Interface sharpening methods for compressible multiphase flow problems: Overview & look ahead

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Outline

Interface sharpening methods for model systems:

1. Passive tracer transport (motivation)
2. Compressible single-phase flow (inviscid)
3. 5-equation 1-velocity, 1-pressure model for compressible two-phase flow
4. 6-equation 1-velocity, 2-pressure model for compressible two-phase flow
5. Model for compressible two-phase flow with drift-flux approximation

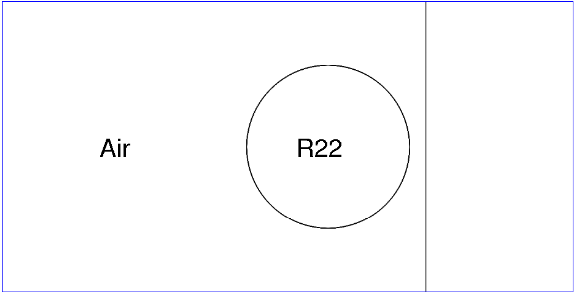
How interface sharpening ?

Higher order method for sharpening interface ?

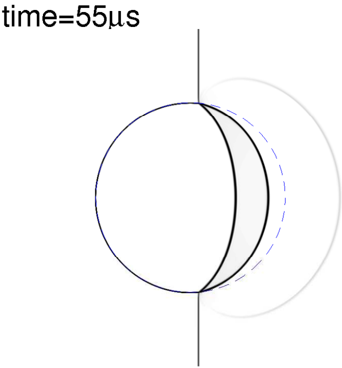
How interface sharpening ?

Higher order method for sharpening interface ?

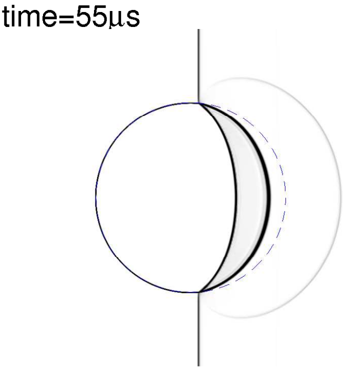
Benchmark test for shock in air & R22 bubble interaction

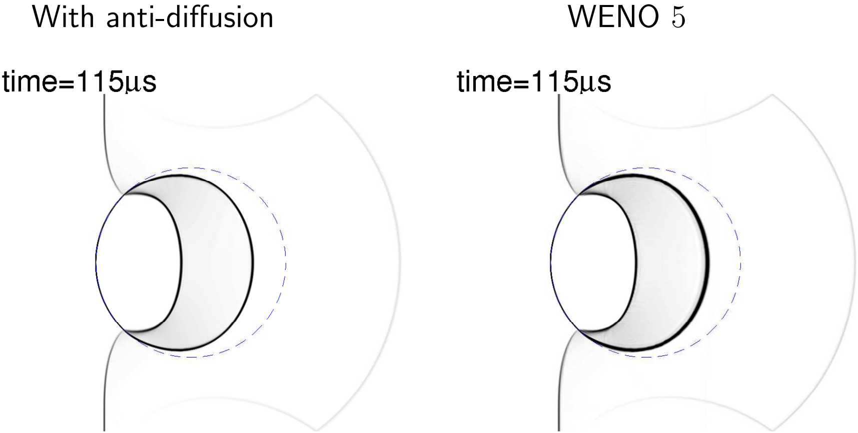


With anti-diffusion

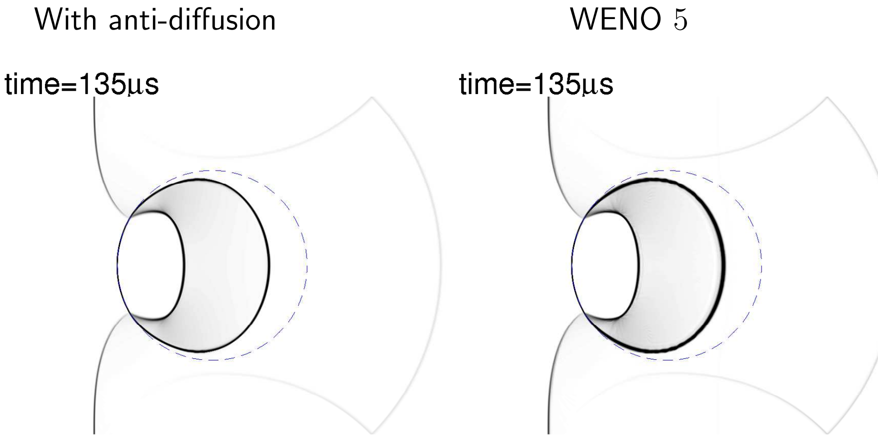


WENO 5

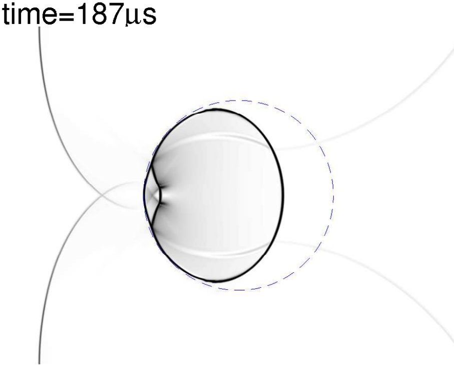




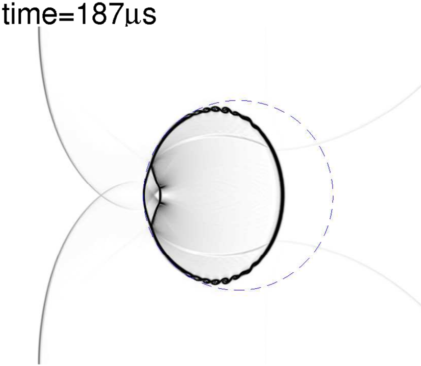
With anti-diffusion
WENO 5
time=115µs
time=115µs


With anti-diffusion
WENO 5
time=135μs
time=135μs

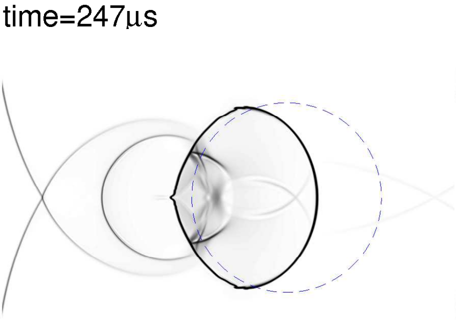
With anti-diffusion



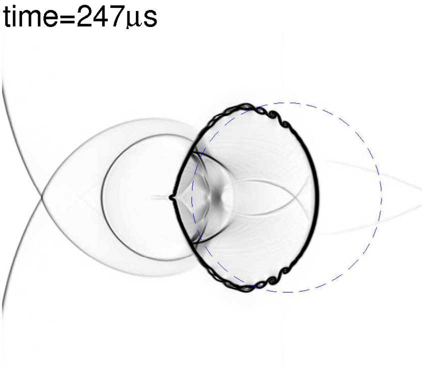
WENO 5



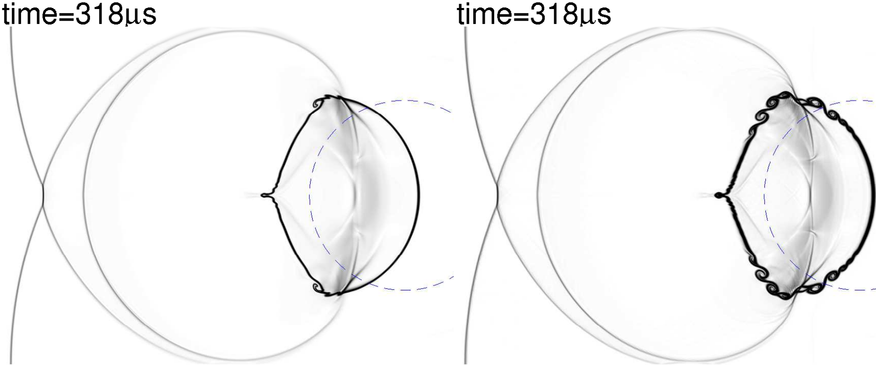
With anti-diffusion



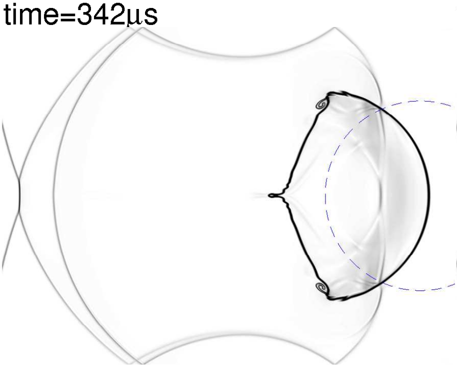
WENO 5



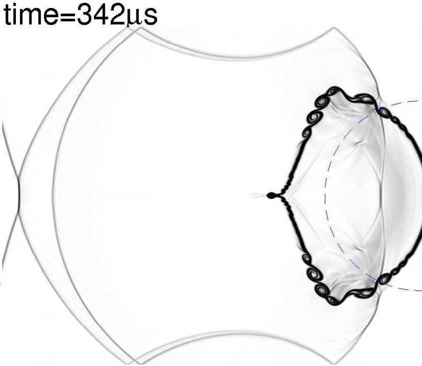
With anti-diffusion | WENO 5



With anti-diffusion

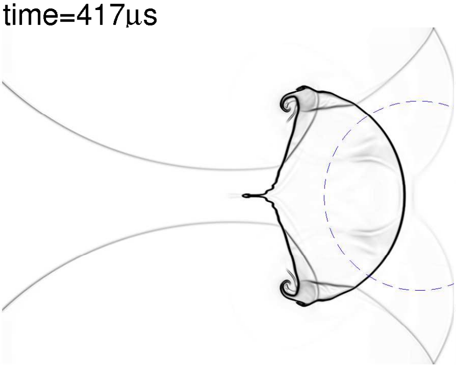


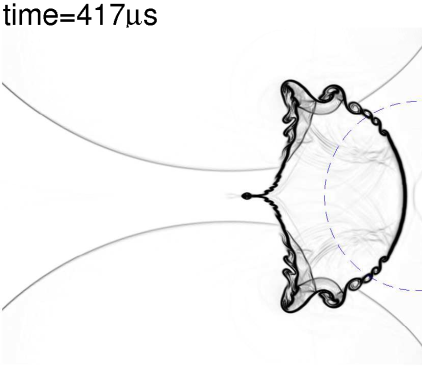
WENO 5



With anti-diffusion

WENO 5

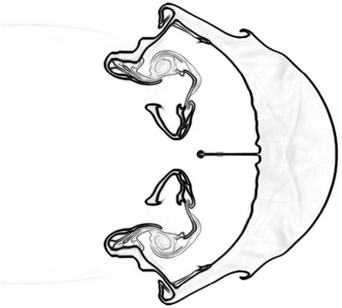




WENO gives more chaotic interface, positivity-preserving in WENO5 with MG EOS (working open issue)

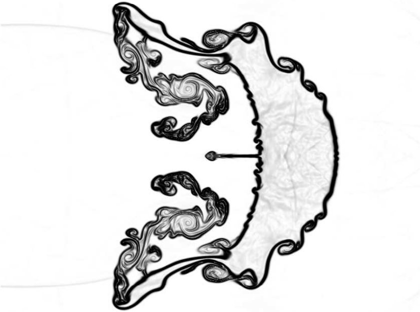
With anti-diffusion

time=1020μs



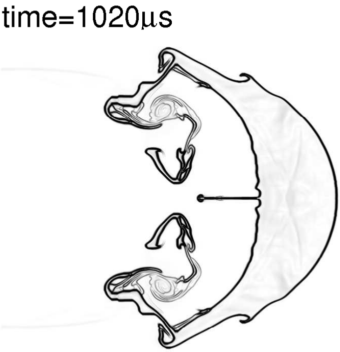
WENO 5

time=1020μs

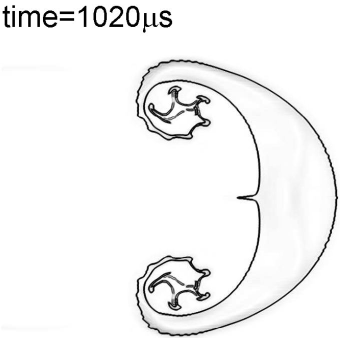


THINC gives more regularized interface

With anti-diffusion

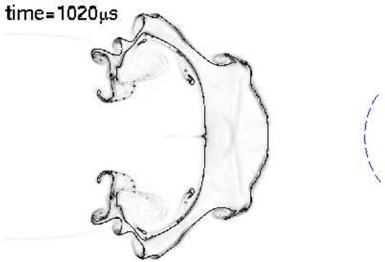


With THINC

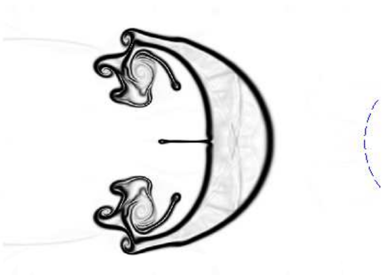


Standard high-resolution method gives poor interface resolution

Volume tracking (Shyue 2006)



2nd order



Shock-contact interaction: Wave speeds diagnosis

Velocity (m/s)	V_s	V_R	V_T	V_{ui}	V_{uf}	V_{di}	V_{df}
Experiment	415	240	540	73	90	78	78
Quirk & Karni	420	254	560	74	90	116	82
Kokh & Lagoutiere	411	243	525	65	86	86	64
Ullah *et al.*	410	246	535	65	86	76	60
Shyue (tracking)	411	243	538	64	87	82	60
Capturing results	410	244	536	65	86	98	76
THINC results	410	244	538	65	86	87	64
Anti-df results	410	244	532	64	85	100	78

Toy problem: Passive tracer transport

Free-surface (or 2-phase) flow modelled by incompressible Navier-Stokes equations read

$$\begin{aligned} \partial_t (\rho \vec{u}) + \mathrm{div} (\rho \vec{u} \otimes \vec{u}) + \nabla p = \nabla \cdot \tau + \rho \vec{g} + \vec{f}_\sigma \\ \partial_t \alpha + \vec{u} \cdot \nabla \alpha = 0 \quad (\text{volume fraction transport}) \\ \mathrm{div}(\vec{u}) = 0 \end{aligned}$$

- Material quantities in 2-phase region determined by

$$z = \alpha z_1 + (1 - \alpha) z_2, \qquad z = \rho,\ \epsilon, \&\ \sigma$$

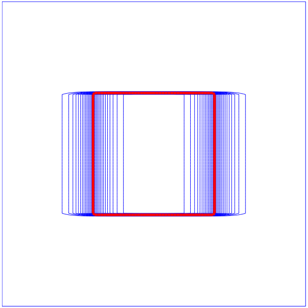
- Source terms are dependent on α also

$$\tau = \epsilon \left(\nabla \vec{u} + \nabla \vec{u}^T \right), \quad \vec{f}_\sigma = -\sigma \kappa \nabla \alpha \quad \text{with } \kappa = \nabla \cdot \left(\frac{\nabla \alpha}{|\nabla \alpha|} \right)$$

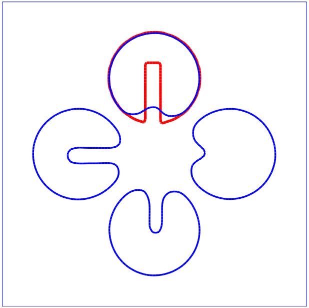
Sharply resolved positivity-preserving α is fundamental

Standard interface capturing results for toy problem, observing poor interface resolution

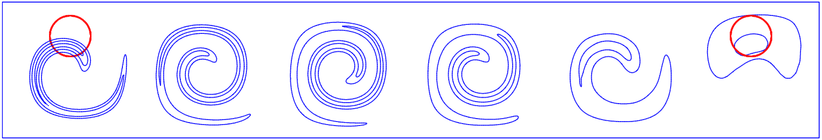
Passive advection



Rotating disc



Vortex in cell



How interface sharpening ? Toy problem

Eulerian interface sharpening methods (*i.e.*, use uniform underlying grid) for volume fraction transport include

1. Differential-based approach
   - Artificial compression: Harten CPAM 1977, Olsson & Kreiss JCP 2005
   - Anti-diffusion: So, Hu & Adams JCP 2011
2. Algebraic-based approach
   - CICSAM (Compressive Interface Capturing Scheme for Arbitrary Meshes): Ubbink & Issa JCP 1999
   - THINC (Tangent of Hyperbola for INterface Capturing): Xiao, Honma & Kono Int. J. Numer. Meth. Fluids 2005

No Lagrangian moving grid or volume tracking cut cells

Differential-based interface sharpening

Use modified volume-fraction transport model as basis

$$\partial_t \alpha + \vec{u} \cdot \nabla \alpha = \frac{1}{\mu_I} \mathcal{D}_\alpha$$

$\mu_I \in \mathbf{R}_+$: free parameter, $\mathcal{D}_\alpha$: interface-sharpening operator

- Compression form (Olsson & Kreiss JCP 2005)

$$\mathcal{D}_\alpha := \nabla \cdot \left[\left(\varepsilon_c \nabla \alpha \cdot \vec{n} - \alpha \left(1 - \alpha \right) \right) \vec{n} \right]$$

$\vec{n} = \nabla \alpha / \|\nabla \alpha\|$, $\varepsilon_c \in \mathbf{R}_+$ (order of mesh size)

- Anti-diffusion form (So, Hu & Adams JCP 2011)

$$\mathcal{D}_\alpha := -\nabla \cdot \left(\varepsilon_d \nabla \alpha \right)$$

$\varepsilon_d \in \mathbf{R}_+^N$ (order of velocity magnitude)

Solution of interface-sharpening model

$$\partial_t \alpha + \vec{u} \cdot \nabla \alpha = \frac{1}{\mu_I} \mathcal{D}_\alpha$$

can be approximated by employing fractional step method

That is, in each time step,

1. Transport step over time step Δt for

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

   by state-of-the-art interface-capturing solver

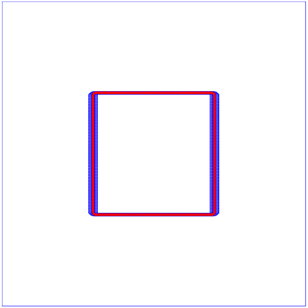
2. Interface-sharpening step over pseudo-time step $\Delta \tau$ for

$$\partial_\tau \alpha = \mathcal{D}_\alpha, \qquad \tau = t/\mu_I$$

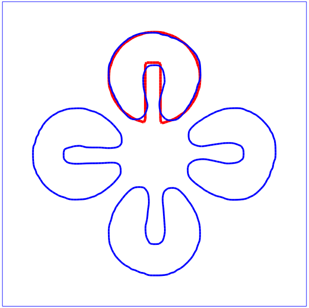
   by explicit finite-difference solver, for example

Passive tracer transport: Anti-diffusion results

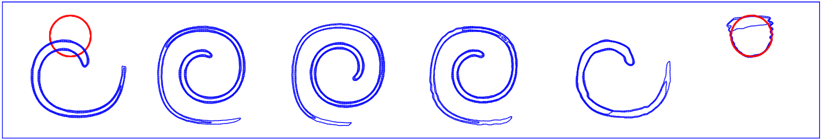
Passive advection



Rotating disc

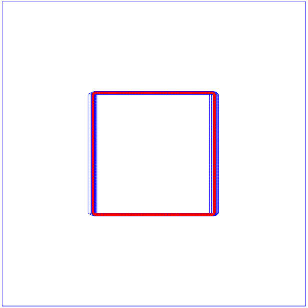


Vortex in cell

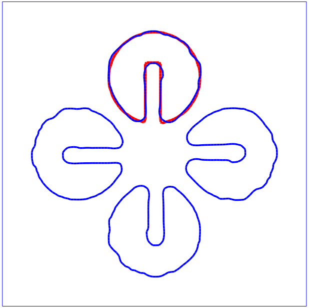


Passive tracer transport: THINC results

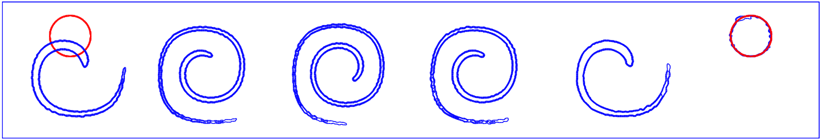
Passive advection



Rotating disc

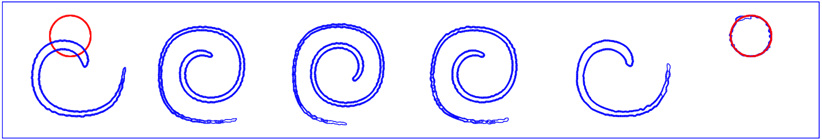


Vortex in cell

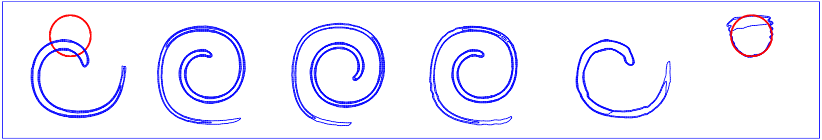


Vortex-in-cell: Comparisons of results

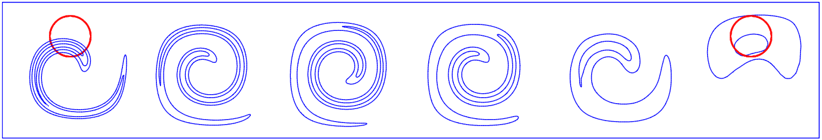
With THINC



With anti-diffusion



Without interface sharpening



THINC-based interface sharpening

In THINC method, original volume-fraction equation

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

is used in each time step as

1. Reconstruct piecewise smooth function $\tilde{\alpha}_i(x, t_n)$ based on THINC reconstruction procedure from cell average $\{\alpha_i^n\}$ at time t_n
2. Construct spatial discretization for $\vec{u} \cdot \alpha$ using interpolated initial data from $\{\tilde{\alpha}_i(x, t_n)\}$ obtained in step 1
3. Employ semi-discrete method to update α^n from current time to next α^{n+1} over time step Δt

THINC reconstruction in step 1 assumes

$$\tilde{\alpha}_i(x) = \alpha_{\min} + \frac{\alpha_{\max} - \alpha_{\min}}{2}\left[1 + \gamma \tanh\left(\beta \frac{x - x_{i-1/2}}{\Delta x} - \bar{x}_i\right)\right]$$

$$\alpha_{\mathcal{M}} = \mathcal{M}\left(\alpha_{i-1}, \alpha_{i+1}\right),\ \mathcal{M} := \min,\ \max,\ \gamma = \mathsf{sgn}\left(\alpha_{i+1} - \alpha_{i-1}\right)$$

β measures sharpeness (given constant) & $\bar{x}_i$ chosen to fulfill

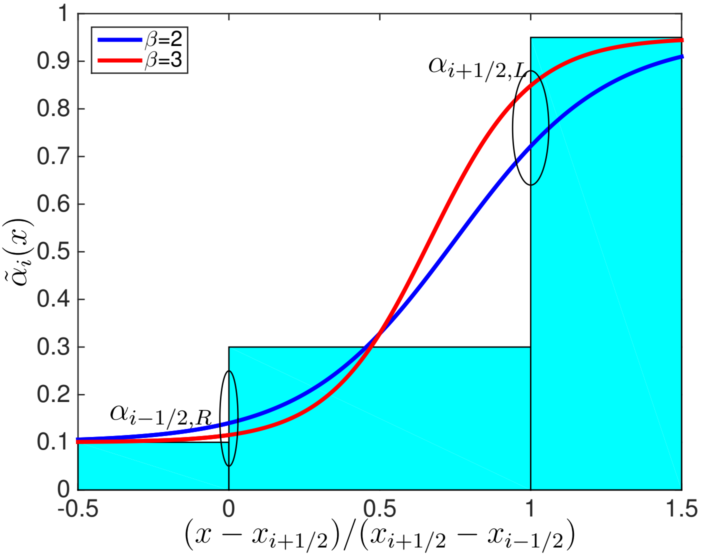
$$\alpha_i = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \tilde{\alpha}_i(x)\, dx$$

For example, cell edges used in step 2 determined by

$$\alpha_{i+1/2,L} = \alpha_{\min} + \frac{\alpha_{\max} - \alpha_{\min}}{2}\left(1 + \gamma \frac{\tanh\beta + C}{1 + C\tanh\beta}\right)$$

$$\alpha_{i-1/2,R} = \alpha_{\min} + \frac{\alpha_{\max} - \alpha_{\min}}{2}\left(1 + \gamma C\right) \qquad (C \text{ not shown})$$

THINC reconstruction: Graphical view



Passive tracer transport: Convergence study

Convergence study of 1-norm errors $\mathcal{E}_1(\alpha)$ as mesh is refined; results for passive advection are shown only

	With THINC		No sharpening		With anti-diffu	
$N \times N$	$\mathcal{E}_1(\alpha)$	Order	$\mathcal{E}_1(\alpha)$	Order	$\mathcal{E}_1(\alpha)$	Order
50×50	9.8840	NaN	91.7486	NaN	4.0436	NaN
100×100	5.1746	0.93	60.6698	0.60	2.0558	0.98
200×200	2.6455	0.97	39.3623	0.62	0.9921	1.05
400×400	1.3373	0.98	25.2699	0.64	0.4414	1.17

Passive tracer transport: CPU timing study

CPU timing in seconds for Passive tracer transport problems (run on HP xw 9400 with AMD Dural-Core Opteron)

Method/Problem	Passive advec.	Rotating disk	Vortex in cell
With THINC	20.5	21.8	280.7
With anti-df	32.1	29.4	383.5
No sharpening	33.2	28.8	344.9
Grid	100×100	100×100	200×200

This validates THINC & anti-diffusion schemes for passive tracer transport

Toy problem: Summary & remarks

1. Anti-diffusion interface sharpening
   - Employed as post-processing step
   - Diffusion coefficient ε_d & parameter μ_I controls interface sharpeness

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   - Parameter β controls interface sharpeness

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   - Employed as pre-processing step
   - Parameter β controls interface sharpeness
3. Hybrid anti-diffusion-THINC is feasible
4. For problems with more than 2 fluid components, interface sharpening based on anti-diffusion appears to be more robust than THINC

Compressible 1-phase flow (inviscid)

Assume inviscid, non-heat conducting, 1-phase, compressible flow in Cartesian coordinates:

$$\partial_t q + \sum_{j=1}^{N} \partial_{x_j} f_j(q) = 0$$

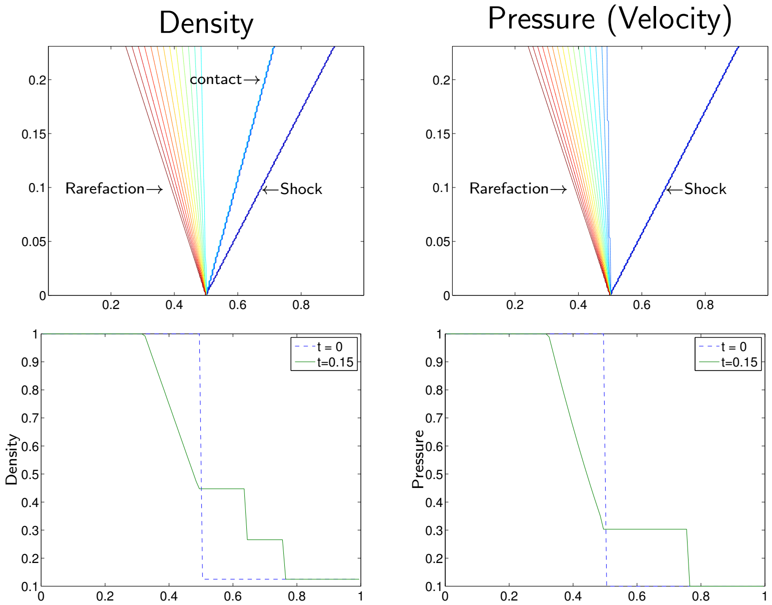
with q & f_j, $j = 1, 2, \ldots, N$, defined by

$$q = (\rho, \rho u_1, \ldots, \rho u_N, E)^T$$
$$f_j = (\rho u_j, \rho u_1 u_j + p\delta_{j1}, \ldots, \rho u_N u_j + p\delta_{jN}, E u_j + p u_j)^T$$

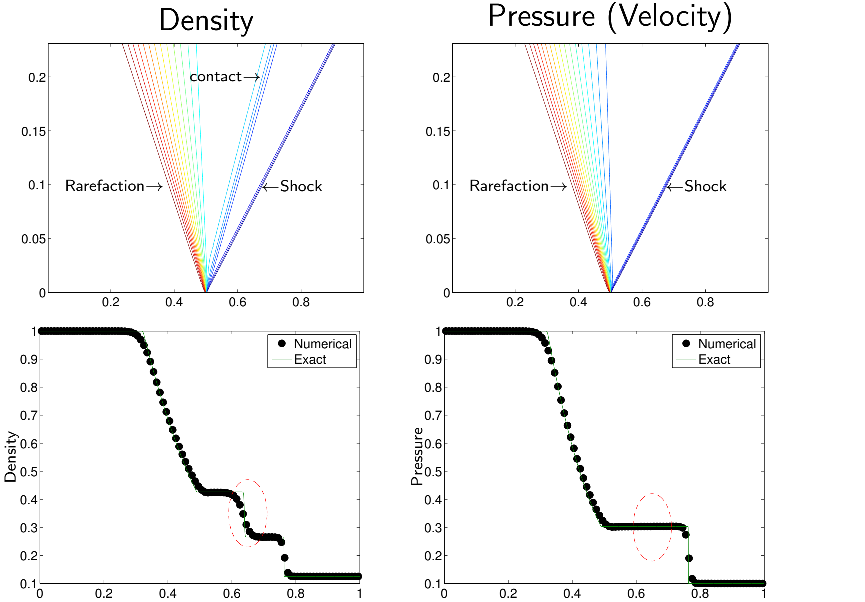
Assume Mie-Grüneisen equation of state

$$p(\rho, e) = p_\infty(\rho) + \Gamma(\rho)\rho\,[e - e_\infty(\rho)]$$

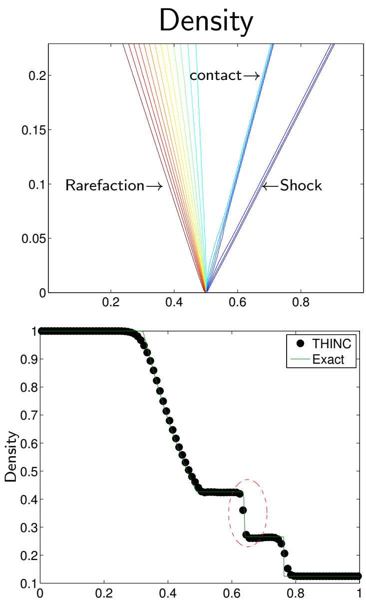
Sod Riemann problem: Exact solution



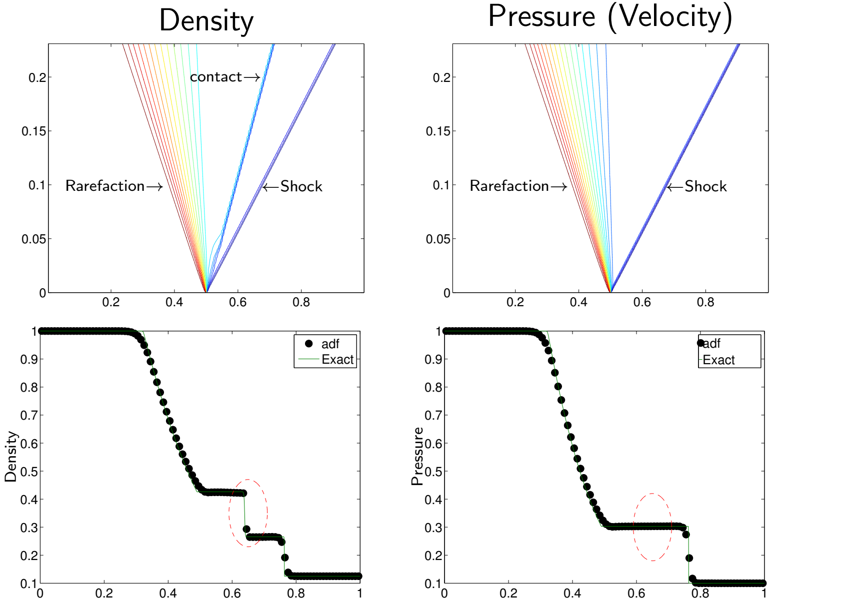
Sod Riemann problem: Interface capturing solution



Sod Riemann problem: THINC solution



Sod Riemann problem: Anti-diffusion solution



How interface sharpening ? Compressible flow

Novel elements (as compared to toy problem for incompressible flow):

1. Robust local interface indicator
   - Physical principles based
     i.e., Flag interface cells by checking jumps of physical quantities nearby (good in $1D$, less effective in $2D$)
   - Tracer transport based
     i.e., Flag interface cells based on classical volume-fraction approach (more effective in $2D$)
2. Consistent interface solution reconstruction (algebraic-based) or post-sharpening (differential-based) to ρ, $\rho\vec{u}$, E, $\cdots$

Interface reconstruction: Compressible 1-phase flow

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

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

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

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

1. Density ρ is reconstructed by basic THINC scheme
2. Momentum $\rho \vec{u}$ is reconstructed by $\vec{u}$ times density in part 1 (see second equation)
3. Total energy E is reconstructed by corrections on total kinetic & internal energy (see third equation)

THINC interface sharpening: Compressible flow

In each time step, our THINC-based interface-sharpening algorithm for compressible flow consists:

1. Reconstruct piecewise polynomial $\tilde{q}_i(x, t_n)$ based on MUSCL/WENO reconstruction procedure from cell average $\{Q^n\}$ at time t_n
2. Modify $\tilde{q}_i(x, t_n)$ for interface cells using variant of THINC scheme from Q^n
3. Construct spatial discretization using interpolated initial data from $\{\tilde{q}_i(x, t_n)\}$ obtained in steps 1 & 2
4. Employ semi-discrete method to update Q^n from current time to next Q^{n+1} over time step Δt

Anti-diffusion: Compressible flow

Anti-diffusion model for compressible 1-phase flow is

$$\partial_t \rho + \mathsf{div}\,(\rho \vec{u}) = \frac{1}{\mu_I} \mathcal{D}_\rho$$

$$\partial_t\,(\rho \vec{u}) + \mathsf{div}\,(\rho \vec{u} \otimes u) + \nabla p = \frac{1}{\mu_I} \mathcal{D}_{\rho \vec{u}}$$

$$\partial_t E + \mathsf{div}\,(E \vec{u} + p \vec{u}) = \frac{1}{\mu_I} \mathcal{D}_E$$

$$\mathcal{D}_\rho := -H_I \nabla \cdot (\varepsilon_d \nabla \rho)$$

$$\mathcal{D}_{\rho u} := u\,\mathcal{D}_\rho, \qquad \mathcal{D}_E := \left[\frac{u \cdot u}{2} + \partial_\rho(\rho e)\right] \mathcal{D}_\rho$$

H_I : Interface indicator $= \begin{cases} 1 & \text{if interface cell,} \\ 0 & \text{otherwise} \end{cases}$

Anti-diffusion method

Anti-diffusion model in compact form

$$\partial_t q + \mathsf{div} f(q) = \frac{1}{\mu_I} \mathcal{D}_q$$

with q, f, & $\mathcal{D}_q$ defined from Euler equations accordingly

In each time step, fractional step is used

1. Solve homogeneous equation without source terms

   $$\partial_t q + \mathsf{div} f(q) = 0$$

   by state-of-the-art solver

2. Interface-sharpening step over pseudo-time

   $$\partial_\tau q = \mathcal{D}_\alpha, \qquad \tau = t/\mu_I$$

   by explicit solver, for example

Compressible 2-phase flow: 7-equation model

7-equation non-equilibrium model of Baer & Nunziato (1986)

$$\partial_t (\alpha\rho)_1 + \text{div}\,(\alpha\rho\vec{u})_1 = 0$$

$$\partial_t (\alpha\rho\vec{u})_1 + \text{div}\,(\alpha\rho\vec{u}\otimes\vec{u})_1 + \nabla(\alpha p)_1 = p_I\nabla\alpha_1 + \lambda\,(\vec{u}_2 - \vec{u}_1)$$

$$\partial_t (\alpha E)_1 + \text{div}\,(\alpha E\vec{u} + \alpha p\vec{u})_1 = p_I\vec{u}_I\cdot\nabla\alpha_1 - \nu p_I\,(p_1 - p_2) + \lambda\vec{u}_I\cdot(\vec{u}_2 - \vec{u}_1)$$

$$\partial_t (\alpha\rho)_2 + \text{div}\,(\alpha\rho\vec{u})_2 = 0$$

$$\partial_t (\alpha\rho\vec{u})_2 + \text{div}\,(\alpha\rho\vec{u}\otimes\vec{u})_2 + \nabla(\alpha p)_2 = -p_I\nabla\alpha_1 - \lambda\,(\vec{u}_2 - \vec{u}_1)$$

$$\partial_t (\alpha E)_2 + \text{div}\,(\alpha E\vec{u} + \alpha p\vec{u})_2 = -p_I\vec{u}_I\cdot\nabla\alpha_1 + \nu p_I\,(p_1 - p_2) - \lambda\vec{u}_I\cdot(\vec{u}_2 - \vec{u}_1)$$

$$\partial_t\alpha_1 + \vec{u}_I\cdot\nabla\alpha_1 = \nu\,(p_1 - p_2)$$

Saturation condition $\alpha_1 + \alpha_2 = 1$

Equation of state $p_k(\rho_k, e_k)$, $k = 1, 2$

p_I & $\vec{u}_I$: interfacial pressure & velocity

- Baer & Nunziato (1986): $p_I = p_2, \quad \vec{u}_I = \vec{u}_1$
- Saurel & Abgrall (JCP 1999, JCP 2003)

$$p_I = \alpha_1 p_1 + \alpha_2 p_2, \quad \vec{u}_I = \frac{\alpha_1\rho_1\vec{u}_1 + \alpha_2\rho_2\vec{u}_2}{\alpha_1\rho_1 + \alpha_2\rho_2}$$

$$p_I = \frac{p_1/Z_1 + p_2/Z_2}{1/Z_1 + 1/Z_2}, \quad \vec{u}_I = \frac{\vec{u}_1 Z_1 + \vec{u}_2 Z_2}{Z_1 + Z_2}, \quad Z_k = \rho_k c_k$$

$$\nu = \frac{S_I}{Z_1 + Z_2}, \quad \lambda = \frac{S_I Z_1 Z_2}{Z_1 + Z_2}, \quad S_I(\text{Interfacial area})$$

ν & λ: relaxation parameters that express rates at which pressure & velocity toward equilibrium respectively

This non-equilibrium model can be used to simulate

1. Mixtures with different phasic pressures, velocities, temperatures

2. Material interfaces

3. Permeable interfaces (*i.e.*, interfaces separating a cloud of dispersed phases such as liquid drops or gases)

4. Cavitation if it is modeled as a simplified mechanical relaxation process, occurring at infinite rate $\mu \to \infty$ & not modeled as a mass transfer process

Reduced 5-equation model

Kapila *et al.* 2001, Murrone *et al.* 2005, & Saurel *et al.* 2008 showed in asymptotic limits of λ & $\nu \to \infty$ *i.e.*, flow towards mechanical equilibrium: $\vec{u}_1 = \vec{u}_2 = \vec{u}$ & $p_1 = p_2 = p$, 7-equation model reduces to 5-equation model

$$\partial_t \left(\alpha_1 \rho_1\right) + \mathrm{div}\left(\alpha_1 \rho_1 \vec{u}\right) = 0$$

$$\partial_t \left(\alpha_2 \rho_2\right) + \mathrm{div}\left(\alpha_2 \rho_2 \vec{u}\right) = 0$$

$$\partial_t \left(\rho \vec{u}\right) + \mathrm{div}\left(\rho \vec{u} \otimes \vec{u}\right) + \nabla p = 0$$

$$\partial_t E + \mathrm{div}\left(E \vec{u} + p \vec{u}\right) = 0$$

$$\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \left(\frac{K_2 - K_1}{K_1/\alpha_1 + K_2/\alpha_2}\right) \mathrm{div}(\vec{u}), \qquad K_i = \rho_i c_i^2$$

Reduced 5-equation model

Kapila *et al.* 2001, Murrone *et al.* 2005, & Saurel *et al.* 2008 showed in asymptotic limits of λ & $\nu \to \infty$ *i.e.*, flow towards mechanical equilibrium: $\vec{u}_1 = \vec{u}_2 = \vec{u}$ & $p_1 = p_2 = p$, 7-equation model reduces to 5-equation model

$$\partial_t (\alpha_1 \rho_1) + \operatorname{div}(\alpha_1 \rho_1 \vec{u}) = 0$$
$$\partial_t (\alpha_2 \rho_2) + \operatorname{div}(\alpha_2 \rho_2 \vec{u}) = 0$$
$$\partial_t (\rho \vec{u}) + \operatorname{div}(\rho \vec{u} \otimes \vec{u}) + \nabla p = 0$$
$$\partial_t E + \operatorname{div}(E\vec{u} + p\vec{u}) = 0$$
$$\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \left(\frac{K_2 - K_1}{K_1/\alpha_1 + K_2/\alpha_2} \right) \operatorname{div}(\vec{u}), \qquad K_i = \rho_i c_i^2$$

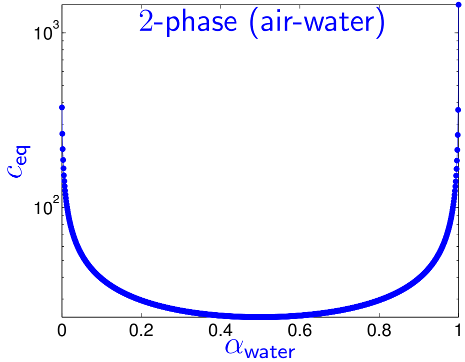
Equilibrium (mixture) pressure p satisfies

$$p = \left(\rho e - \sum_{k=1}^{2} \alpha_k \rho_k e_{\infty,k}(\rho_k) + \sum_{k=1}^{2} \alpha_k \frac{p_{\infty,k}(\rho_k)}{\Gamma_k(\rho_k)} \right) \Big/ \sum_{k=1}^{2} \frac{\alpha_k}{\Gamma_k(\rho_k)}$$

Reduced 5-equation model is hyperbolic with non-monotonic equilibrium sound speed c_{eq}:

$$\frac{1}{\rho c_{\text{eq}}^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2} \qquad \text{(Wood's formula)}$$

yielding stiffness in equations & numerical solver



5-equation transport model

For nearly single-phase flow, where $\alpha_1 \approx 0$ or 1, Allaire, Clerc, & Kokh (JCP 2002) proposed using

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

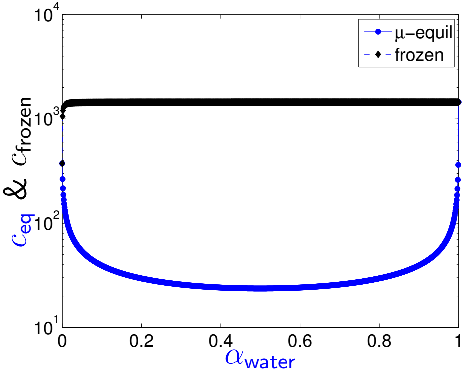
Mixture pressure p computed in same manner as before

Phasic entropy $\mathcal{S}_k$ satisfies relation

$$\left(\frac{\partial p_1}{\partial \mathcal{S}_1}\right)_{\rho_1}\frac{D\mathcal{S}_1}{Dt} - \left(\frac{\partial p_2}{\partial \mathcal{S}_2}\right)_{\rho_2}\frac{D\mathcal{S}_2}{Dt} = \left(\rho_1 c_1^2 - \rho_2 c_2^2\right)\mathsf{div}(\vec{u}) \neq 0$$

Model is hyperbolic, but with monotone frozen sound speed

$$\rho c_{\text{frozen}}^2 = \sum_{k=1}^{2} \alpha_k \rho_k c_k^2$$



Interface reconstruction: 5-equation model

Assume equilibrium pressure p, velocity $\vec{u}$, & phasic density ρ_k for each interface cell

1. Volume fraction α_1 is reconstructed by basic THINC scheme, denoted by $\tilde{\alpha}_1$
2. Reconstruct phasic & mixture density $\alpha_i \rho_i$ & ρ by
$$\widetilde{\alpha_i \rho_i} = \tilde{\alpha}_i \rho_i, \quad i = 1, 2, \quad \tilde{\rho} = \tilde{\alpha}_1 \rho_1 + (1 - \tilde{\alpha}_1) \rho_2$$
3. Reconstruct momentum $\rho \vec{u}$ by
$$\widetilde{\rho \vec{u}} = \tilde{\rho} \vec{u}$$
4. Reconstruct total energy E by
$$\tilde{E} = \frac{1}{2} \tilde{\rho} \vec{u} \cdot \vec{u} + \tilde{\alpha}_1 \rho_1 e_1 + (1 - \tilde{\alpha}_1) \rho_2 e_2$$

5-equation transport model: Anti-diffusion

5-equation transport model with anti-diffusion

$$\partial_t (\alpha_1 \rho_1) + \mathsf{div} (\alpha_1 \rho_1 \vec{u}) = \frac{1}{\mu_I} \mathcal{D}_{\alpha_1 \rho_1}$$

$$\partial_t (\alpha_2 \rho_2) + \mathsf{div} (\alpha_2 \rho_2 \vec{u}) = \frac{1}{\mu_I} \mathcal{D}_{\alpha_2 \rho_2}$$

$$\partial_t (\rho u) + \mathsf{div} (\rho \vec{u} \otimes \vec{u}) + \nabla p = \frac{1}{\mu_I} \mathcal{D}_{\rho u}$$

$$\partial_t E + \mathsf{div} (E \vec{u} + p \vec{u}) = \frac{1}{\mu_I} \mathcal{D}_E$$

$$\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \frac{1}{\mu_I} \mathcal{D}_{\alpha_1}$$

Exist two ways to set $\mathcal{D}_z$, $z = \alpha_1 \rho_1, \ldots, \alpha_1$, in literature

1. α-ρ based (Shyue 2011)

$$\mathcal{D}_{\alpha_1} := -\nabla \cdot (\varepsilon_d \nabla \alpha_1), \quad \mathcal{D}_{\alpha_k \rho_k} := -H_I \nabla \cdot (\varepsilon_d \nabla \alpha_k \rho_k)$$

$$\mathcal{D}_\rho := \sum_{k=1}^{2} \mathcal{D}_{\alpha_k \rho_k}, \quad \mathcal{D}_{\rho \vec{u}} := \vec{u} \mathcal{D}_\rho, \quad K = \frac{1}{2} \vec{u} \cdot \vec{u}$$

$$\mathcal{D}_E := K \mathcal{D}_\rho + \sum_{k=1}^{2} \partial_{\alpha_k \rho_k} (\rho_k e_k) \mathcal{D}_{\alpha_k \rho_k} + \sum_{k=1}^{2} \rho_k e_k \mathcal{D}_{\alpha_k}$$

2. α-based only (So, Hu, & Adams JCP 2012)

$$\mathcal{D}_{\alpha_1} := -\nabla \cdot (\varepsilon_d \nabla \alpha_1), \quad \mathcal{D}_{\alpha_k \rho_k} := \rho_k \mathcal{D}_{\alpha_k}, \quad \mathcal{D}_{\alpha_2} := -\mathcal{D}_{\alpha_1}$$

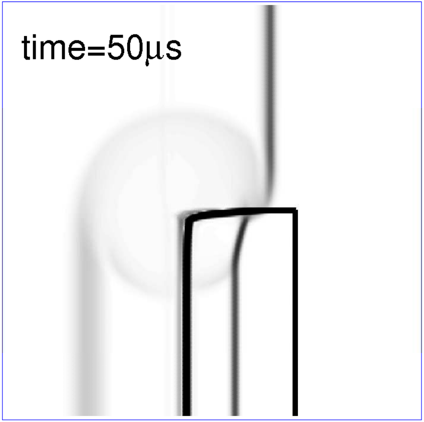
$$\mathcal{D}_\rho := \sum_{k=1}^{2} \mathcal{D}_{\alpha_k \rho_k}, \ \mathcal{D}_{\rho \vec{u}} := \vec{u} \mathcal{D}_\rho, \ \mathcal{D}_E := K \mathcal{D}_\rho + \sum_{k=1}^{2} \rho_k e_k \mathcal{D}_{\alpha_k}$$

$\mathcal{D}_{\alpha_1} := \nabla \cdot \left[\left(\varepsilon_c \nabla \alpha_1 \cdot \vec{n} - \alpha_1 \left(1 - \alpha_1 \right) \right) \vec{n} \right]$ applicable

Shock(morb)-contact(moly) interaction

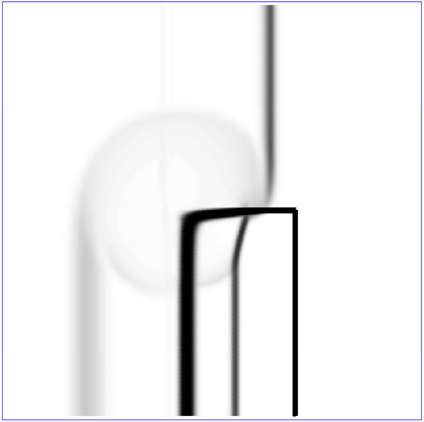
With THINC

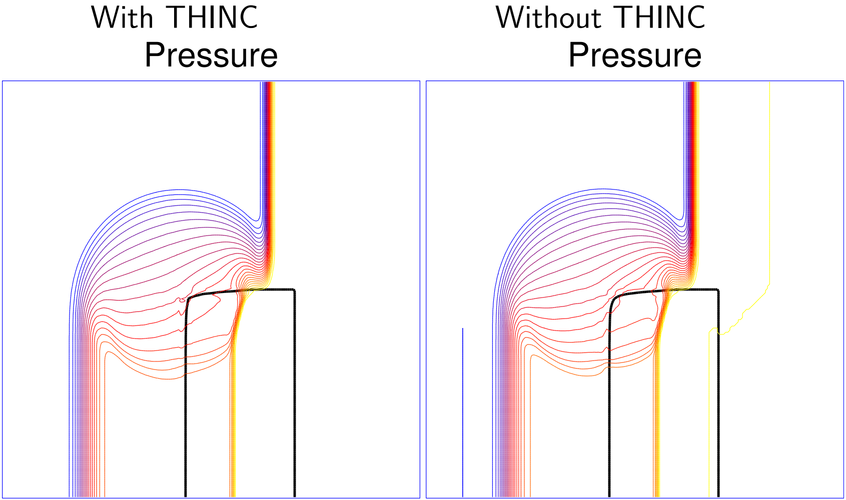
Density



Without THINC

Density

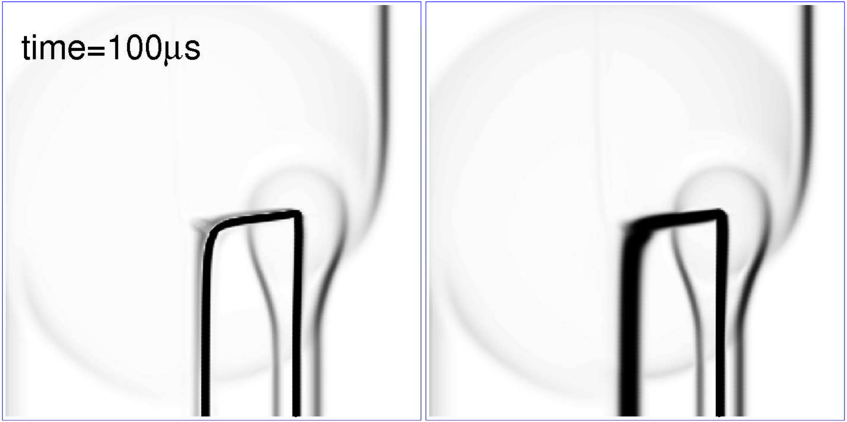


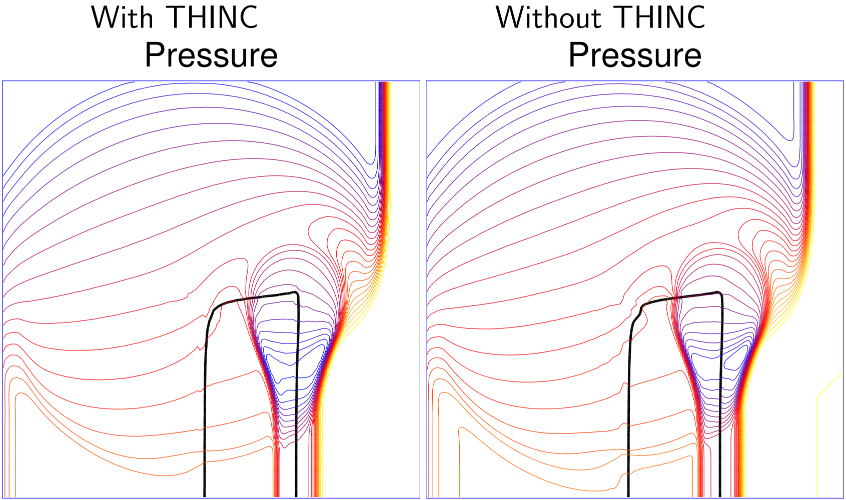


With THINC
Pressure
Without THINC
Pressure

With THINC
Density

Without THINC
Density





With THINC
Pressure
Without THINC
Pressure

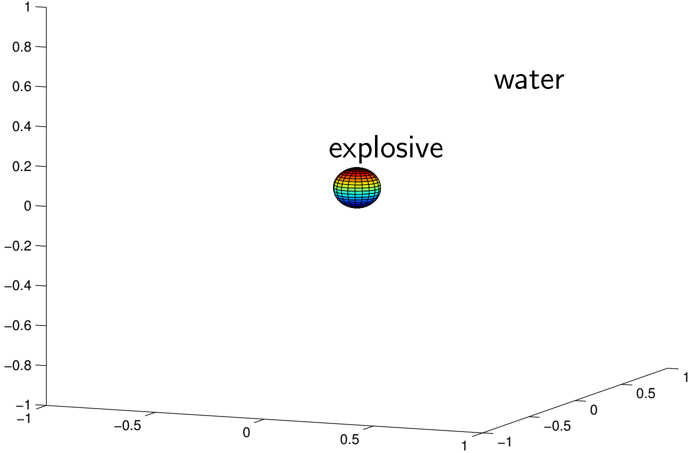
5-equation model: Axisymmetric case

Axisymmetric version of reduced 5-equation model reads

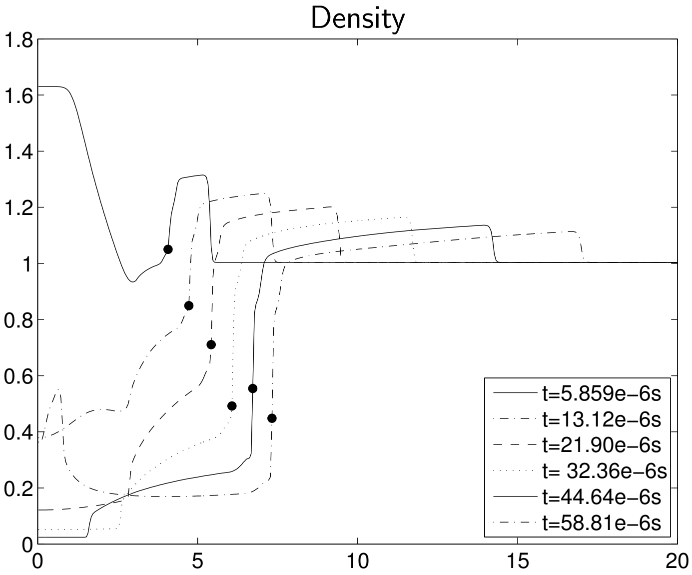
$$
\begin{aligned}
&\partial_t \left(A(x)\alpha_1\rho_1\right) + \partial_x \left(A(x)\alpha_1\rho_1 u\right) = 0 \\
&\partial_t \left(A(x)\alpha_2\rho_2\right) + \partial_x \left(A(x)\alpha_2\rho_2 u\right) = 0 \\
&\partial_t \left(A(x)\rho u\right) + \partial_x \left(A(x)\rho u^2\right) + A(x)\partial_x p = 0 \\
&\partial_t \left(A(x)E\right) + \partial_x \left(A(x)Eu + A(x)pu\right) = 0 \\
&\partial_t \alpha_1 + \partial_x \left(\alpha_1 u\right) = \frac{\alpha_1 \bar{K}}{K_1}\partial_x u + \left(\frac{\alpha_1 \bar{K}}{K_1} - \alpha_1\right)\frac{A'(x)}{A(x)}\partial_x u
\end{aligned}
$$

where $1/\bar{K} = \sum_{i=1}^{2} \alpha_i / K_i, \quad K_i = \rho_i c_i^2$

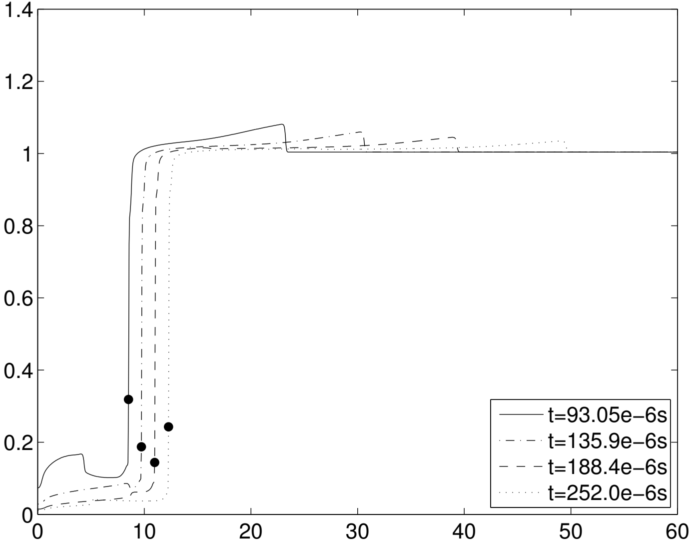
Spherical UNDEX (Wardlaw)



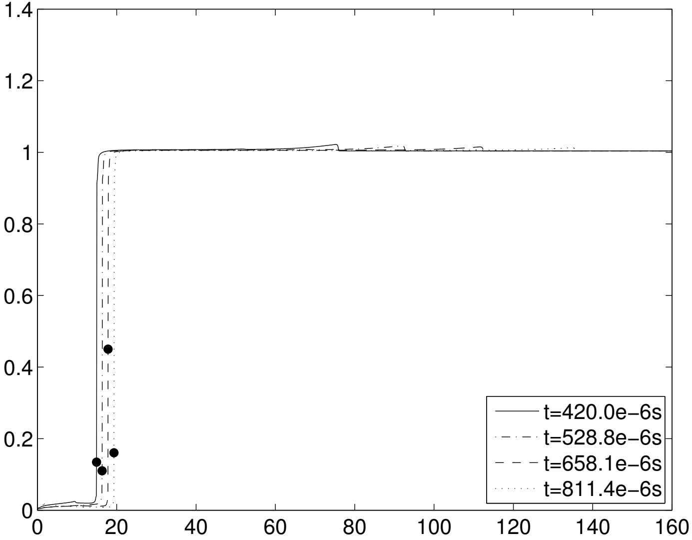
Spherical UNDEX: Initial phase



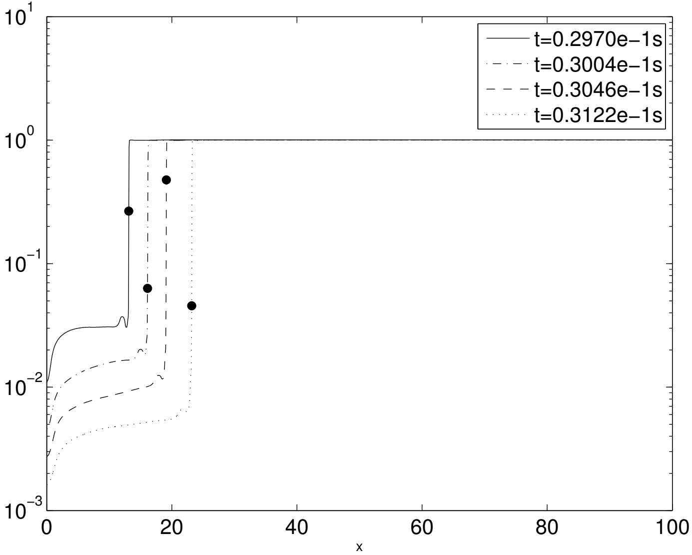
Spherical UNDEX: Shock-contact interaction phase



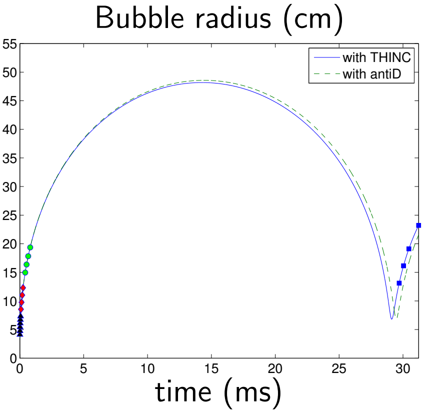
Spherical UNDEX: Incompressible phase

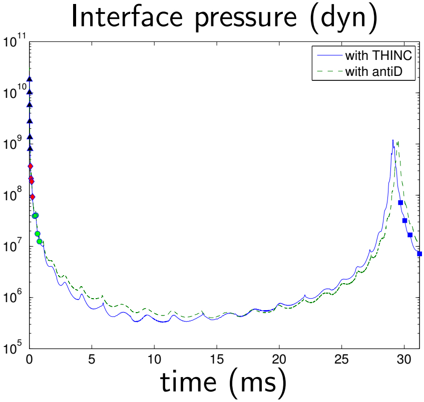


Spherical UNDEX: bubble collapse & rebound



Spherical UNDEX test: Diagnosis





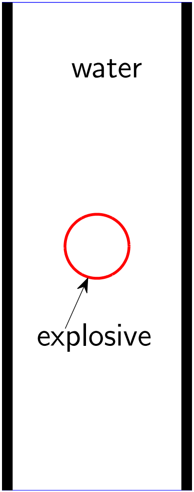
Spherical UNDEX test: Diagnosis

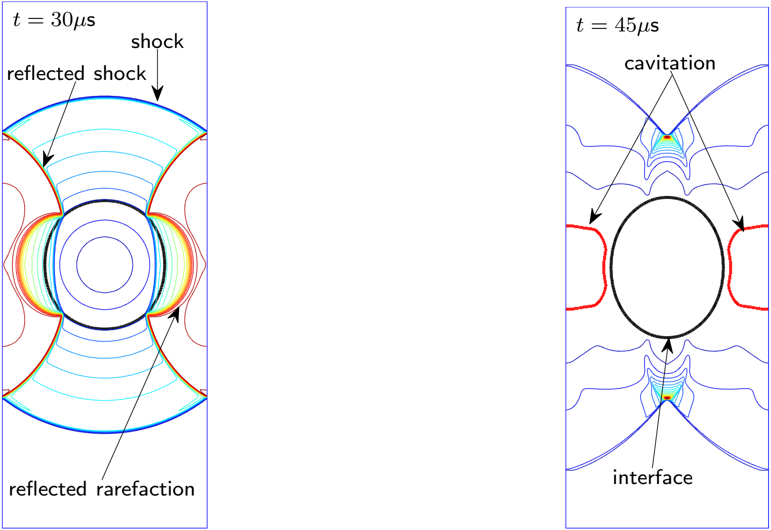
Table: Quantitative study of maximum bubble radius $r_{\max}$ & period of bubble oscillation T_b for spherical underwater explosion

	$r_{\max}$(cm)	error (%)	T_b(ms)	error (%)
Experiment	48.10	0	29.8	0
Incompressible	66.49	38.2	39.1	31.2
Luo *et al.*	48.75	1.4	29.7	0.3
Wardlaw	46.40	3.5	29.8	0
THINC	48.17	0.1	29.1	2.3
Anti-diffusion	48.57	0.1	29.5	1.1

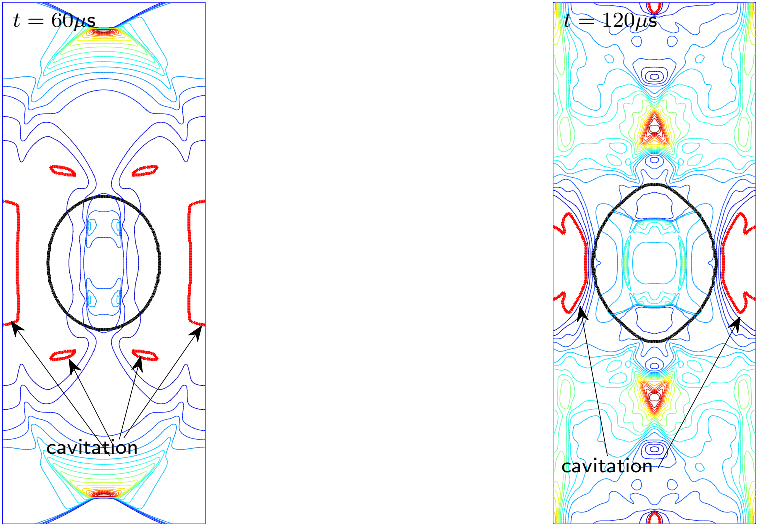
Underwater explosions: cylindrical wall

High pressure gaseous explosive in water (cylindrical case)

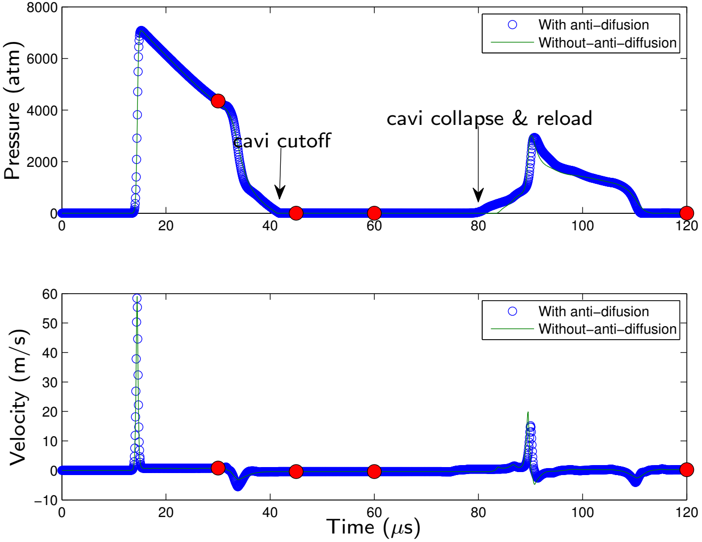




$t = 30\mu$s
shock
reflected shock
reflected rarefaction
$t = 45\mu$s
cavitation
interface



$t = 60\mu s$
cavitation
$t = 120\mu s$
cavitation



Pressure (atm)
With anti−difusion
Without−anti−diffusion
cavi cutoff
cavi collapse & reload
8000
6000
4000
2000
0
0
20
40
60
80
100
120
Velocity (m/s)
With anti−difusion
Without−anti−diffusion
60
50
40
30
20
10
0
−10
0
20
40
60
80
100
120
Time (μs)

6-equation model: Alternative to 5-equation model

Non-equilibrium 6-equation model of Saurel *et al.* (JCP 2009):

$$\partial_t (\alpha_1 \rho_1) + \text{div}(\alpha_1 \rho_1 \vec{u}) = 0$$
$$\partial_t (\alpha_2 \rho_2) + \text{div}(\alpha_2 \rho_2 \vec{u}) = 0$$
$$\partial_t (\rho \vec{u}) + \text{div}(\rho \vec{u} \otimes \vec{u}) + \nabla (\alpha_1 p_1 + \alpha_2 p_2) = 0$$
$$\partial_t (\alpha_1 \rho_1 e_1) + \text{div}(\alpha_1 \rho_1 e_1 \vec{u}) + \alpha_1 p_1 \nabla \cdot \vec{u} = -p_I \nu (p_1 - p_2)$$
$$\partial_t (\alpha_2 \rho_2 e_2) + \text{div}(\alpha_2 \rho_2 e_2 \vec{u}) + \alpha_2 p_2 \nabla \cdot \vec{u} = p_I \nu (p_1 - p_2)$$
$$\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \nu (p_1 - p_2)$$

Model is hyperbolic with monotone frozen sound speed & is equivalent to reduced 5-equation model asymptotically as $\nu \to \infty$ (*i.e.*, $p_1 \to p_2$)

Pelanti & Shyue (2012) proposed

$$\begin{aligned}
\partial_t\left(\alpha_1\rho_1\right) + \mathsf{div}(\alpha_1\rho_1\vec{u}) &= 0\\
\partial_t\left(\alpha_2\rho_2\right) + \mathsf{div}(\alpha_2\rho_2\vec{u}) &= 0\\
\partial_t(\rho\vec{u}) + \mathsf{div}(\rho\vec{u}\otimes\vec{u}) + \nabla\left(\alpha_1 p_1 + \alpha_2 p_2\right) &= 0\\
\partial_t\left(\alpha_1 E_1\right) + \mathsf{div}\left(\alpha_1 E_1\vec{u} + \alpha_1 p_1\vec{u}\right) + \mathcal{B}\left(q, \nabla q\right) &= -\nu p_I\left(p_1 - p_2\right)\\
\partial_t\left(\alpha_2 E_2\right) + \mathsf{div}\left(\alpha_2 E_2\vec{u} + \alpha_2 p_2\vec{u}\right) - \mathcal{B}\left(q, \nabla q\right) &= \nu p_I\left(p_1 - p_2\right)\\
\partial_t\alpha_1 + \vec{u}\cdot\nabla\alpha_1 &= \nu\left(p_1 - p_2\right)
\end{aligned}$$

$$\mathcal{B} = -\vec{u}\left(\left(Y_2 p_1 + Y_1 p_2\right)\nabla\alpha_1 + \alpha_1 Y_2\nabla p_1 - \alpha_2 Y_1\nabla p_2\right)$$

Use phasic total energy instead of phasic internal energy; numerically easy to retain mixture total energy consistency

Interface reconstruction: 6-equation model

Assume equilibrium pressure p, velocity $\vec{u}$, & phasic density ρ_k for each interface cell again

1. Reconstruct volume fraction α_1, phasic density $\alpha_i\rho_i$, total density ρ, momentum $\rho\vec{u}$, in same manner as for 5-equation model
2. Reconstruct phasic total energy $\alpha_i E_i$ by

$$\widetilde{\alpha_i E_i} = \frac{1}{2}\tilde{\alpha}_i\rho_i\vec{u}\cdot\vec{u} + \tilde{\alpha}_i\rho_i e_i$$

6-equation model: Anti-diffusion

$$\partial_t\left(\alpha_1\rho_1\right)+\mathsf{div}(\alpha_1\rho_1\vec{u})=\frac{1}{\mu_I}\mathcal{D}_{\alpha_1\rho_1}$$

$$\partial_t\left(\alpha_2\rho_2\right)+\mathsf{div}(\alpha_2\rho_2\vec{u})=\frac{1}{\mu_I}\mathcal{D}_{\alpha_2\rho_2}$$

$$\partial_t(\rho\vec{u})+\mathsf{div}(\rho\vec{u}\otimes\vec{u})+\nabla\left(\alpha_1p_1+\alpha_2p_2\right)=\frac{1}{\mu_I}\mathcal{D}_{\rho u}$$

$$\partial_t\left(\alpha_1E_1\right)+\mathsf{div}\left(\alpha_1E_1\vec{u}+\alpha_1p_1\vec{u}\right)+\mathcal{B}\left(q,\nabla q\right)=-\nu p_I\left(p_1-p_2\right)+\frac{1}{\mu_I}\mathcal{D}_{\alpha_1E_1}$$

$$\partial_t\left(\alpha_2E_2\right)+\mathsf{div}\left(\alpha_2E_2\vec{u}+\alpha_2p_2\vec{u}\right)-\mathcal{B}\left(q,\nabla q\right)=\nu p_I\left(p_1-p_2\right)+\frac{1}{\mu_I}\mathcal{D}_{\alpha_2E_2}$$

$$\partial_t\alpha_1+\vec{u}\cdot\nabla\alpha_1=\nu\left(p_1-p_2\right)+\frac{1}{\mu_I}\mathcal{D}_{\alpha_1}$$

Write 6-equation model in compact form as

$$\partial_t q + \mathsf{div}(f(q)) + w(q, \nabla q) = \psi_{\mu_I}(q) + \psi_\nu(q)$$

Compute approximate solution based on fractional step:

1. Homogeneous hyperbolic step

$$\partial_t q + \mathsf{div}(f(q)) + w(q, \nabla q) = 0$$

2. Source-terms relaxation step

$$\partial_t q = \psi_{\mu_I}(q) + \psi_\nu(q)$$

Pressure relaxation $\nu \to \infty$

Continue by considering pressure relaxation with

$$\partial_t q = \psi_\nu(q), \qquad \text{as} \quad \nu \to \infty$$

Current ODE system is

$$\begin{aligned}
\partial_t \left(\alpha\rho\right)_1 &= 0 \\
\partial_t \left(\alpha\rho\vec{u}\right)_1 &= 0 \\
\partial_t \left(\alpha\rho E\right)_1 &= -\nu p_I \left(p_1 - p_2\right) \\
\partial_t \left(\alpha\rho\right)_2 &= 0 \\
\partial_t \left(\alpha\rho\vec{u}\right)_2 &= 0 \\
\partial_t \left(\alpha\rho E\right)_2 &= \nu p_I \left(p_1 - p_2\right) \\
\partial_t \alpha_1 &= \nu \left(p_1 - p_2\right)
\end{aligned}$$

Combining energy & volume fraction equations, we have

$$\partial_t \left(\alpha\rho E\right)_k = -p_I \partial_t \alpha_k$$

yielding (after using mass & momentum equations)

$$\partial_t \left(\alpha\rho e\right)_k = -p_I \partial_t \alpha_k \qquad \text{or} \qquad \alpha_k \rho_k \partial_t e_k = -p_I \partial_t \alpha_k$$

Integration wrt t over Δt, we have

$$\alpha_k \rho_k \left(e_k - e_{k0}\right) = -\int_{\alpha_{k0}}^{\alpha_k} p_I d\alpha_k = -\bar{p}_I \left(\alpha_k - \alpha_{k0}\right)$$

or

$$e_k = e_{k0} - \bar{p}_I \left(\frac{1}{\rho_k} - \frac{1}{\rho_{k0}}\right), \qquad k = 1, 2$$

Combining EOS $e_k(\bar{p}_I, \rho_k)$ with

$$e_k = e_{k0} - \bar{p}_I \left(\frac{1}{\rho_k} - \frac{1}{\rho_{k0}} \right),$$

we find phasic density ρ_k as a function of $\bar{p}_I$, *i.e.*,

$$\rho_k(\bar{p}_I), \qquad k = 1, 2$$

Use saturation condition

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

leads to algebraic equation for $\bar{p}_I$ (relaxed pressure)

Having relaxed $\bar{p}_I = p_1 = p_2$ & so ρ_k, α_k, conservative vector q can be updated (EOS should be imposed)

Future perspective I

Consider 6-equation model with heat & mass transfer of form

$$
\begin{aligned}
&\partial_t (\alpha_1 \rho_1) + \mathsf{div}(\alpha_1 \rho_1 \vec{u}) = \dot{m} \\
&\partial_t (\alpha_2 \rho_2) + \mathsf{div}(\alpha_2 \rho_2 \vec{u}) = -\dot{m} \\
&\partial_t (\rho \vec{u}) + \mathsf{div}(\rho \vec{u} \otimes \vec{u}) + \nabla (\alpha_1 p_1 + \alpha_2 p_2) = 0 \\
&\partial_t (\alpha_1 E_1) + \mathsf{div} (\alpha_1 E_1 \vec{u} + \alpha_1 p_1 \vec{u}) + \mathcal{B}(q, \nabla q) = \\
&\qquad - \nu p_I (p_1 - p_2) + \mathcal{Q} + e_I \dot{m} \\
&\partial_t (\alpha_2 E_2) + \mathsf{div} (\alpha_2 E_2 \vec{u} + \alpha_2 p_2 \vec{u}) - \mathcal{B}(q, \nabla q) = \\
&\qquad \nu p_I (p_1 - p_2) - \mathcal{Q} - e_I \dot{m} \\
&\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \mu (p_1 - p_2) + \frac{\dot{m}}{\rho_I}
\end{aligned}
$$

Assume $\mu, \theta, \nu \to \infty$: instantaneous 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:
   $\mathcal{Q} := \theta\,(T_2 - T_1)$
   - θ expresses rate towards thermal equilibrium $T_1 \to T_2$,

3. Mass transfer via thermo-chemical relaxation:
   $\dot{m} := \nu\,(g_2 - g_1)$
   - ν expresses rate towards diffusive equilibrium $g_1 \to g_2$, & is nonzero only at 2-phase mixture & metastable state, *i.e.*,

$$\nu = \begin{cases} \infty & \epsilon_1 \leq \alpha_1 \leq 1 - \epsilon_1 \ \& \ T_{\text{liquid}} > T_{\text{sat}} \\ 0 & \text{otherwise} \end{cases}$$

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Liquid-vapor phase change depends strongly on numerical resolution of α_k

Dodecane 2-phase Riemann problem

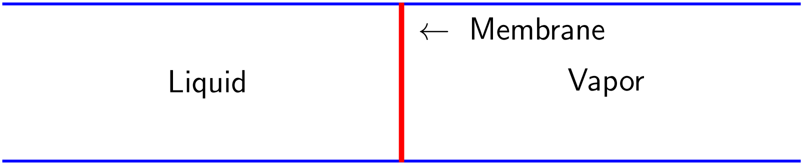
Saurel *et al.* (JFM 2008) & Zein *et al.* (JCP 2010):

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

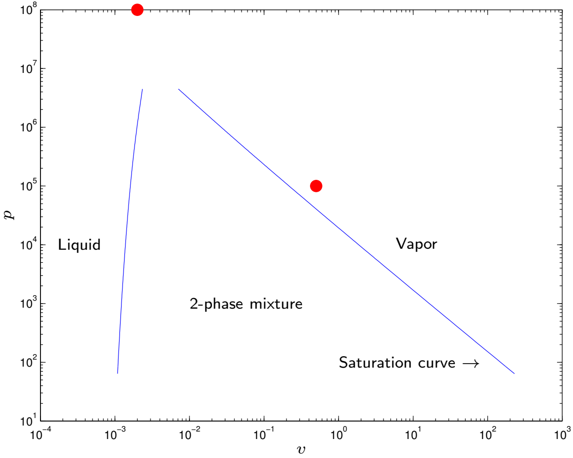
$$(\rho_v, \rho_l, u, p, \alpha_v)_L = \left(2\text{kg/m}^3,\ 500\text{kg/m}^3,\ 0,\ 10^8\text{Pa},\ 10^{-8}\right)$$

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

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

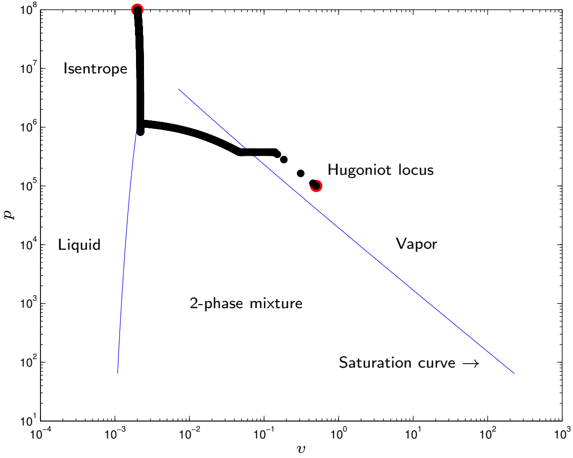


Dodecane 2-phase problem: Phase diagram

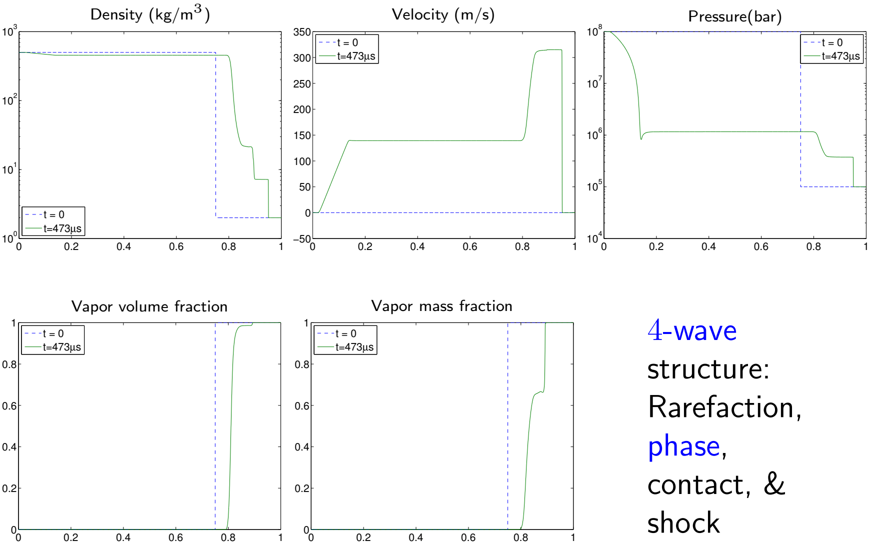


Dodecane 2-phase problem: Phase diagram

Wave path in p-v phase diagram

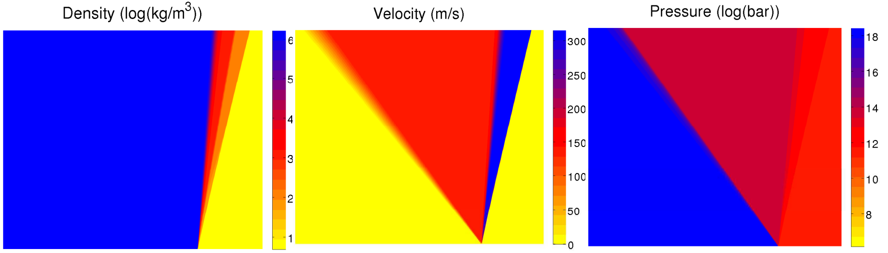


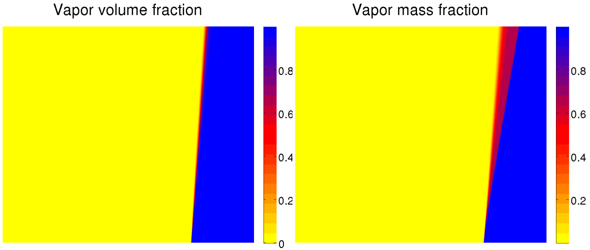
Dodecane 2-phase problem: Sample solution



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

Dodecane 2-phase problem: Sample solution





All physical quantities are discon-tinuous across phase boundary

Future perspective II

Consider barotropic 1-pressure, 1-velocity compressible 2-phase flow model with drift flux approximation

$$\partial_t \left(\alpha_1\rho_1\right) + \mathsf{div}(\alpha_1\rho_1\vec{u}) = \mathsf{div}\left(\rho Y_1 Y_2 \vec{u}_R\right) \qquad \text{(Continuity } \alpha_1\rho_1\text{)}$$

$$\partial_t \left(\alpha_2\rho_2\right) + \mathsf{div}(\alpha_2\rho_2\vec{u}) = -\mathsf{div}\left(\rho Y_1 Y_2 \vec{u}_R\right) \qquad \text{(Continuity } \alpha_2\rho_2\text{)}$$

$$\partial_t(\rho\vec{u}) + \mathsf{div}(\rho\vec{u}\otimes\vec{u}) + \nabla p = 0 \qquad \text{(Momentum)}$$

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Equilibrum pressure p computed by solving

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

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Darcy law model for relative velocity $\vec{u}_R$ assumes

$$\vec{u}_R = \frac{1}{\lambda}\alpha_1\alpha_2\left(\frac{\rho_2-\rho_1}{\rho}\right)\nabla p$$

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Accurate resolution of dissipative source terms & so mathematical model requires good approximation of α_k

Rather than solving saturation condition for p, we may consider model that includes volume fraction equation explicitly as

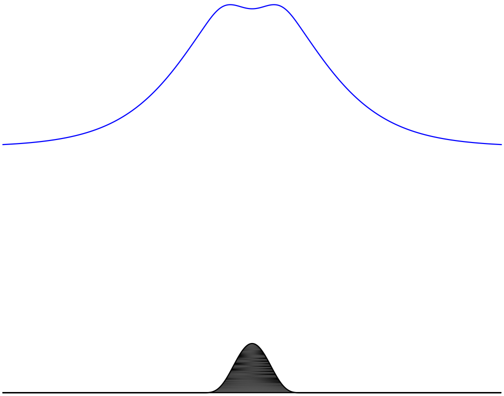
$$\partial_t (\alpha_1\rho_1) + \mathsf{div}(\alpha_1\rho_1\vec{u}) = \mathsf{div}\,(\rho Y_1 Y_2 \vec{u}_R)$$
$$\partial_t (\alpha_2\rho_2) + \mathsf{div}(\alpha_2\rho_2\vec{u}) = -\mathsf{div}\,(\rho Y_1 Y_2 \vec{u}_R)$$
$$\partial_t(\rho\vec{u}) + \mathsf{div}(\rho\vec{u}\otimes\vec{u}) + \nabla(\alpha_1 p_1 + \alpha_2 p_2) = 0$$
$$\partial_t\alpha_1 + \vec{u}\cdot\nabla\alpha_1 - \rho c_w^2 \frac{\alpha_1\alpha_2}{\rho_1 c_1^2 \rho_2 c_2^2}\left(\rho_2 c_2^2 - \rho_1 c_1^2\right)\mathsf{div}(\vec{u}) =$$
$$\rho c_w^2 \frac{\alpha_1\alpha_2}{\rho_1 c_1^2 \rho_2 c_2^2}\left(\frac{\rho_1 c_1^2}{\alpha_1\rho_1} + \frac{\rho_2 c_2^2}{\alpha_2\rho_2}\right)\mathsf{div}(\rho Y_1 Y_2 \vec{u}_R)$$

Here c_w is Wood sound speed defined by

$$\frac{1}{\rho c_{\mathsf{w}}^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2} \qquad \text{(Wood's formula)}$$

Water wave problem

Existence or non-existence of 2-bump solution in water wave via computer aided proof in 2-phase (air-water) direct numerical simulation



Future perspective III

Hyperelasticity flow $\cdots$

Future perspective III

Hyperelasticity flow $\cdots$

Thank you