Volume of fluid methods for compressible multiphase flow

II: Eulerian interface sharpening approach

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Objective

Recall that our aim is to discuss a class of volume of fluid (vs. level set, MAC, particles) methods for interface problems with application to compressible multiphase flow

1. Adaptive moving grid approach (last lecture)
   - Cartesian grid embedded volume tracking
   - Moving mapped grid interface capturing

2. Eulerian interface sharpening approach (this lecture)
   - Artificial interface compression method
   - Anti-diffusion method

Outline

- Review interface sharpening techniques for viscous incompressibe two-phase flow
  - Artificial interface compression
  - Anti-diffusion
- Extend method to compressible multiphase flow
  - Interface only problem
  - Problem with shock wave

This is a work in progress since August 2011

Incompressible 2-phase flow: Review

Consider unsteady, incompressible, viscous, immiscible 2-phase flow with governing equations

$$\nabla \cdot \vec{u} = 0 \qquad \text{(Continuity)}$$

$$\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p = \nabla \cdot \tau + \rho \vec{g} + \vec{f}_\sigma \qquad \text{(Momentum)}$$

$$\partial_t \alpha + \vec{u} \cdot \nabla \alpha = 0 \qquad \text{(Volume fraction transport)}$$

Material quantities in 2-phase coexistent region are often computed by α-based weighted average as

$$\rho = \alpha \rho_1 + (1 - \alpha) \rho_2, \quad \epsilon = \alpha \epsilon_1 + (1 - \alpha) \epsilon_2,$$

where

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

Interface sharpening techniques

Typical interface sharpening methods for incompressible flow include:

- 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
  - Improved THINC
- PDE based approah
  - Artificial compression: Harten CPAM 1977, Olsson & Kreiss JCP 2005
  - Anti-diffusion: So, Hu & Adams JCP 2011

Artificial interface compression

Our first interface-sharpening model concerns artificial compression proposed by Olsson & Kreiss

$$\partial_t \alpha + \vec{u} \cdot \nabla \alpha = \frac{1}{\mu} \nabla \cdot \vec{n} \left[D \left(\nabla \alpha \cdot \vec{n} \right) - \alpha \left(1 - \alpha \right) \right]$$

where $\vec{n} = \nabla \alpha / |\nabla \alpha|$, $\quad D > 0$, $\quad \mu \gg 1$

Standard fractional step method may apply as

1. Advection step over a time step

$$\partial_t \alpha + \vec{u} \cdot \nabla \alpha = 0 \qquad \text{or} \qquad \partial_t \alpha + \nabla \cdot (\alpha \vec{u}) = 0$$

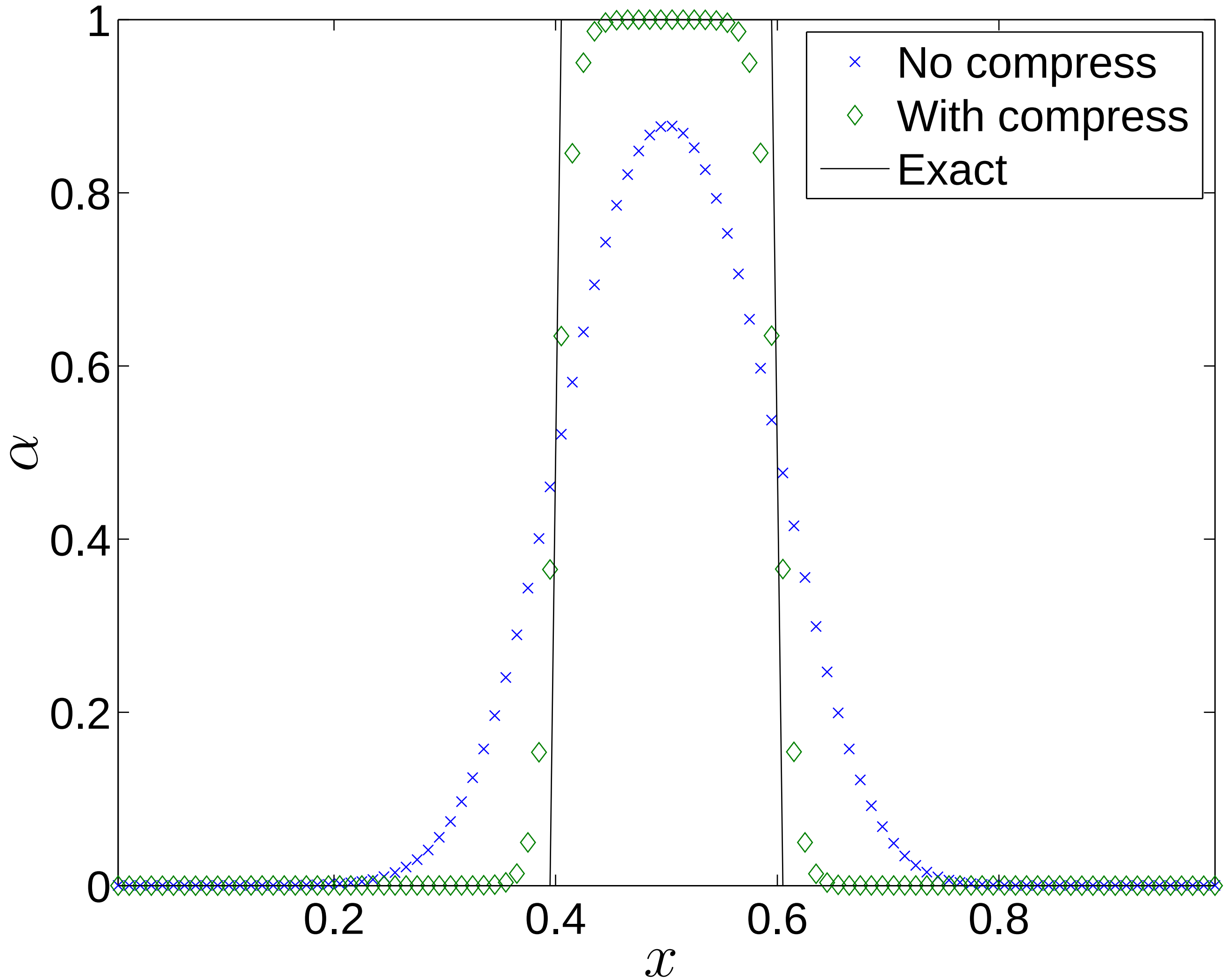
since by assumption $\nabla \cdot \vec{u} = 0$

2. Interface compression step to

$$\partial_\tau \alpha = \nabla \cdot \vec{n} \left[D \left(\nabla \alpha \cdot \vec{n} \right) - \alpha \left(1 - \alpha \right) \right], \quad \tau = t/\mu$$

Square wave passive advection

Square-wave pluse moving with $u = 1$ after 4 periodic cycle



Interface compression: 1D case

To see why this approach works, consider 1D model

$$\partial_t \alpha + u \partial_x \alpha = \frac{1}{\mu} \partial_x \vec{n} \cdot \left[D \left(\partial_x \alpha \cdot \vec{n} \right) - \alpha \left(1 - \alpha \right) \right], \quad x \in \mathbb{R}, \quad t > 0$$

with $\vec{n} = 1$ & initial $\alpha(x, 0) = \alpha_0(x) = 1/\left(1 + \exp\left(-x/D\right)\right)$.
Exact solution for this initial value problem is simply

$$\alpha(x, t) = \alpha_0(x - ut)$$

while solution with perturbed data $\tilde{\alpha}_0(x) = \alpha_0(x) + \delta(x)$ is

$$\alpha(\xi, \tau) = \tilde{\alpha}_0\left(\xi + \xi_0\right) \qquad \text{as} \quad \tau \to \infty \quad (\xi = x - ut, \tau = t/\mu)$$

If perturbation is zero mass $\int_{-\infty}^{\infty} \delta(\xi, 0) d\xi = 0$ (which is true if model is solved conservatively), we have true solution with $\xi_0 = 0$, see Sattinger (1976) & Goodman (1986)

Interface compression: Multi-D case

Let $K = D\nabla\alpha \cdot \vec{n} - \alpha\,(1-\alpha)$ with $\vec{n} = \nabla\alpha/|\nabla\alpha|$. In interface-compression step, we solve

$$\partial_\tau \alpha = \nabla \cdot \vec{n}\left[D\left(\nabla\alpha \cdot \vec{n}\right) - \alpha\,(1-\alpha)\right] = K\nabla \cdot \vec{n} + \vec{n} \cdot \nabla K$$

& reach τ-steady state solution as $\mu \to \infty$, yielding $K = 0$ & 1D profile in coordinate normal to interface $n^\perp$ as

$$\alpha = 1/\left(1 + \exp\left(-n^\perp/D\right)\right) = \left(1 + \tanh\left(n^\perp/2D\right)\right)/2$$

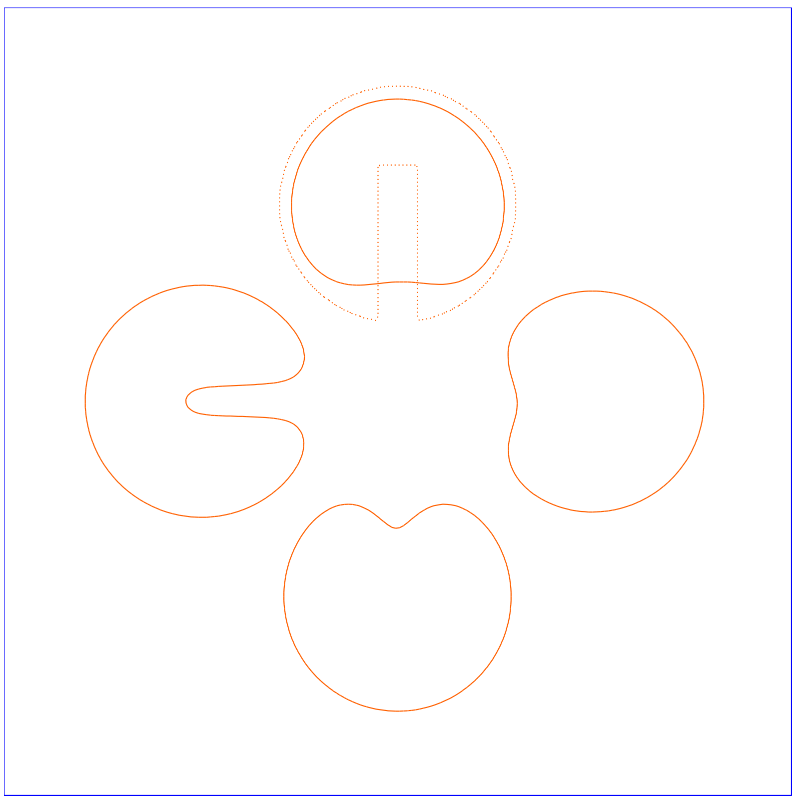
When μ finite, $K \neq 0$, *i.e.*, $K\nabla \cdot \vec{n} + \vec{n} \cdot \nabla K \neq 0$, α & so interface would be changed both normally & tangentially depending on both strength & accuracy of curvature $\nabla \cdot \vec{n}$ evaluation numerically

Zalesak's rotating disc

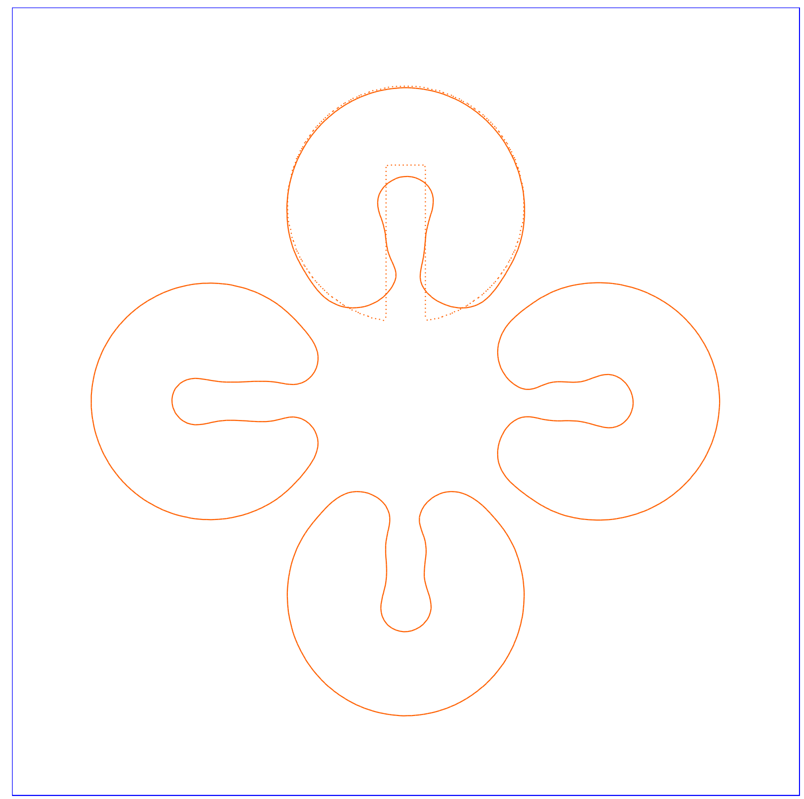
Contours $\alpha = 0.5$ at 4 different times within 1 period in that

$$\vec{u} = (1/2 - y, x - 1/2)$$

No compression



With compression

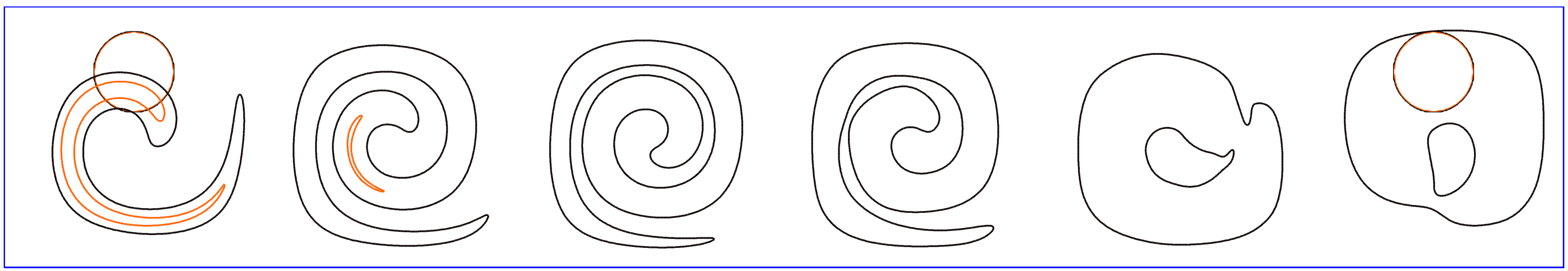


Vortex in cell

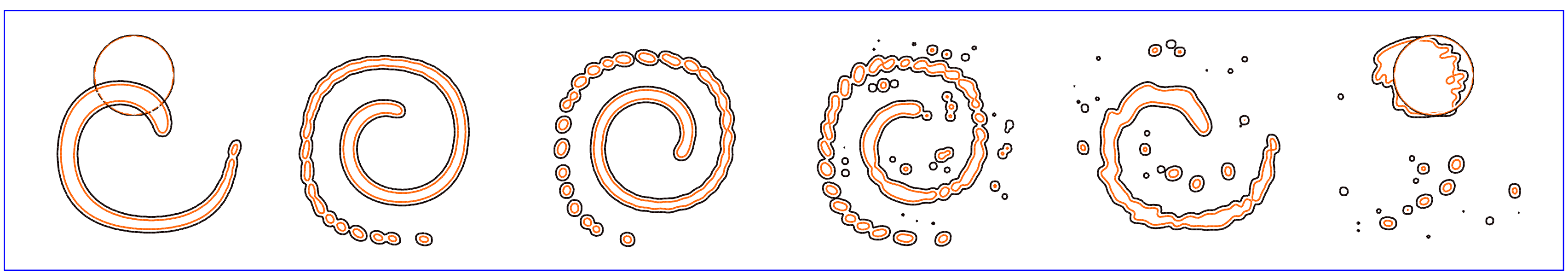
Contours $\alpha = (0.05, 0.5, 0.95)$ at 6 different times in 1 period

$$\vec{u} = \left(-\sin^2(\pi x)\sin(2\pi y), \sin(2\pi x)\sin^2(\pi y)\right)\cos(\pi t/8)$$

No compression



With compression



Interface compression runs

Methods used here are very elementary, *i.e.*,

1. Use Clawpack for advection in Step 1

2. Use simple first order explicit method for interface compression in Step 2
   - Diffusion coefficient $D = \varepsilon \min_{\forall i} \Delta x_i$
   - Time step $\Delta\tau$

$$\Delta\tau \leq \frac{1}{2D} \sum_{i=1}^{d} \Delta x_i^2$$

   - Stopping criterion: simple 1-norm error measure

Extension to compressible flow

Shukla, Pantano & Freund (JCP 2010) proposed extension of interface-compression method for incompressible flow to compressible flow governed by reduced 2-phase model as

$$\partial_t (\alpha_1 \rho_1) + \nabla \cdot (\alpha_1 \rho_1 \vec{u}) = 0$$

$$\partial_t (\alpha_2 \rho_2) + \nabla \cdot (\alpha_2 \rho_2 \vec{u}) = 0$$

$$\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p = 0$$

$$\partial_t (\rho E) + \nabla \cdot (\rho E \vec{u} + p \vec{u}) = 0$$

$$\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \frac{1}{\mu} \vec{n} \cdot \nabla \left(D \nabla \alpha_1 \cdot \vec{n} - \alpha_1 (1 - \alpha_1) \right)$$

$$\partial_t \rho + \nabla \cdot (\rho \vec{u}) = \frac{1}{\mu} H(\alpha_1) \vec{n} \cdot \left(\nabla \left(D \nabla \rho \cdot \vec{n} \right) - (1 - 2\alpha_1) \nabla \rho \right)$$

Mixture pressure is computed based on isobaric closure

Compressible flow: Density correction

To see how density compression term comes from, we assume $\nabla\rho\cdot\vec{n}\sim\nabla\alpha_1\cdot\vec{n}$ & consider case when

$$K = D\nabla\alpha_1\cdot\vec{n}-\alpha_1\left(1-\alpha_1\right)\approx 0 \quad\Longrightarrow\quad D\nabla\alpha_1\cdot\vec{n}\approx\alpha_1(1-\alpha_1)$$

yielding density diffusion normal to interface as

$$\nabla\left(D\nabla\rho\cdot\vec{n}\right)\cdot\vec{n}\approx\nabla\left(\alpha_1(1-\alpha_1)\right)\cdot\vec{n}=\left(1-2\alpha_1\right)\nabla\alpha_1\cdot\vec{n}$$

$$\sim\left(1-2\alpha_1\right)\nabla\rho\cdot\vec{n}$$

Analogously, we write density equation with correction as

$$\partial_t\rho+\nabla\cdot\left(\rho\vec{u}\right)=\frac{1}{\mu}H(\alpha_1)\vec{n}\cdot\left(\nabla\left(D\nabla\rho\cdot\vec{n}\right)-\left(1-2\alpha_1\right)\nabla\rho\right)$$

$H(\alpha_1)=\tanh\left(\alpha_1(1-\alpha_1)/D\right)^2$ is localized-interface function

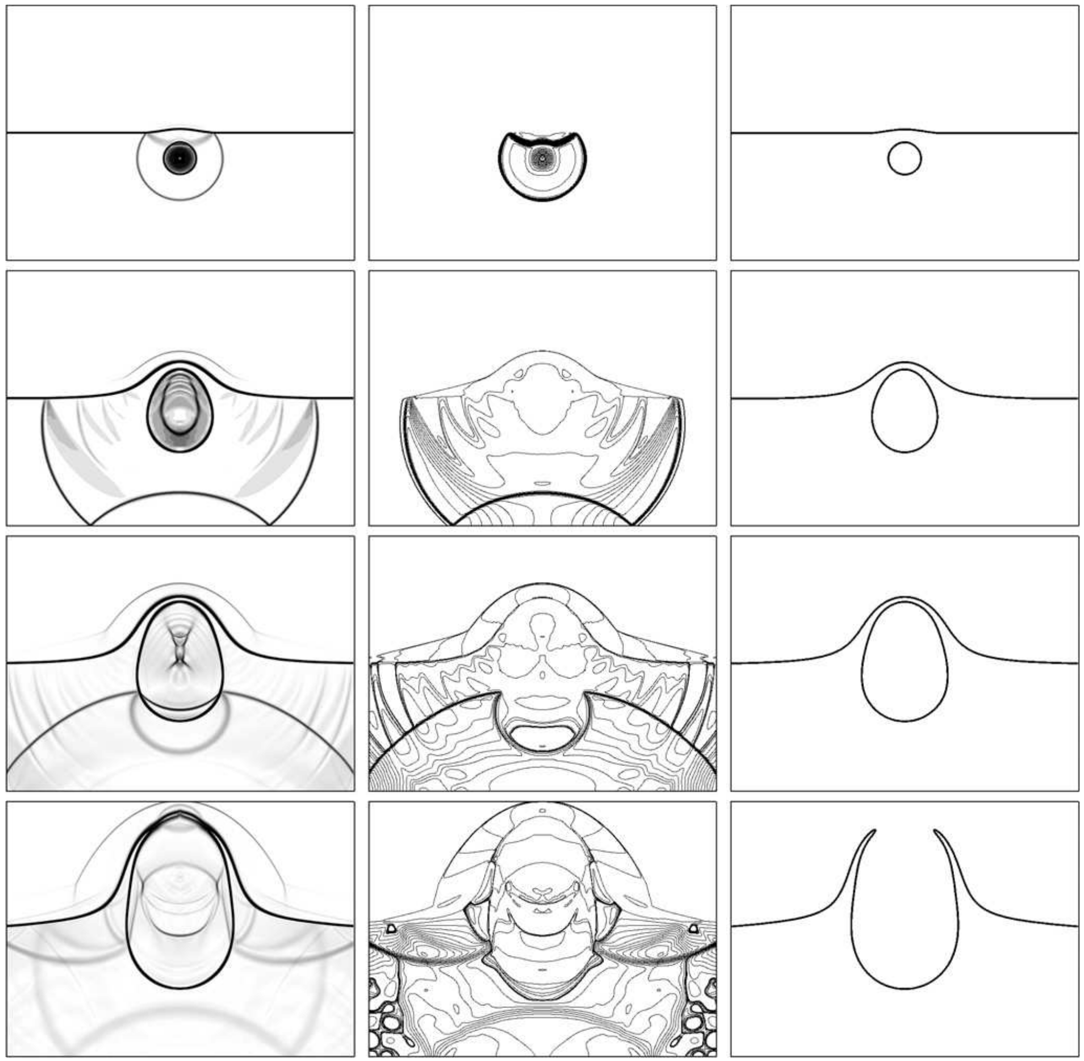
Shukla *et al.* interface compression

In each time step, Shukla's interface-compression algorithm for compressible 2-phase flow consists of following steps:

1. Solve model equation without interface-compression terms by state-of-the-art shock capturing method
2. Compute promitive variable $w = (\rho_1, \rho_2, \rho, \vec{u}, p, \alpha_1)$ from conservative variables $q = (\alpha_1\rho_1, \alpha_2\rho_2, \rho\vec{u}, \rho E, \alpha_1)$
3. Iterate interface & density compression equations to τ-steady state until convergence
4. Update conserved variables at end of time step from primitive variables in step 2 & new values of ρ , α_1 from step 3

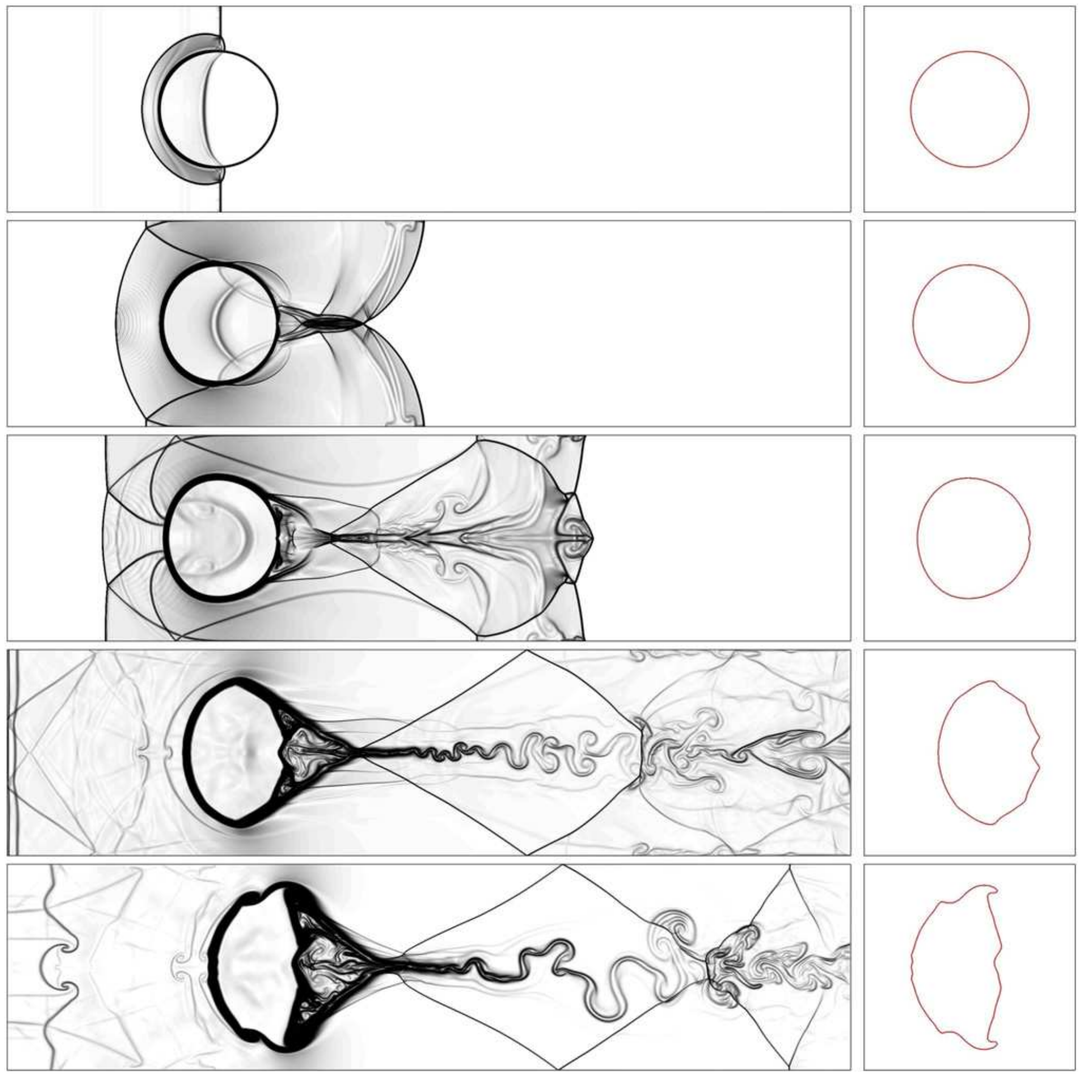
Underwater explosion

Solution adpated from Shukla's paper (JCP 2010)



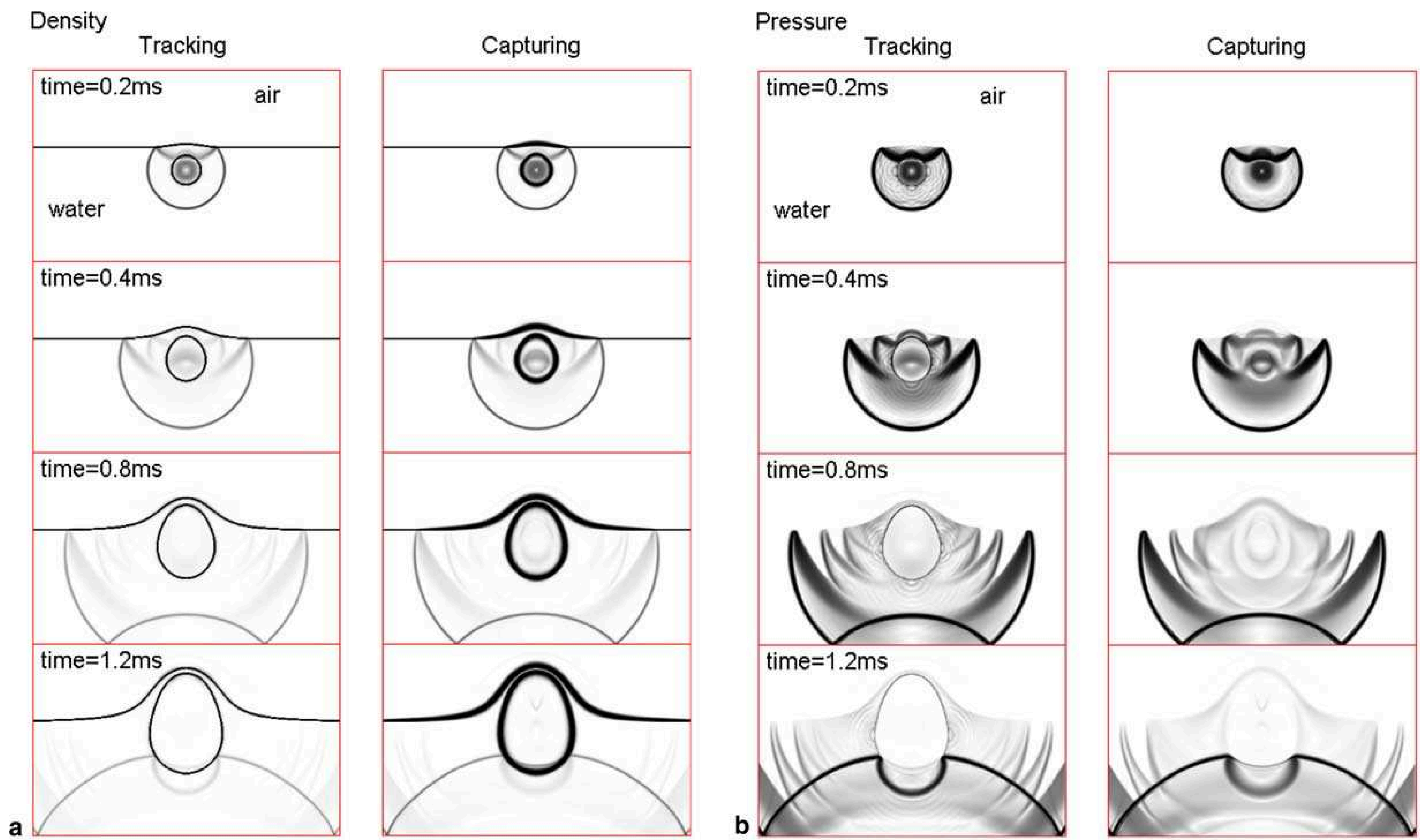
Shock in air & water cylinder

Solution adpated from Shukla's paper (JCP 2010)



Underwater explosion (revisit)

Solution adpated from Shyue's paper (JCP 2006)



Shukla *et al.* algorithm: Remark

In Shukla's results there are noises in pressure contours for UNDEX means poor calculation of pressure near interface

To understand method better, consider simple interface only problem where p & $\vec{u}$ are constants in domain, while ρ & material quantities in EOS have jumps across interfaces

Assume consistent approximation in step 1 for model equation without interface-compression, yielding

$$\text{smeared} \quad (\alpha_1\rho_1, \alpha_2\rho_2, \alpha_1)^* \qquad \& \qquad \text{constant} \quad (\vec{u}, p)^*$$

In step 3, $\rho^* = (\alpha_1\rho_1)^* + (\alpha_2\rho_2)^*$ & α_1^* are compressed to $\tilde{\rho}$ & $\tilde{\alpha}_1$, which in step 4, for total mass & momentum, we set

$$(\rho, \rho u)^{n+1} = (\tilde{\rho}, \tilde{\rho}\vec{u}^*) \quad \Longrightarrow \quad \vec{u}^{n+1} = \tilde{\rho}\vec{u}^* / \tilde{\rho} = \vec{u}^* \quad \text{as expected}$$

Shukla *et al.* algorithm: Remark

In addition, for total energy, we set

$$(\rho E)^{n+1} = \left(\frac{1}{2}\rho|\vec{u}|^2 + \rho e\right)^{n+1} = \frac{1}{2}\tilde{\rho}|\vec{u}^*|^2 + \widetilde{\rho e}(?)$$

Consider stiffened gas EOS for phasic pressure $p_k = (\gamma_k - 1)(\rho e)_k - \gamma_k \mathcal{B}_k$, $k = 1, 2$. We then have

$$\widetilde{\rho e} = \sum_{k=1}^{2} \alpha_k \rho_k e_k = \sum_{k=1}^{2} \tilde{\alpha}_k \frac{p^* + \gamma_k \mathcal{B}_k}{\gamma_k - 1}$$
$$= p^* \sum_{k=1}^{2} \frac{\tilde{\alpha}_k}{\gamma_k - 1} + \sum_{k=1}^{2} \tilde{\alpha}_k \frac{\gamma_k \mathcal{B}_k}{\gamma_k - 1}$$

yielding equilibrium pressure $p^{n+1} = p^*$ if

$$\left(\frac{1}{\gamma - 1}\right)^{n+1} = \sum_{k=1}^{2} \frac{\tilde{\alpha}_k}{\gamma_k - 1} \quad \& \quad \left(\frac{\gamma \mathcal{B}}{\gamma - 1}\right)^{n+1} = \sum_{k=1}^{2} \tilde{\alpha}_k \frac{\gamma_k \mathcal{B}_k}{\gamma_k - 1}$$

Shukla *et al.* algorithm: Remark

Next example concerns linearized Mie-Grüneisen EOS for phasic pressure $p_k = (\gamma_k - 1)\,(\rho e)_k + (\rho_k - \rho_{0k})\,\mathcal{B}_k$

$$\widetilde{\rho e} = \sum_{k=1}^{2} \alpha_k \rho_k e_k = \sum_{k=1}^{2} \frac{\tilde{\alpha}_k p^*}{\gamma_k - 1} - \left(\tilde{\alpha}_k \rho_k^* - \tilde{\alpha}_k \rho_{0k}\right) \frac{\mathcal{B}_k}{\gamma_k - 1}$$

$$= p^* \sum_{k=1}^{2} \frac{\tilde{\alpha}_k}{\gamma_k - 1} - \sum_{k=1}^{2} \left(\tilde{\alpha}_k \rho_k^* - \tilde{\alpha}_k \rho_{0k}\right) \frac{\mathcal{B}_k}{\gamma_k - 1}$$

yielding equilibrium pressure $p^{n+1} = p^*$ if

$$\left(\frac{1}{\gamma - 1}\right)^{n+1} = \sum_{k=1}^{2} \frac{\tilde{\alpha}_k}{\gamma_k - 1} \quad \& \quad \left(\frac{(\rho - \rho_0)\mathcal{B}}{\gamma - 1}\right)^{n+1} = \sum_{k=1}^{2} \left(\tilde{\alpha}_k \rho_k^* - \tilde{\alpha}_k \rho_{0k}\right) \frac{\mathcal{B}_k}{\gamma_k - 1}$$

Shukla *et al.* algorithm: Remark

In Shukla *et al.* algorithm, there is a consistent problem as

$$\sum_{k=1}^{2}(\alpha_k\rho_k)^{n+1} = \sum_{k=1}^{2}\tilde{\alpha}_k\rho_k^{*} \neq \tilde{\rho} = \rho^{n+1}$$

One way to remove this inconsistency is to include compression terms in $\alpha_k\rho_k$, $k = 1, 2$, via

$$\partial_t(\alpha_k\rho_k) + \nabla\cdot(\alpha_k\rho_k\vec{u}) = \frac{1}{\mu}H(\alpha_1)\vec{n}\cdot(\nabla(D\nabla(\alpha_k\rho_k)\cdot\vec{n}) - (1-2\alpha_1)\nabla(\alpha_k\rho_k))$$

We set $\rho^{n+1} = \sum_{k=1}^{2}(\alpha_k\rho_k)^{n+1} = \sum_{k=1}^{2}\tilde{\alpha}_k\tilde{\rho}_k$

Validation of this approach is required

Anti-diffusion interface sharpening

Alternative interface-sharpening model is anti-diffusion proposed by So, Hu & Adams (JCP 2011)

$$\partial_t \alpha + \vec{u} \cdot \nabla \alpha = -\frac{1}{\mu} \nabla \cdot (D \nabla \alpha), \qquad D > 0, \quad \mu \gg 1$$

Standard fractional step method may apply again as

1. Advection step over a time step

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

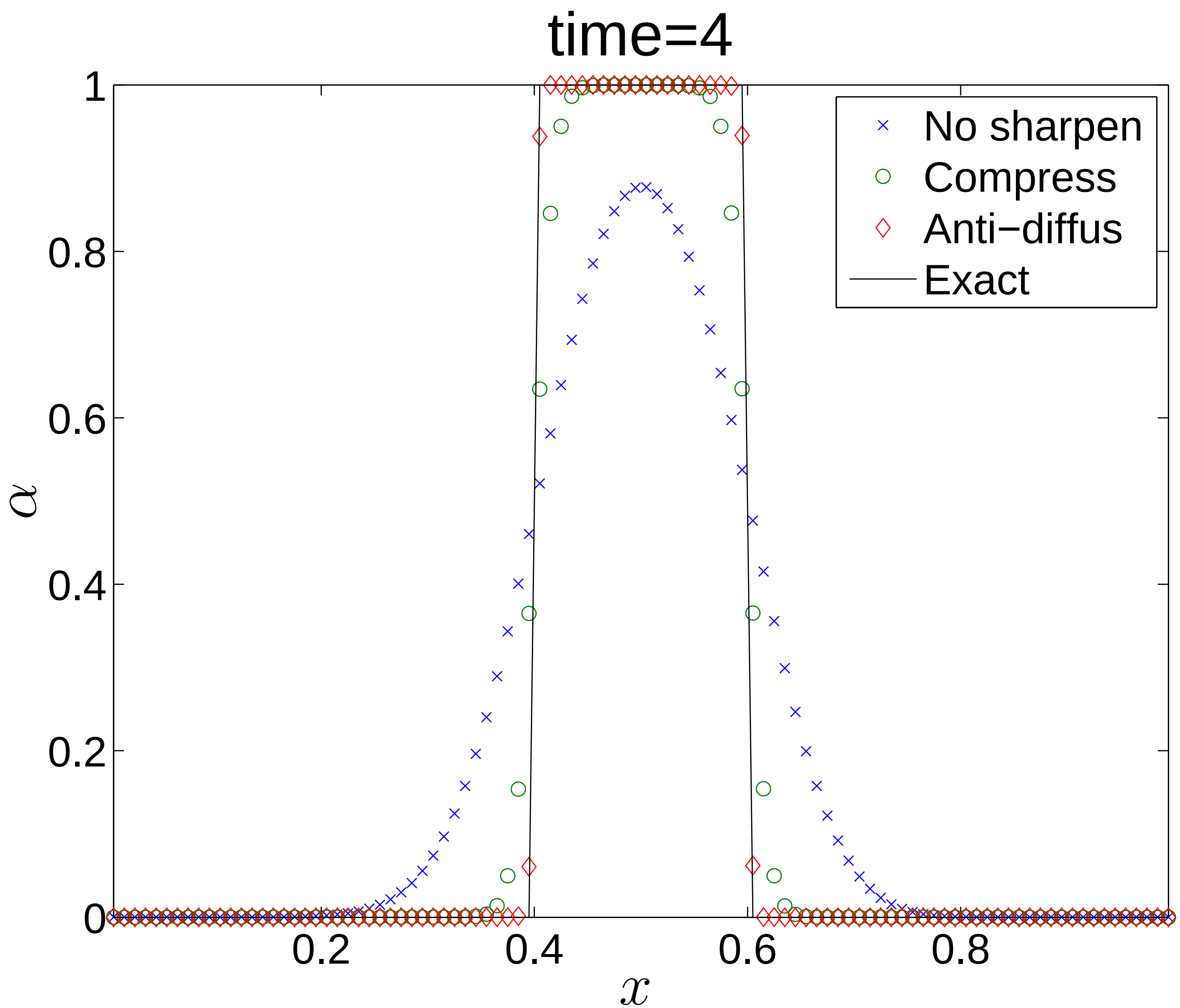
2. Anti-diffusion step towards “sharp layer”

$$\partial_\tau \alpha = -\nabla \cdot (D \nabla \alpha) \quad \text{or} \quad \partial_\tau \alpha = -\nabla \cdot \vec{n} \left(D \nabla \alpha \cdot \vec{n} \right), \quad \tau = t/\mu$$

Numerical regularization is required such as employ MINMOD limiter to stabilize $\nabla \alpha$ in discretization, Breuß *et al.* (’05, ’07)

Square wave passive advection (revisit)

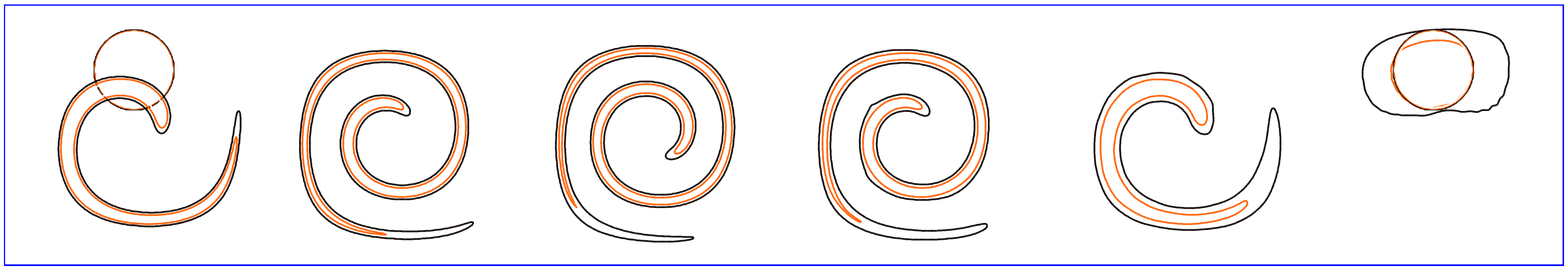
Square-wave pluse moving with $u = 1$ after 4 periodic cycle



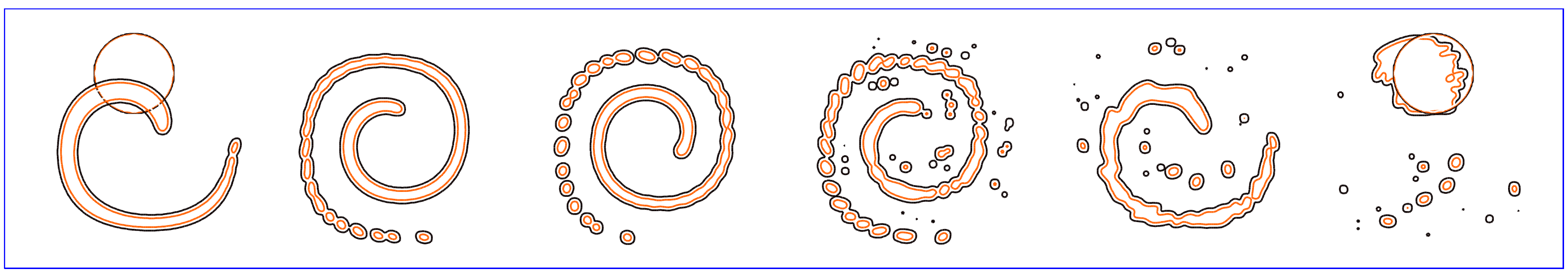
Vortex in cell (revisit)

Contours $\alpha = (0.05, 0.5, 0.95)$ at 6 different times in 1 period

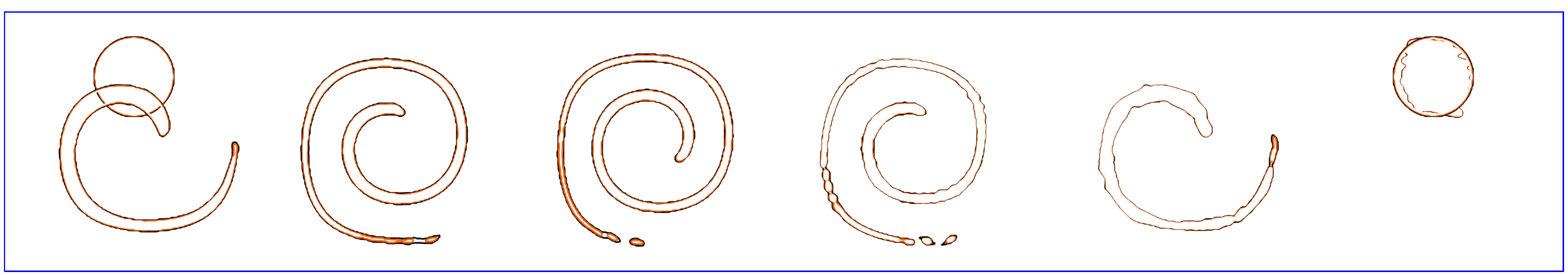
No interface sharpening (second order)



With interface compression



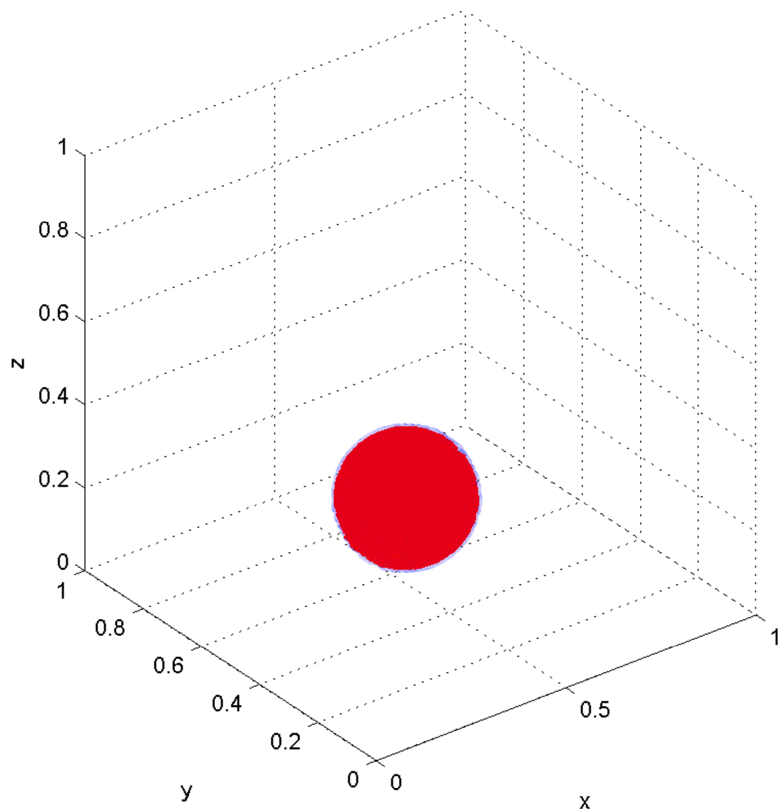
With anti-diffusion



Deformation flow in 3D

In this test, consider velocity field

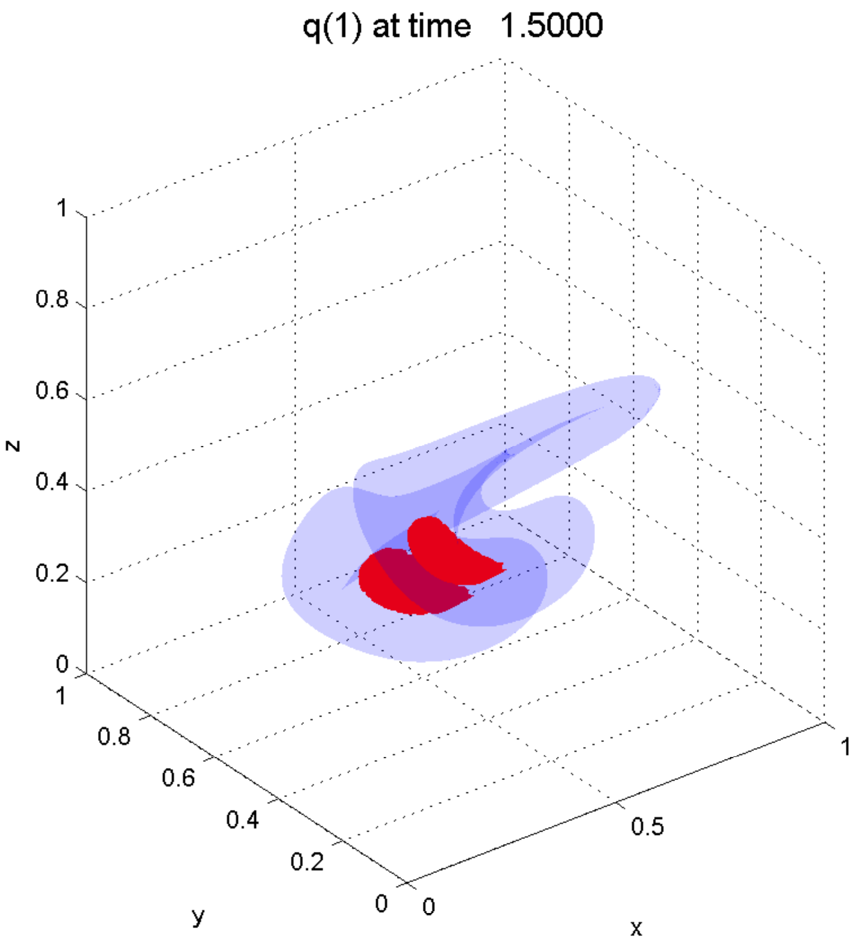
$$\vec{u} = \Big(2\sin^2(\pi x)\sin(2\pi y)\sin(2\pi z), -\sin(2\pi x)\sin^2(\pi y)\sin(2\pi z), -\sin(2\pi x)\sin(2\pi y)\sin^2(\pi z)\Big)\cos(\pi t/3)$$

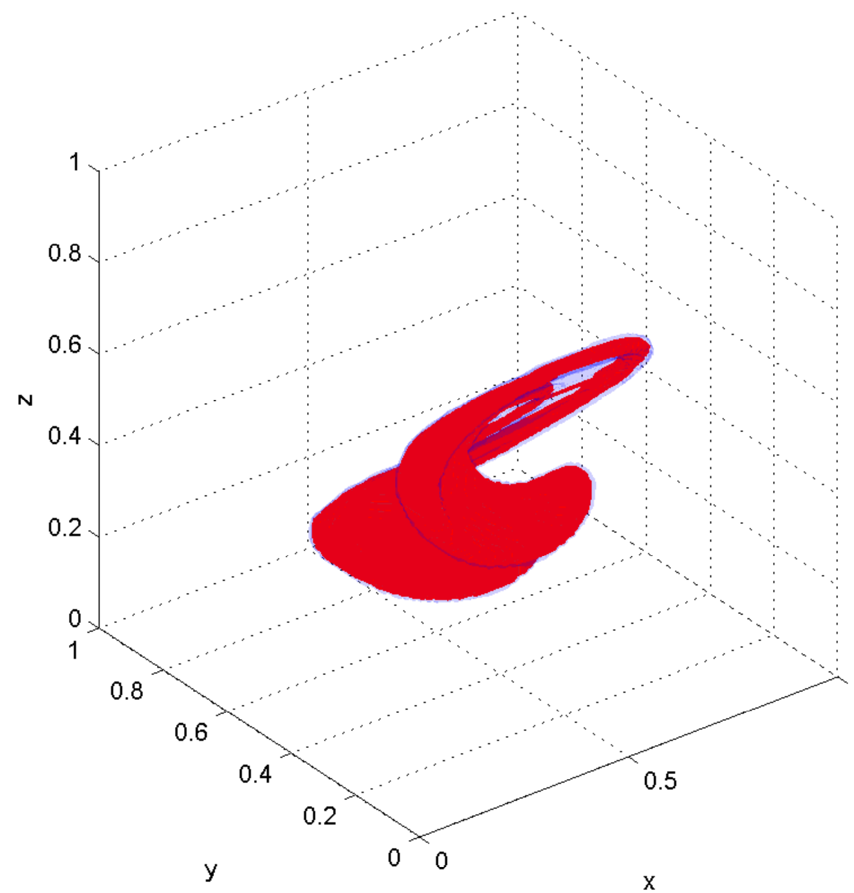


Deformation flow in 3D

No anti-diffusion

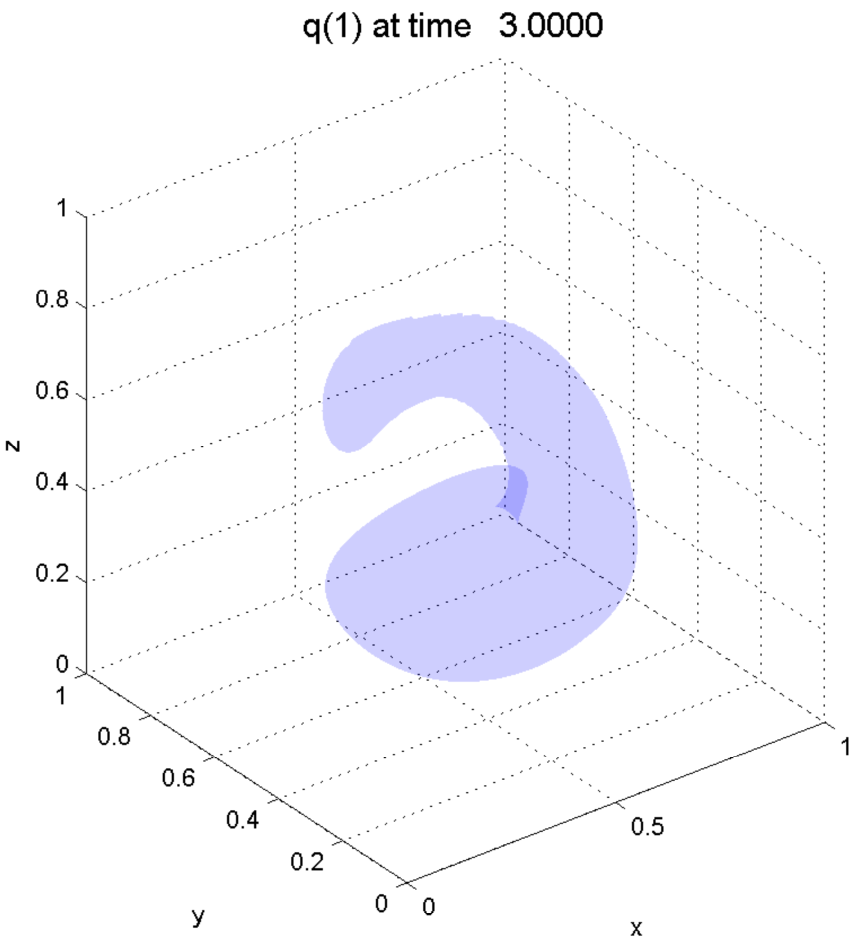
With anti-diffusion



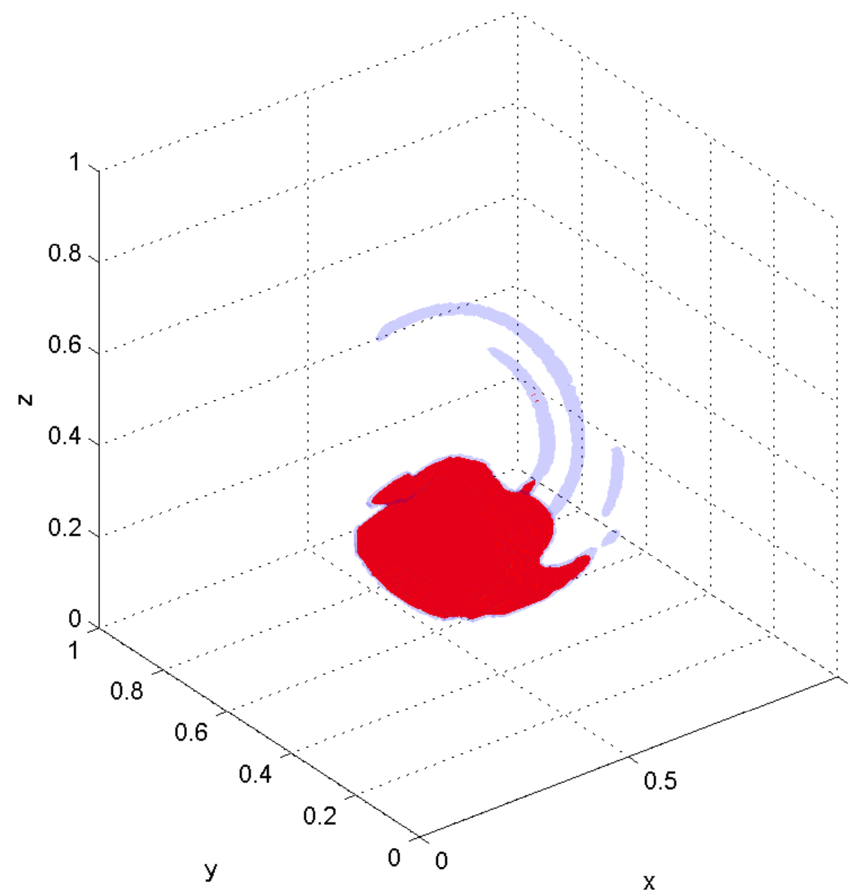


Deformation flow in 3D

No anti-diffusion

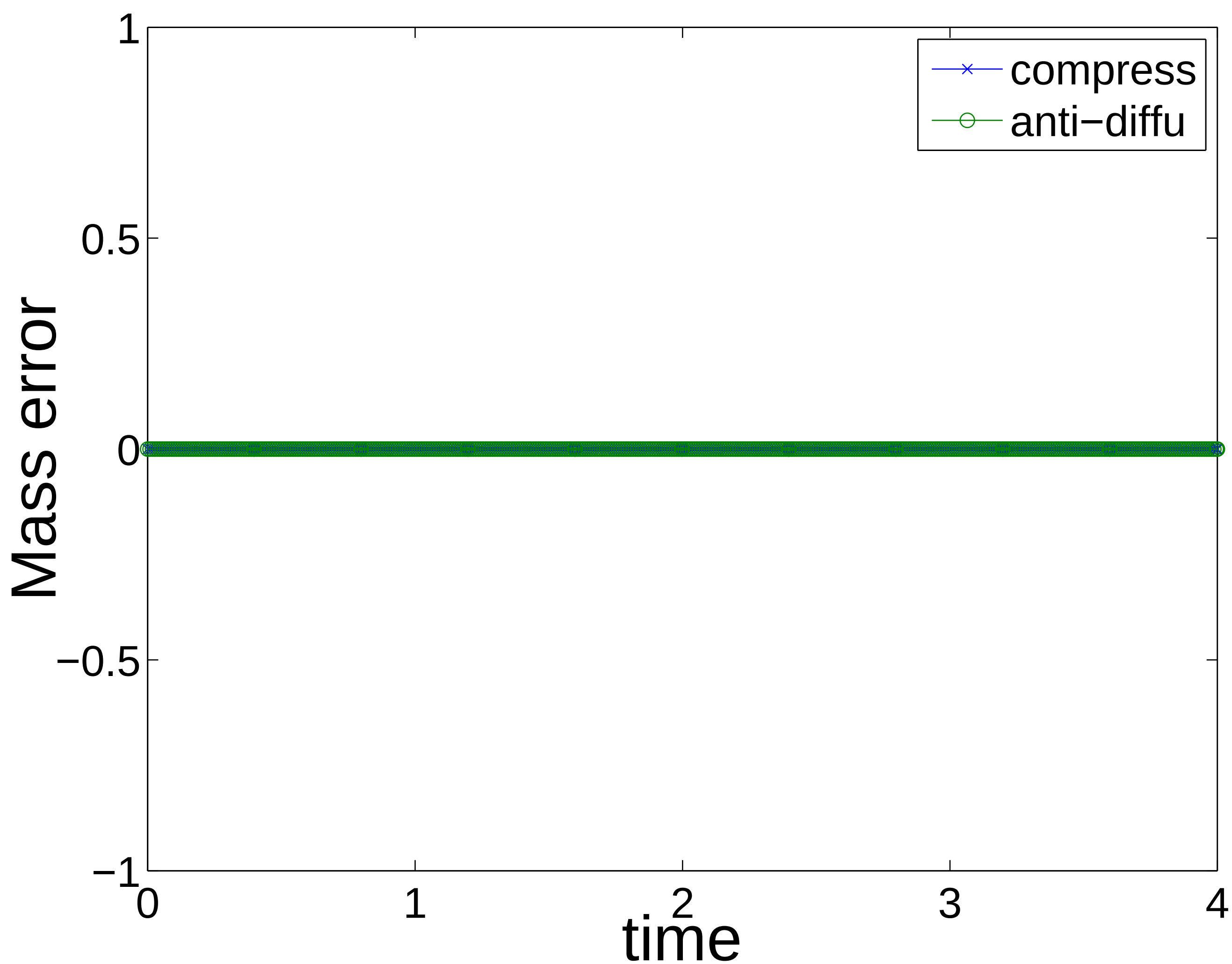


With anti-diffusion



Passive advection: Conservation

Mass error for sample interface sharpening methods



Anti-diffusion runs

Methods used here are the same as artificial interface compression runs, *i.e.*,

1. Use Clawpack for advection in Step 1
2. Use first order explicit method for anti-diffusion in Step 2
   - Diffusion coefficient $D = \max |\vec{u}|$
   - Time step $\Delta\tau$

$$\Delta\tau \leq \frac{1}{2D}\sum_{i=1}^{d}\Delta x_i^2$$

   - Stopping criterion: some measure of interface sharpness

Positivity & accuracy

In compressible multiphase flow, positivity of volume fraction, *i.e.*, $\alpha_k \geq 0$, $\forall k$, is of fundamental importance ; this is because it provides, in particular,

1. information on interface location
2. information on thermodynamic states such as ρe & p in numerical "mixture" region & so ρ_k from $\alpha_k \rho_k$

It is known & have been mentioned many times in this conference that devise of oscillation-free higher-order method is still an open problem (if I have stated correctly)

In this regards, interface-sharpening of some kind should be a useful tool as opposed to higher-order methods or other volume-of-fluid methods

Anti-diffusion to compressible flow

Reduced 2-phase model with anti-diffusion (Shyue 2011)

$$
\begin{aligned}
&\partial_t \alpha_1 + \vec{u}\cdot\nabla\alpha_1 = -\frac{1}{\mu}\nabla\cdot\left(D\nabla\alpha_1\right)\\
&\partial_t\left(\alpha_1\rho_1\right) + \nabla\cdot\left(\alpha_1\rho_1\vec{u}\right) = -\frac{1}{\mu}H(\alpha_1)\nabla\cdot\left(D\nabla\alpha_1\rho_1\right)\\
&\partial_t\left(\alpha_2\rho_2\right) + \nabla\cdot\left(\alpha_2\rho_2\vec{u}\right) = -\frac{1}{\mu}H(\alpha_1)\nabla\cdot\left(D\nabla\alpha_2\rho_2\right)\\
&\partial_t\left(\rho\vec{u}\right) + \nabla\cdot\left(\rho\vec{u}\otimes\vec{u}\right) + \nabla p = -\frac{1}{\mu}H(\alpha_1)\vec{u}\,\nabla\cdot\left(D\nabla\rho\right)\\
&\partial_t\left(\rho E\right) + \nabla\cdot\left(\rho E\vec{u} + p\vec{u}\right) =\\
&\qquad\qquad -\frac{1}{\mu}H(\alpha_1)\mathcal{L}\left(\frac{1}{2}\rho|\vec{u}|^2\right) - \frac{1}{\mu}H(\alpha_1)\mathcal{L}\left(\rho e\right)
\end{aligned}
$$

Denote $\mathcal{L}$ as an diffusion operator

Anti-diffusion to compressible flow

To find $\mathcal{L}\left(\frac{1}{2}\rho|\vec{u}|^2\right)$, assuming $|\vec{u}|^2$ is constant, we observe

$$\nabla\left(\frac{1}{2}\rho|\vec{u}|^2\right) = \frac{1}{2}|\vec{u}|^2\nabla\rho \quad \text{yielding} \quad \mathcal{L}\left(\frac{1}{2}\rho|\vec{u}|^2\right) = \frac{1}{2}|\vec{u}^2|\nabla\cdot(D\nabla\rho)$$

To find $\mathcal{L}(\rho e)$, we need to know equation of state. Now in stiffened gas case with $p_k = (\gamma_k - 1)(\rho e)_k - \gamma_k \mathcal{B}_k$,

$$\nabla(\rho e) = \nabla\left(\sum_{k=1}^{2}\alpha_k\rho_k e_k\right) = \nabla\left(\sum_{k=1}^{2}\alpha_k\frac{p+\gamma_k\mathcal{B}_k}{\gamma_k - 1}\right)$$

$$= \sum_{k=1}^{2}\left(\frac{p+\gamma_k\mathcal{B}_k}{\gamma_k - 1}\right)\nabla\alpha_k = \left(\frac{p+\gamma_1\mathcal{B}_1}{\gamma_1 - 1} - \frac{p+\gamma_2\mathcal{B}_2}{\gamma_2 - 1}\right)\nabla\alpha_1$$

$$= \beta\,\nabla\alpha_1 \quad \text{yielding} \quad \mathcal{L}(\rho e) = \beta\,\nabla\cdot(D\nabla\alpha_1)$$

Anti-diffusion to compressible flow

We next consider case with linearized Mie-Grüneisen EOS $p_k = (\gamma_k - 1)(\rho e)_k + (\rho_k - \rho_{0k})\mathcal{B}_k \; k = 1, 2$, & proceed same procedure as before

$$\nabla(\rho e) = \nabla\left(\sum_{k=1}^{2} \alpha_k \rho_k e_k\right) = \nabla\left(\sum_{k=1}^{2} \alpha_k \frac{p - (\rho_k - \rho_{0k})\mathcal{B}_k}{\gamma_k - 1}\right)$$

$$= \sum_{k=1}^{2} \frac{p + \rho_{0k}\mathcal{B}_k}{\gamma_k - 1} \nabla\alpha_k + \sum_{k=1}^{2} \frac{\mathcal{B}_k}{\gamma_k - 1} \nabla(\alpha_k \rho_k)$$

$$= \beta_0 \nabla\alpha_1 + \sum_{k=1}^{2} \beta_k \nabla(\alpha_k \rho k)$$

We choose $\mathcal{L}(\rho e) = \beta_0 \, \nabla \cdot (D\nabla\alpha_1) + \sum_1^2 \beta_k \, \nabla \cdot (D\nabla\alpha_k\rho_k)$

Anti-diffusion to compressible flow

Write anti-diffusion model in compact form

$$\partial_t q + \nabla \cdot \vec{f} + B \nabla q = -\frac{1}{\mu}\psi(q)$$

with q, $\vec{f}$, B, & ψ defined (not shown)

In each time step, proposed anti-diffusion algorithm for compressible 2-phase flow consists of following steps:

1. Solve model equation without anti-diffusion terms

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

2. Iterate model equation with anti-diffusion terms

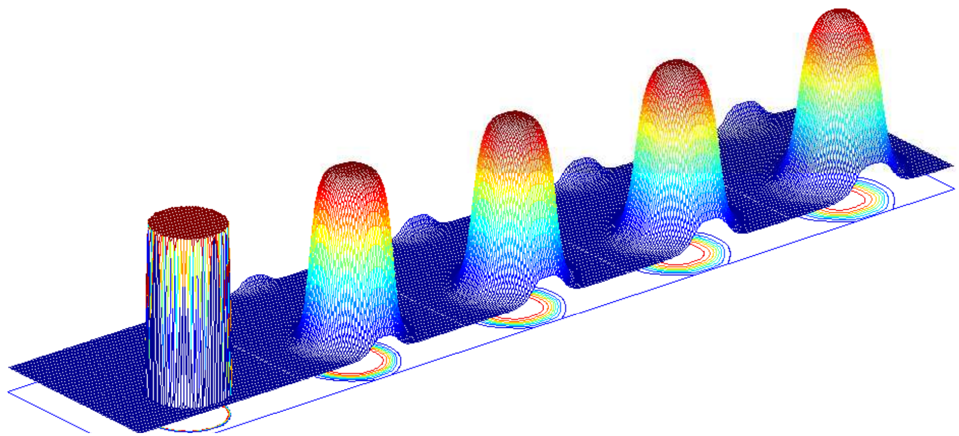
$$\partial_\tau q = \psi(q)$$

to τ-steady state until convergence

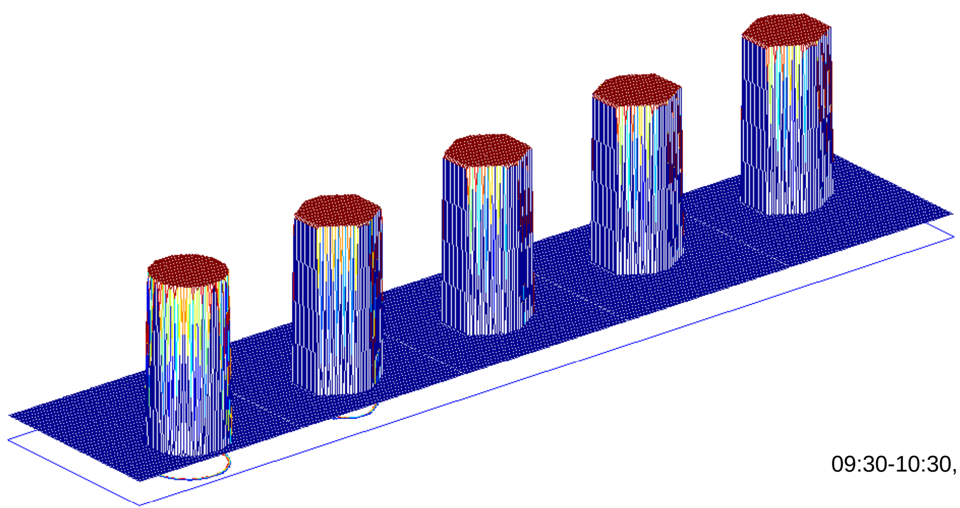
Circular water column advection

Density surface plot (Moving speed $\vec{u} = (1, 1/10)$)

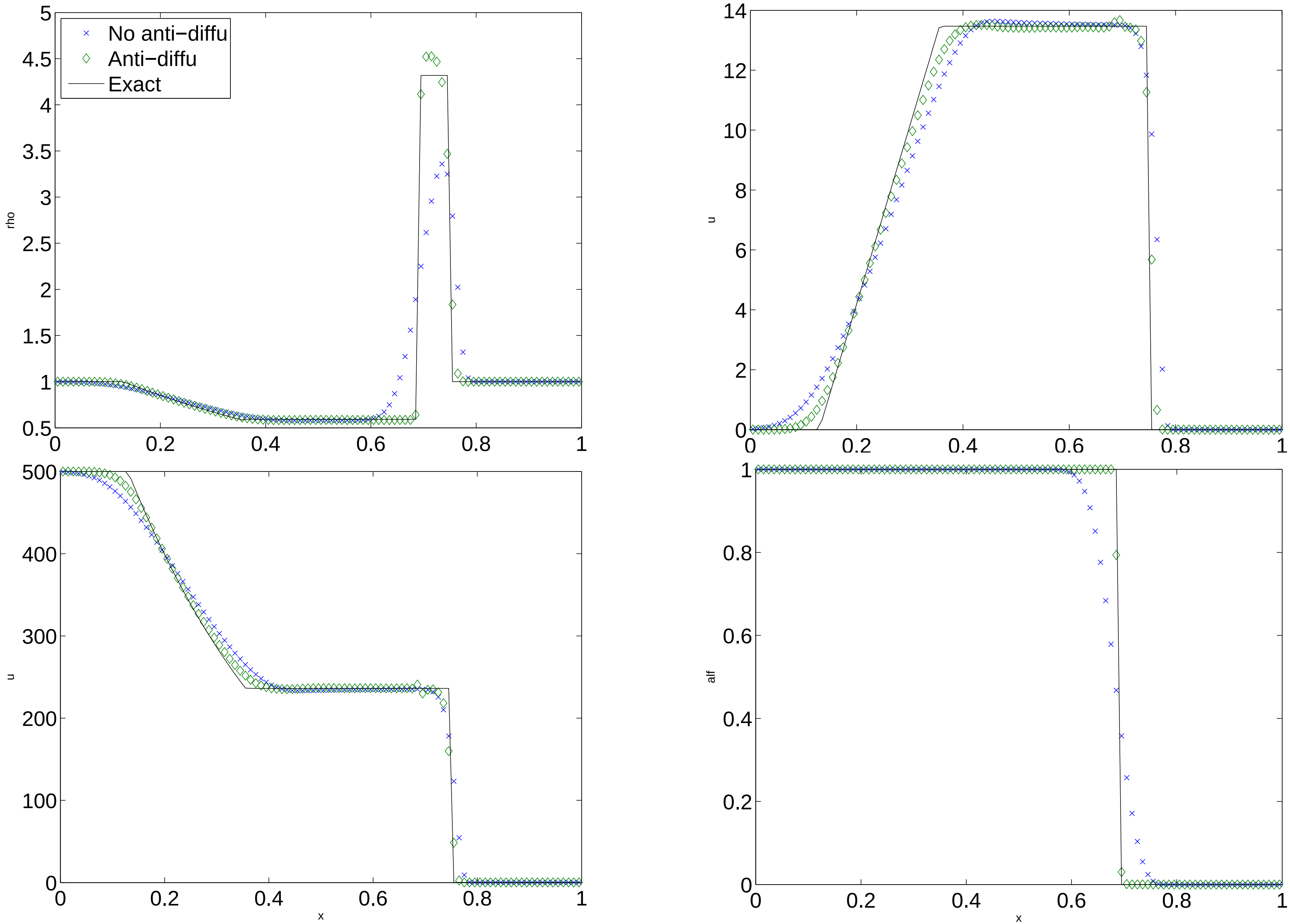
No anti-diffusion



With anti-diffusion



Air-Helium Riemann problem



Future perspectives

- Effect of local interface identification $H(\alpha)$
  - Algebraic approach

$$H(\alpha) = \begin{cases} \tanh\left(\alpha(1-\alpha)/D\right)^2 & \text{(Shukla \textit{et al.})} \\ \tanh\left(\sqrt{\alpha(1-\alpha)/D}\right) \end{cases}$$

  - PDE approach
- Anti-diffusion on moving mapped grid
- Extension to other multiphase model

Thank you