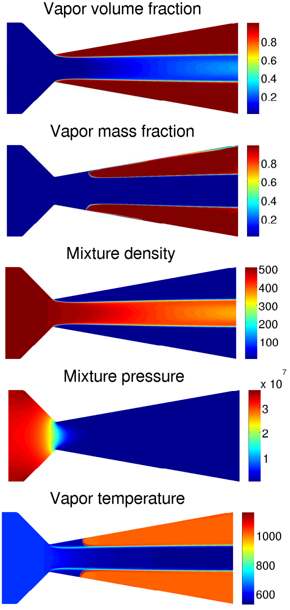
All physical quantities are discon-tinuous across phase boundary

High-pressure fuel injector

With thermo-chemical relaxation



No thermo-chemical relaxation



Thank you