Numerical Methods for Compressible Multicomponent Flow with Moving Interfaces and Boundaries

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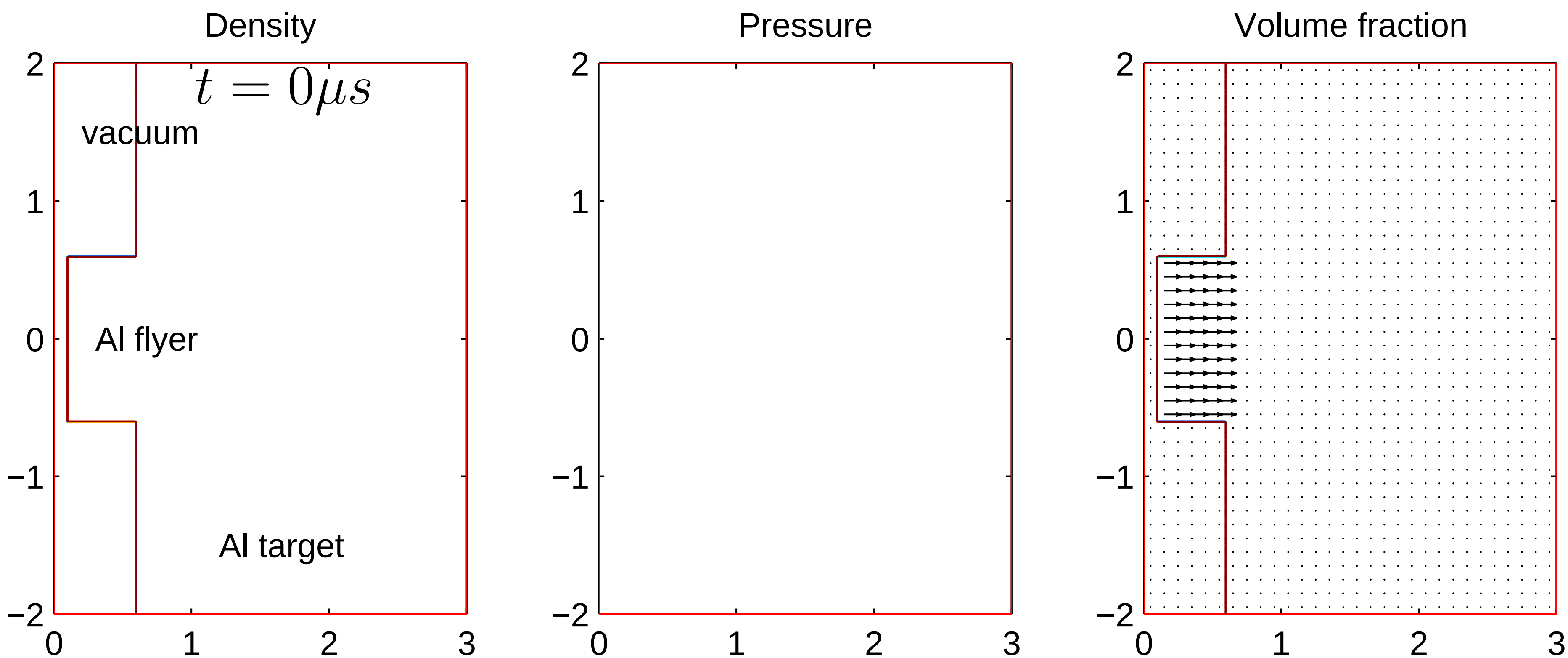
Illustrative Example 1

- Flying Aluminum-plate problem
- Vacuum-Al boundary



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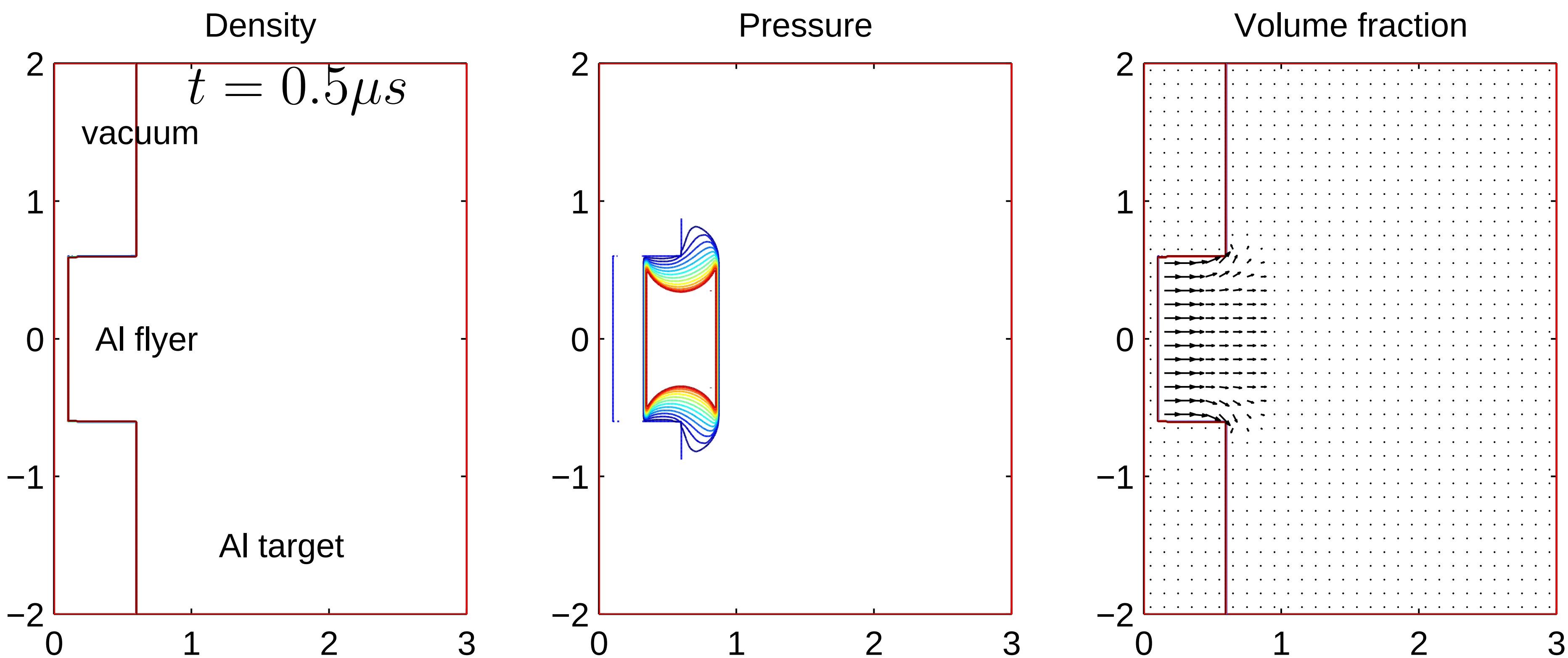

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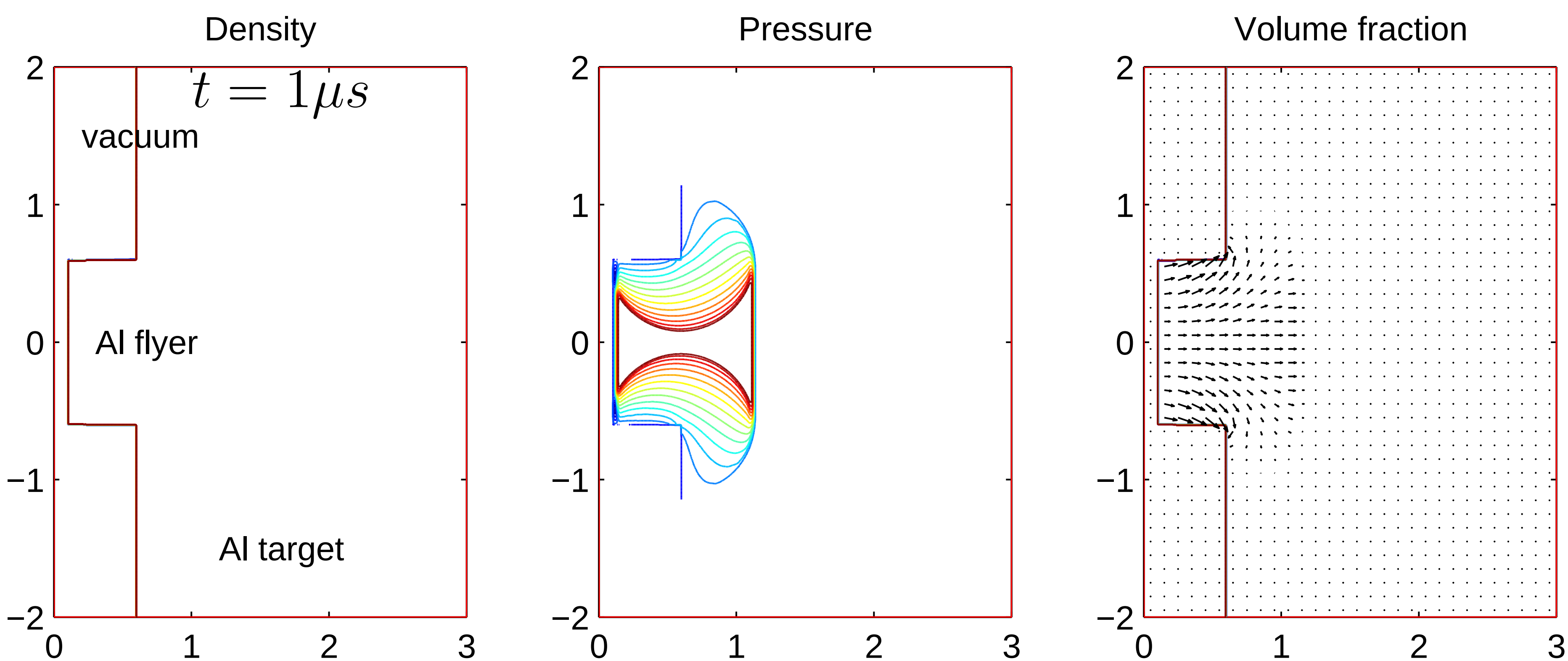

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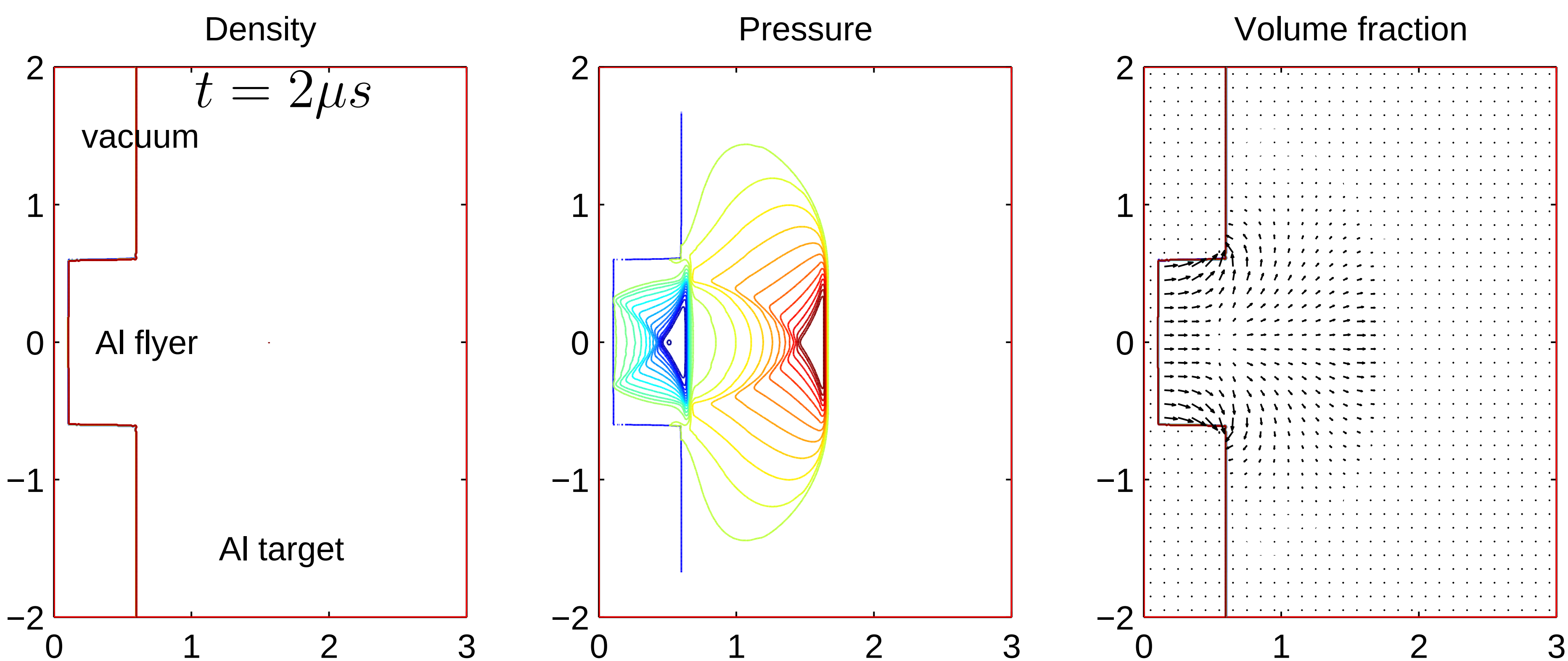

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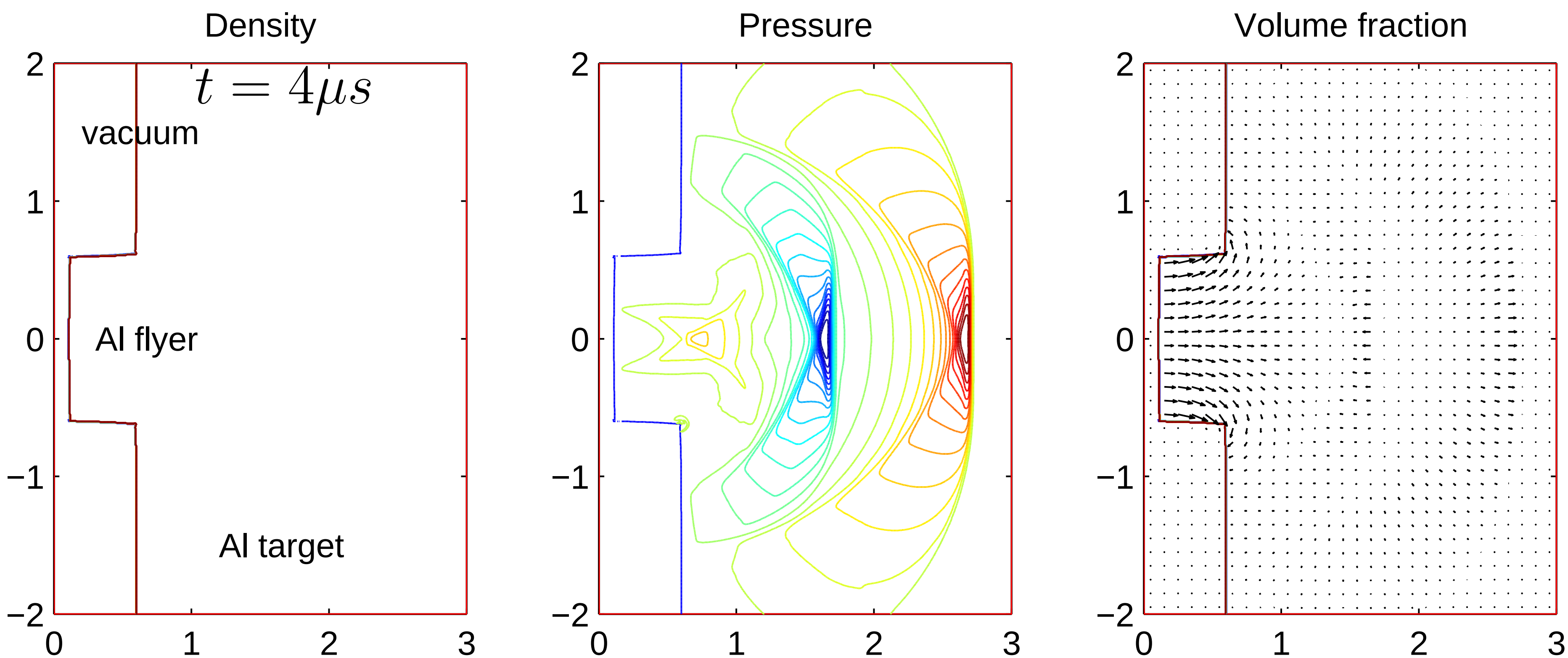
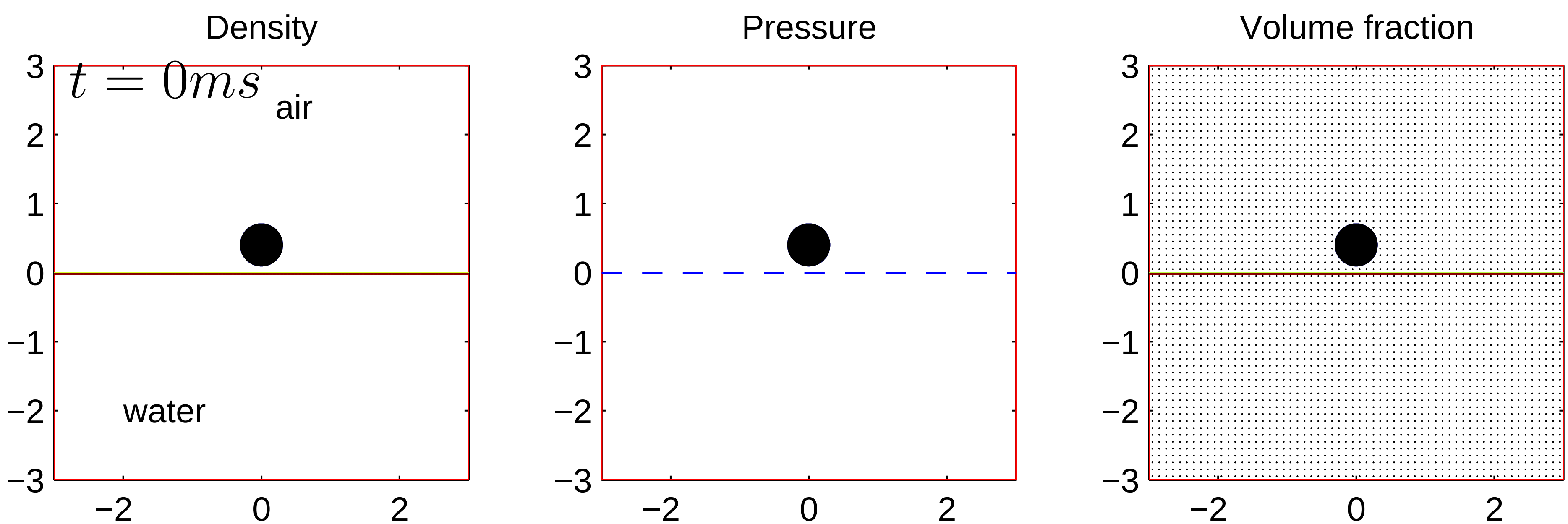


Illustrative Example 2

- Flying rigid-cylinder in partially air-filled water tank
- Air-water interface & moving rigid boundary



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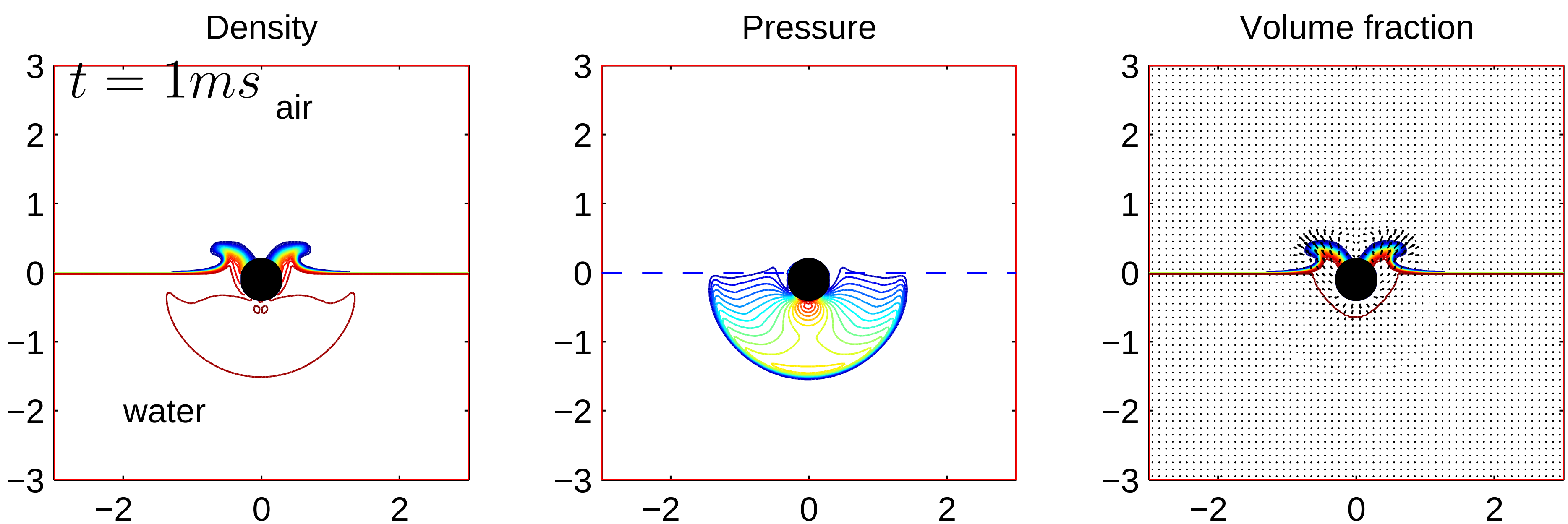

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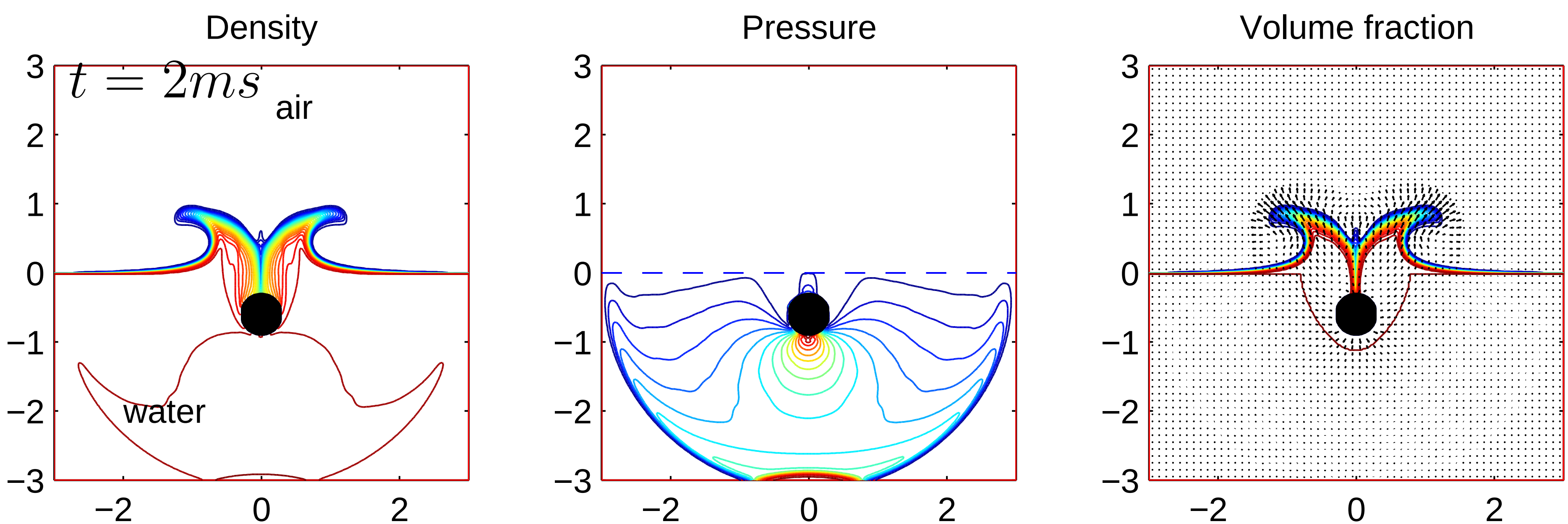

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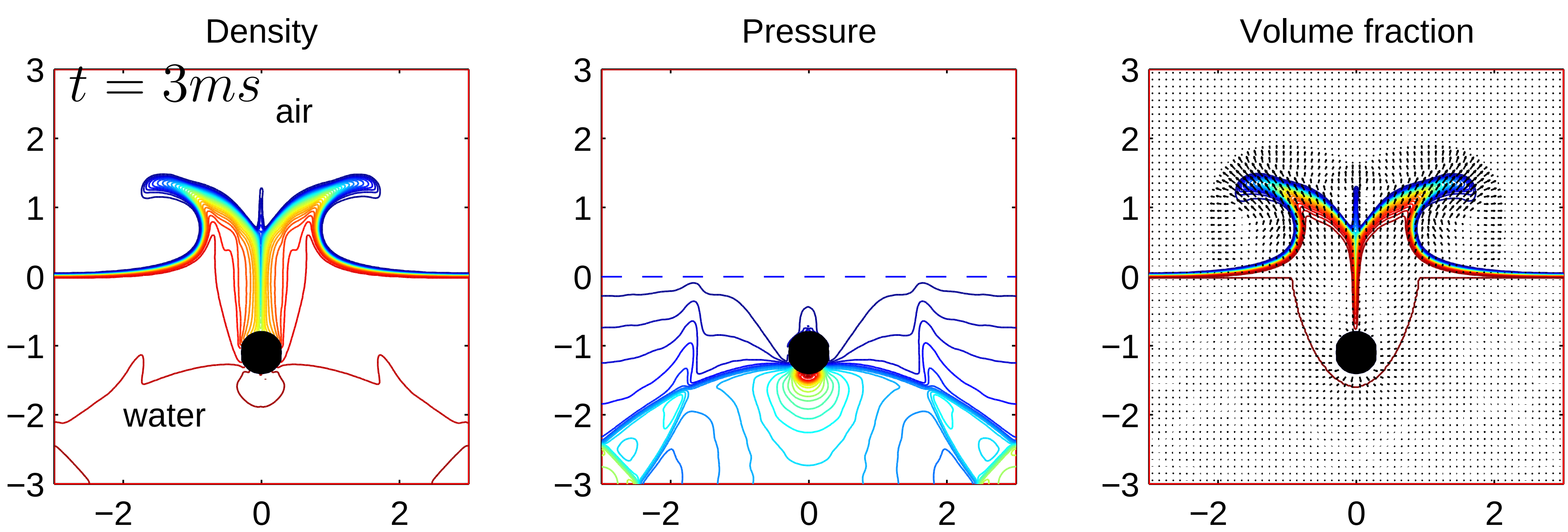

Overview

- Mathematical model
  - Fluid-mixture type equations of motion for homogeneous two-phase flow
  - Mie-Grüneisen EOS for real materials
- Numerical techniques
  - Finite volume method based on wave propagation
    - Surface tracking for moving boundaries
    - Volume tracking for moving interfaces
- Numerical results
- Future work

Two Phase Flow Problem

Ignore physical effects such as viscosity, surface tension, mass diffusion, and so on

- Each fluid component k, $k = 1, 2$, satisties
  - Eulerian conservation laws

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

  - Mie-Grüneisen equation of state

$$p(\rho, e) = p_{\text{ref}}(\rho) + \rho\, \Gamma(\rho) \left[e - e_{\text{ref}}(\rho) \right]$$

Mie-Grüneisen Equations of State

Typical examples are:

- $(p_{\text{ref}}, e_{\text{ref}})$ lies along an isentrope

Mie-Grüneisen Equations of State

Typical examples are:

- $(p_{\text{ref}}, e_{\text{ref}})$ lies along an isentrope
  1. Jones-Wilkins-Lee EOS for gaseous explosives

$$\Gamma(V) = \gamma - 1$$

$$e_{\text{ref}}(V) = e_0 + \frac{\mathcal{A}\ V_0}{\mathcal{R}_1} \exp\left(\frac{-\mathcal{R}_1 V}{V_0}\right) + \frac{\mathcal{B}\ V_0}{\mathcal{R}_2} \exp\left(\frac{-\mathcal{R}_2 V}{V_0}\right)$$

$$p_{\text{ref}}(V) = p_0 + \mathcal{A}\ \exp\left(\frac{-\mathcal{R}_1 V}{V_0}\right) + \mathcal{B}\ \exp\left(\frac{-\mathcal{R}_2 V}{V_0}\right)$$

Here $V = 1/\rho$

Mie-Grüneisen Equations of State

Typical examples are:

- $(p_{\text{ref}}, e_{\text{ref}})$ lies along an isentrope
  2. Cochran-Chan EOS for solid explosives

$$\Gamma(V) = \Gamma_0 = \gamma - 1$$

$$e_{\text{ref}}(V) = e_0 + \frac{-\mathcal{A}\, V_0}{1-\mathcal{E}_1}\left[\left(\frac{V}{V_0}\right)^{1-\mathcal{E}_1} - 1\right] + \frac{\mathcal{B}\, V_0}{1-\mathcal{E}_2}\left[\left(\frac{V}{V_0}\right)^{1-\mathcal{E}_2} - 1\right]$$

$$p_{\text{ref}}(V) = p_0 + \mathcal{A}\left(\frac{V}{V_0}\right)^{-\mathcal{E}_1} - \mathcal{B}\left(\frac{V}{V_0}\right)^{-\mathcal{E}_2}$$

Mie-Grüneisen Equations of State

- $(p_{\text{ref}}, e_{\text{ref}})$ lies along a Hugoniot locus
  - Assume linear shock speed u_s & particle velocity u_p

$$u_s = c_0 + s\,u_p$$

  - We may derive the relations

$$\Gamma(V) = \Gamma_0 \left(\frac{V}{V_0}\right)^{\alpha}$$

$$p_{\text{ref}}(V) = p_0 + \frac{{c_0}^2(V_0 - V)}{[V_0 - s(V_0 - V)]^2}$$

$$e_{\text{ref}}(V) = e_0 + \frac{1}{2}\left[p_{\text{ref}}(V) + p_0\right](V_0 - V)$$

Material Quantities for Model EOS

JWL EOS	ρ_0(kg/m^3)	$\mathcal{A}$(GPa)	$\mathcal{B}$(GPa)	$\mathcal{R}_1$	$\mathcal{R}_2$	Γ
TNT1	1630	371.2	3.23	4.15	0.95	0.30
TNT2	1630	548.4	9.375	4.94	1.21	1.28
Water	1004	1582	-4.67	8.94	1.45	1.17
CC EOS	ρ_0(kg/m^3)	$\mathcal{A}$(GPa)	$\mathcal{B}$(GPa)	$\mathcal{E}_1$	$\mathcal{E}_2$	Γ
TNT	1840	12.87	13.42	4.1	3.1	0.93
Copper	8900	145.67	147.75	2.99	1.99	2
Shock EOS	ρ_0(kg/m^3)	c_0(m/s)	s	Γ_0	α	
Aluminum	2785	5328	1.338	2.0	1	
Copper	8924	3910	1.51	1.96	1	

Two-Phase Flow Model

- Model derivation based on averaging theory of Drew (Theory of Multicomponent Fluids, D.A. Drew & S. L. Passman, Springer, 1999)

Namely, introduce indicator function χ_k as

$$\chi_k(M,t) = \begin{cases} 1 & \text{if } M \text{ belongs to phase } k \\ 0 & \text{otherwise} \end{cases}$$

Denote $< \psi >$ as volume averaged for flow variable ψ,

$$\langle \psi \rangle = \frac{1}{V} \int_V \psi \, dV$$

Gauss & Leibnitz rules

$$\langle \chi_k \nabla \psi \rangle = \langle \nabla(\chi_k \psi) \rangle - \langle \psi \nabla \chi_k \rangle \quad \& \quad \langle \chi_k \psi_t \rangle = \langle (\chi_k \psi)_t \rangle - \langle \psi (\chi_k)_t \rangle$$

Two-Phase Flow Model (Cont.)

Take product of each conservation (or balance) law with χ_k & perform averaging process. In case of mass conservation equation, for example, we have

$$\langle \chi_k \rho_k \rangle_t + \nabla \cdot < \chi_k \rho_k \vec{u}_k >= \langle \rho_k (\chi_k)_t + \rho_k \vec{u}_k \cdot \nabla \chi_k \rangle$$

Since χ_k is governed by

$$(\chi_k)_t + \vec{u}_0 \cdot \nabla \chi_k = 0, \qquad \vec{u}_0\text{: interface velocity}$$

yielding averaged equation for mass

$$\langle \chi_k \rho_k \rangle_t + \nabla \cdot < \chi_k \rho_k \vec{u}_k >= \langle \rho_k \left(\vec{u}_k - \vec{u}_0 \right) \cdot \nabla \chi_k \rangle$$

Analogously, we may derive averaged equation for momentum, energy, & entropy (not shown here)

Two-Phase Flow Model (Cont.)

In summary, averaged model system, we have, are

$$\langle \chi_k \rho_k \rangle_t + \nabla \cdot < \chi_k \rho_k \vec{u}_k >= \langle \rho_k \left(\vec{u}_k - \vec{u}_0 \right) \cdot \nabla \chi_k \rangle$$

$$\langle \chi_k \rho_k \vec{u}_k \rangle_t + \nabla \cdot < \chi_k \rho_k \vec{u}_k \otimes \vec{u}_k > + \nabla \langle \chi_k p_k \rangle = \langle p_k \nabla \chi_k \rangle + \langle \rho_k \vec{u}_k \left(\vec{u}_k - \vec{u}_0 \right) \cdot \nabla \chi_k \rangle$$

$$\langle \chi_k \rho_k E_k \rangle_t + \nabla \cdot < \chi_k \rho_k E_k \vec{u}_k + \chi_k p_k \vec{u}_k >= \langle p_k \vec{u}_k \cdot \nabla \chi_k \rangle + \langle \rho_k E \left(\vec{u}_k - \vec{u}_0 \right) \cdot \nabla \chi_k \rangle$$

$$\langle \chi_k \rangle_t + \langle \vec{u}_k \cdot \nabla \chi_k \rangle = \langle \left(\vec{u}_k - \vec{u}_0 \right) \cdot \nabla \chi_k \rangle$$

Existence of interfacial source terms
Mathematical as well as numerical modelling these terms are essential & difficult for multiphase flow problems

Homogeneous Two-Phase Flow Model

- Assume homogeneous flow (*i.e.*, across interfaces: $p_k = p$ & $\vec{u}_k = \vec{u}$, $k = 0, 1, 2$)
- Introduce volume fraction $\alpha_k = V_k / V$ ($\alpha_1 + \alpha_2 = 1$)

By dropping all interfacial terms, we may obtain a simplified model as

$$
\begin{aligned}
&(\alpha_k \rho_k)_t + \nabla \cdot (\alpha_k \rho_k \vec{u}) = 0 \\
&(\alpha_k \rho_k \vec{u})_t + \nabla \cdot (\alpha_k \rho_k \vec{u} \otimes \vec{u}) + \nabla (\alpha_k p) = p \nabla \alpha_k \\
&(\alpha_k \rho_k E_k)_t + \nabla \cdot (\alpha_k \rho_k E_k \vec{u} + \alpha_k p \vec{u}) = p \vec{u} \cdot \nabla \alpha_k \\
&(\alpha_k)_t + \vec{u} \cdot \nabla \alpha_k = 0
\end{aligned}
$$

for $k = 1, 2$

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Alternatively, a simplified model as

$$
\begin{aligned}
&(\alpha_k \rho_k)_t + \nabla \cdot (\alpha_k \rho_k \vec{u}) = 0 \\
&(\rho \vec{u})_t + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p = 0 \\
&(\rho E)_t + \nabla \cdot (\rho E \vec{u} + p \vec{u}) = 0 \\
&(\alpha_k)_t + \vec{u} \cdot \nabla \alpha_k = 0
\end{aligned}
$$

Here $\rho = \sum_{k=1}^{2} \alpha_k \rho_k, \quad \rho E = \sum_{k=1}^{2} \alpha_k \rho_k E_k$

Homogeneous Flow Model (Cont.)

- Mixture equation of state: $p = p(\alpha_2,\ \alpha_1\rho_1,\ \alpha_2\rho_2,\ \rho e)$
- Isobaric closure: $p_1 = p_2 = p$
  - For a class of EOS, explicit formula for p is available (examples are given next)
  - For some complex EOS, from $(\alpha_2, \rho_1, \rho_2, \rho e)$ in model equations we recover p by solving

$$p_1(\rho_1, \rho_1 e_1) = p_2(\rho_2, \rho_2 e_2) \quad \& \quad \sum_{k=1}^{2} \alpha_k \rho_k e_k = \rho e$$

- This homogeneous two-phase model was called a five-equation model by Allaire, Clerc, & Kokh (JCP 2002) or a volume-fraction model by Shyue (JCP 1998)

Homogeneous Flow Model (Cont.)

- Polytropic ideal gas: $p_k = (\gamma_k - 1)\rho_k e_k$

$$\rho e = \sum_{k=1}^{2} \alpha_k \rho_k e_k = \sum_{k=1}^{2} \alpha_k \frac{p}{\gamma_k - 1} \quad \Longrightarrow \quad p = \rho e \Big/ \sum_{k=1}^{2} \frac{\alpha_k}{\gamma_k - 1}$$

- Van der Waals gas: $p_k = (\frac{\gamma_k - 1}{1 - b_k \rho_k})(\rho_k e_k + a_k \rho_k^2) - a_k \rho_k^2$

$$\rho e = \sum_{k=1}^{2} \alpha_k \rho_k e_k = \sum_{k=1}^{2} \alpha_k \left[\left(\frac{1 - b_k \rho_k}{\gamma_k - 1} \right) (p + a_k \rho_k^2) - a_k \rho_k^2 \right] \quad =$$

$$p = \left[\rho e - \sum_{k=1}^{2} \alpha_k \left(\frac{1 - b_k \rho_k}{\gamma_k - 1} - 1 \right) a_k \rho_k^2 \right] \Big/ \sum_{k=1}^{2} \alpha_k \left(\frac{1 - b_k \rho_k}{\gamma_k - 1} \right)$$

Homogeneous Flow Model (Cont.)

- Two-molecular vibrating gas: $p_k = \rho_k R_k T(e_k)$, T satisfies

$$e = \frac{RT}{\gamma - 1} + \frac{RT_{\text{vib}}}{\exp\left(T_{\text{vib}}/T\right) - 1}$$

As before, we now have

$$\rho e = \sum_{k=1}^{2} \alpha_k \rho_k e_k = \sum_{k=1}^{2} \alpha_k \left[\left(\frac{\rho_k R_k T_k}{\gamma_k - 1} \right) + \frac{\rho_k R_k T_{\text{vib},k}}{\exp\left(T_{\text{vib},k}/T_k\right) - 1} \right]$$

$$= \sum_{k=1}^{2} \alpha_k \left[\left(\frac{p}{\gamma_k - 1} \right) + \frac{p_{\text{vib},k}}{\exp\left(p_{\text{vib},k}/p\right) - 1} \right] \quad \text{(Nonlin. eq.)}$$

Homogeneous Flow Model (Cont.)

- It can be shown entropies, $\mathcal{S}_k$, $k = 1, 2$, satisfy

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

- Murrone & Guillard (JCP 2005) propsed a reduced two-phase flow model in which

$$(\alpha_2)_t + \vec{u} \cdot \nabla \alpha_2 = \alpha_1 \alpha_2 \left(\frac{\rho_1 c_1^2 - \rho_2 c_2^2}{\sum_{k=1}^{2} \alpha_k \rho_k c_k^2}\right)$$

and now phase entropies satisfy

$$\frac{D\mathcal{S}_k}{Dt} = \frac{\partial \mathcal{S}_k}{\partial t} + \vec{u} \cdot \nabla \mathcal{S}_k = 0, \quad \text{for} \quad k = 1, 2$$

Homogeneous Flow Model (Cont.)

- Model system is hyperbolic under suitable thermodynamic stability condition (see below)
- In the model, when $\alpha_2 = 0$ (or $= 1$), ρ_2 (or ρ_1) can not be recovered from α_2 & $\alpha_2\rho_2$ (or α_1 & $\alpha_1\rho_1$).
- It is not absolutely clear in the model how to compute nonlinear term ρ^ι, $\iota > 1$ from α_k & $\alpha_k\rho_k$
- This formulation of model equation would not work when one fluid component is adiabatic, but the other fluid component is not
- Surely, there are other set of model systems proposed in the literature that are robust for homogeneous flow

Thermodynamic Stability

- Fundamental derivative of gas dynamics

$$\mathcal{G} = -\frac{V}{2}\frac{(\partial^2 p/\partial V^2)_S}{(\partial p/\partial V)_S}, \qquad S : \text{specific entropy}$$

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- Assume fluid state satisfy $\mathcal{G} > 0$ for thermodynamic stability, *i.e.*,

$$(\partial^2 p/\partial V^2)_S > 0 \qquad \& \qquad (\partial p/\partial V)_S < 0$$

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  - $(\partial^2 p/\partial V^2)_S > 0$ means convex EOS

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  - $(\partial^2 p/\partial V^2)_S > 0$ means convex EOS
  - $(\partial p/\partial V)_S < 0$ means real speed of sound, for

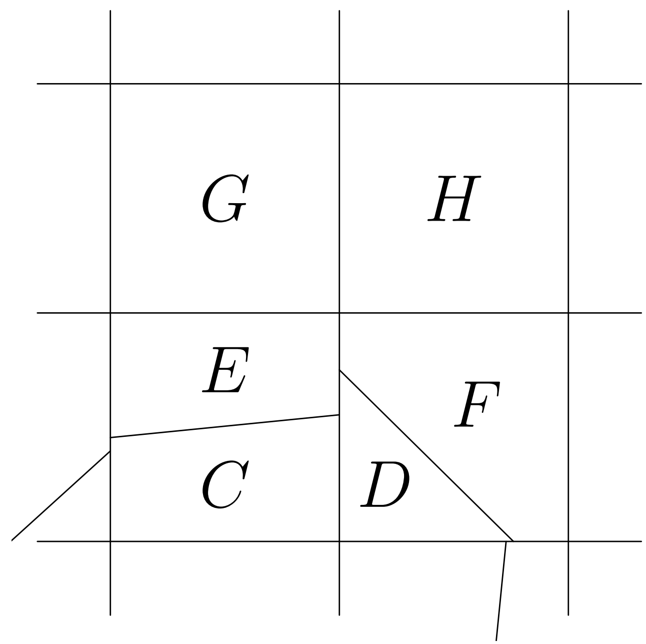
$$c^2 = \left(\frac{\partial p}{\partial \rho}\right)_S = -V^2 \left(\frac{\partial p}{\partial V}\right)_S > 0$$

Finite Volume Wave Propagation Method

- Finite volume method, Q_S^n gives approximate value of cell average of solution q over cell S at time t_n

$$Q_S^n \approx \frac{1}{\mathcal{M}(S)} \int_S q(X, t_n)\, dV$$

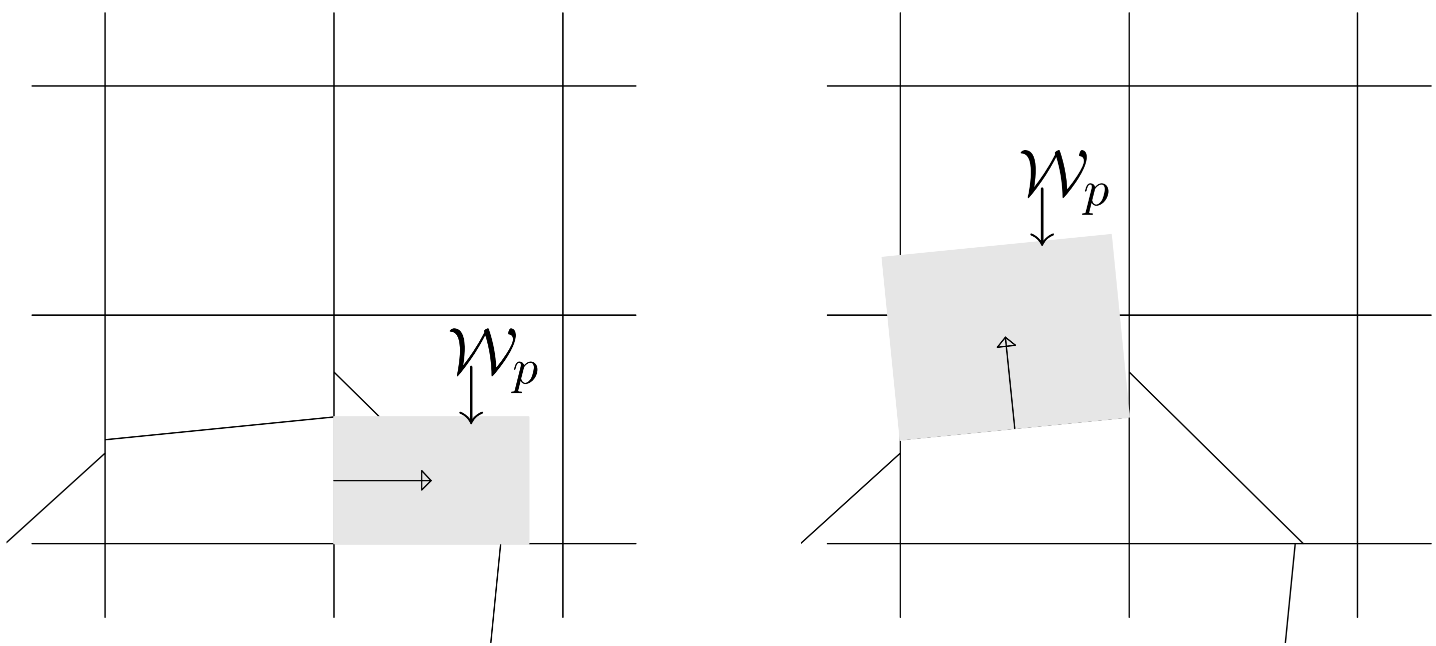
$\mathcal{M}(S)$: measure (area in 2D or volume in 3D) of cell S



Wave Propagation Method (cont.)

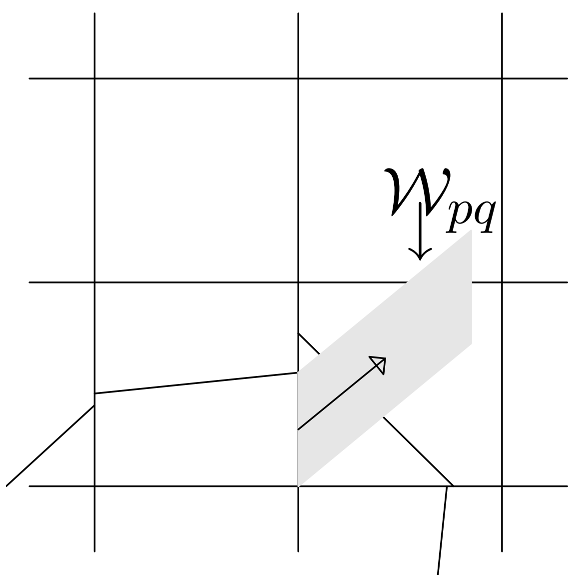
- First order version: Piecewise constant wave update
  - Godunov-type method: Solve Riemann problem at each cell interface in normal direction & use resulting waves to update cell averages

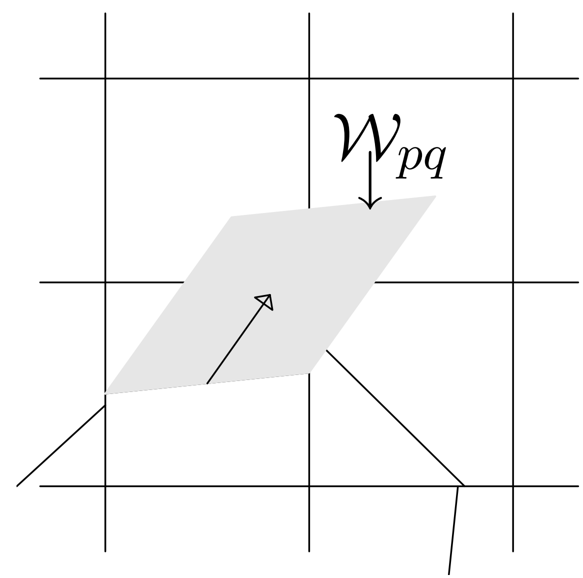
$$Q_S^{n+1} := Q_S^{n+1} - \frac{\mathcal{M}\left(\mathcal{W}_p \cap S\right)}{\mathcal{M}(S)} R_p, \qquad R_p \text{ being jump from RP}$$



Wave Propagation Method (cont.)

- First order version: Transverse-wave included
  - Use transverse portion of equation, solve Riemann problem in transverse direction, & use resulting waves to update cell averages as usual
  - Stability of method is typically improved, while conservation of method is maintained

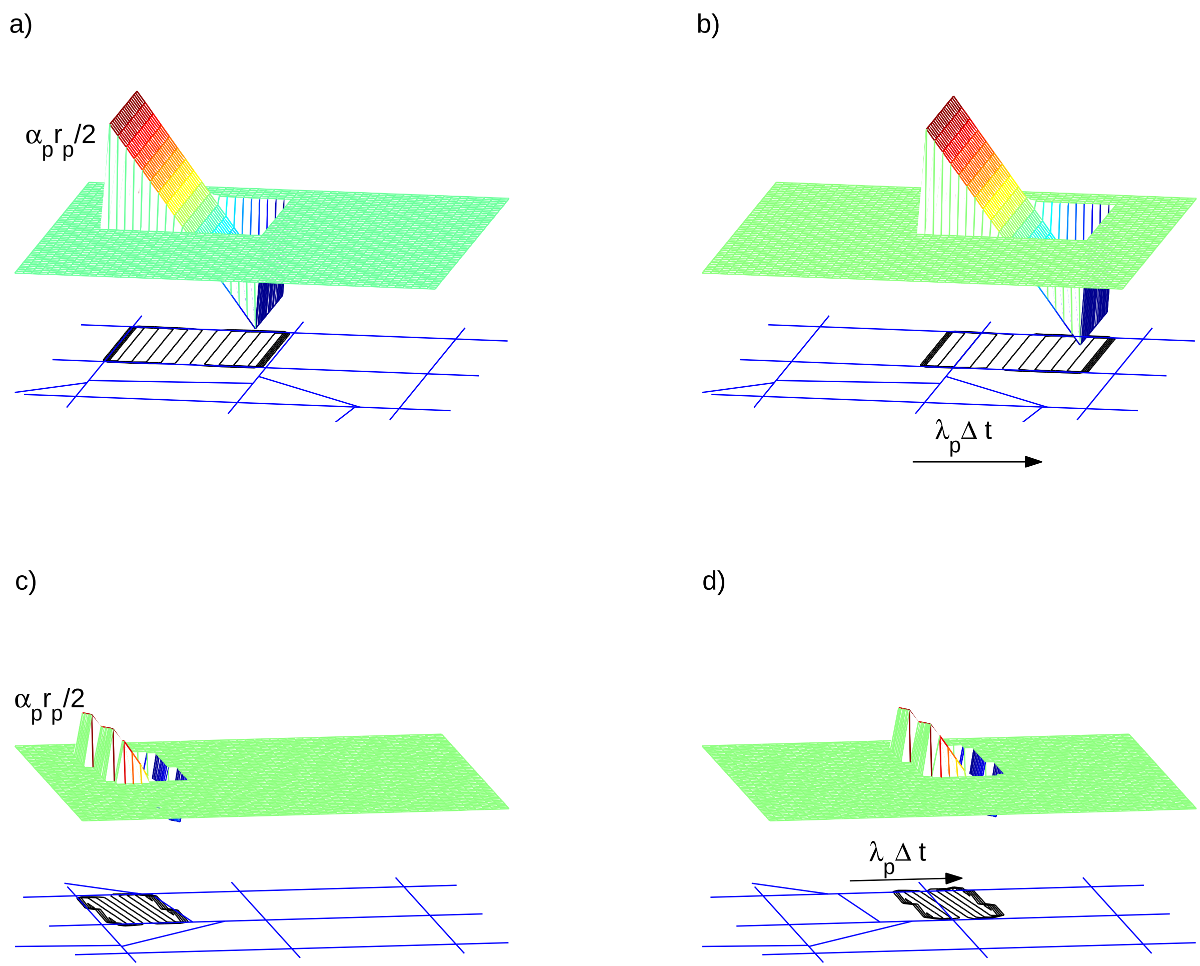




Wave Propagation Method (cont.)

- High resolution version: Piecewise linear wave update

wave before propagation after propagation



Volume Tracking Algorithm

1. Volume moving procedure
   (a) Volume fraction update
   Take a time step on current grid to update cell averages of volume fractions at next time step
   (b) Interface reconstruction
   Find new interface location based on volume fractions obtained in (a) using an interface reconstruction scheme. Some cells will be subdivided & values in each subcell must be initialized.
2. Physical solution update
   Take same time interval as in (a), but use a method to update cell averages of multicomponent model on new grid created in (b)

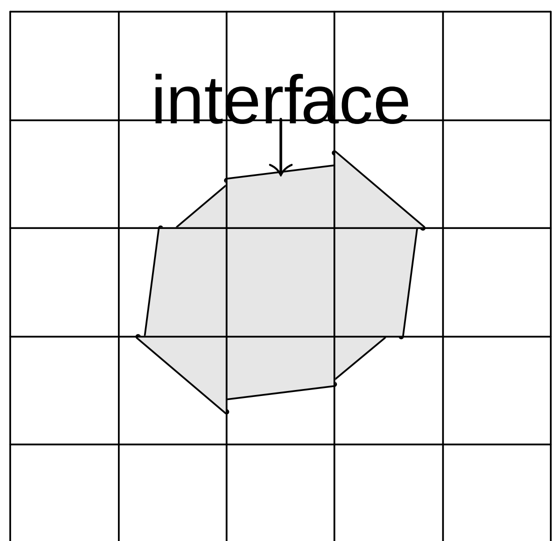
Interface Reconstruction Scheme

- Given volume fractions on current grid, piecewise linear interface reconstruction (PLIC) method does:
  1. Compute interface normal
     - Gradient method of Parker and Youngs
     - Least squares method of Puckett
  2. Determine interface location by iterative bisection

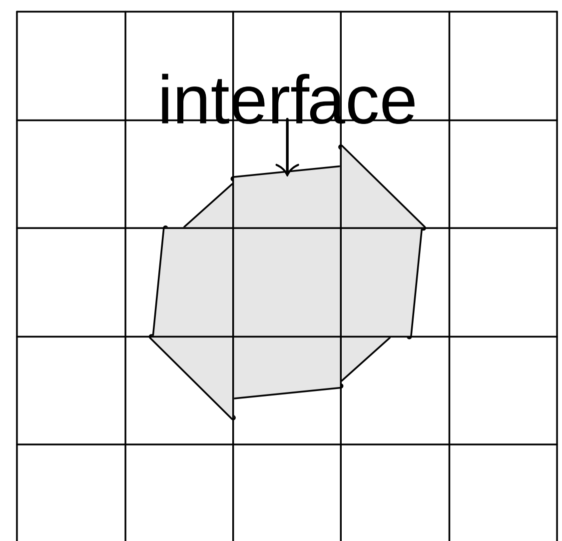
Data set

0	0	0	0	0
0	0.09	0.51	0.29	0
0	0.68	1	0.68	0
0	0.29	0.51	0.09	0
0	0	0	0	0

Parker & Youngs



Puckett



Volume Moving Procedure

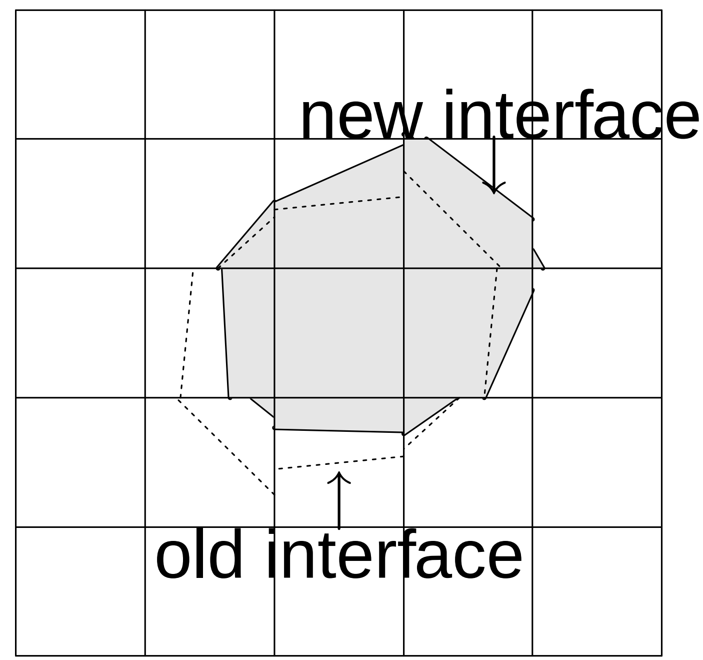
(a) Volume fractions given in previous slide are updated with uniform $(u,v)=(1,1)$ over $\Delta t = 0.06$

(b) New interface location is reconstructed

(a)

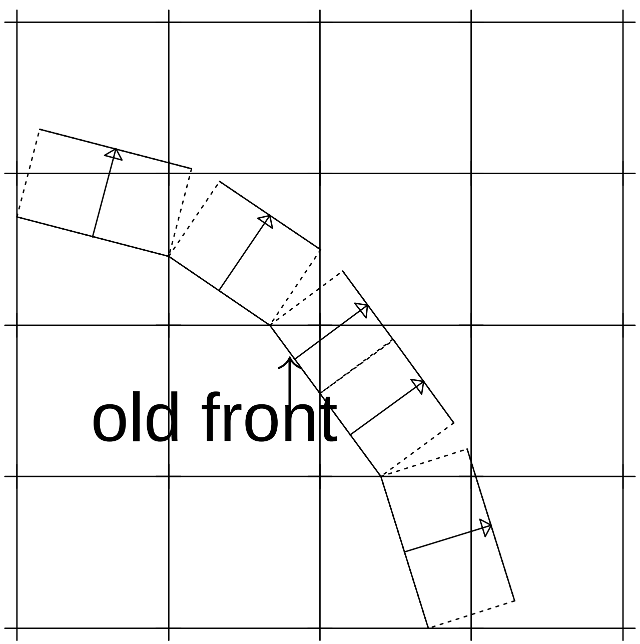
0	0	0	$1(-3)$	0
0	0.11	0.72	0.74	$5(-3)$
0	0.38	1	0.85	0
0	0.01	0.25	0.06	0
0	0	0	0	0

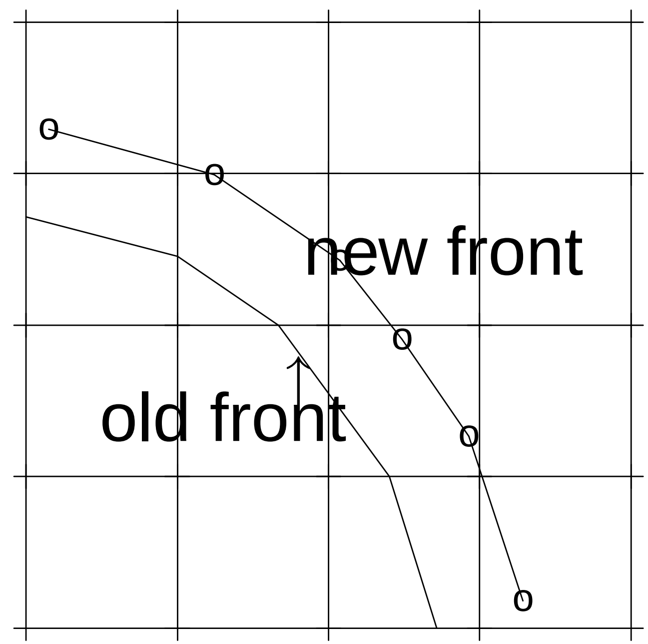
(b)



Surface Moving Procedure

- Solve Riemann problem at tracked interfaces & use resulting waves to find new location of interface at the next time step





Interface Conditions

- For tracked segments representing rigid (solid wall) boundary (stationary or moving), appropriate boundary states are assigned for fictitious subcells in each time step
- For tracked segments representing material interfaces, jump conditions across interfaces are satisfied only in an approximate manner, & would not be imposed explicitly in each time step

Stability Issues

- Choose time step Δt based on uniform grid mesh size Δx, Δy as

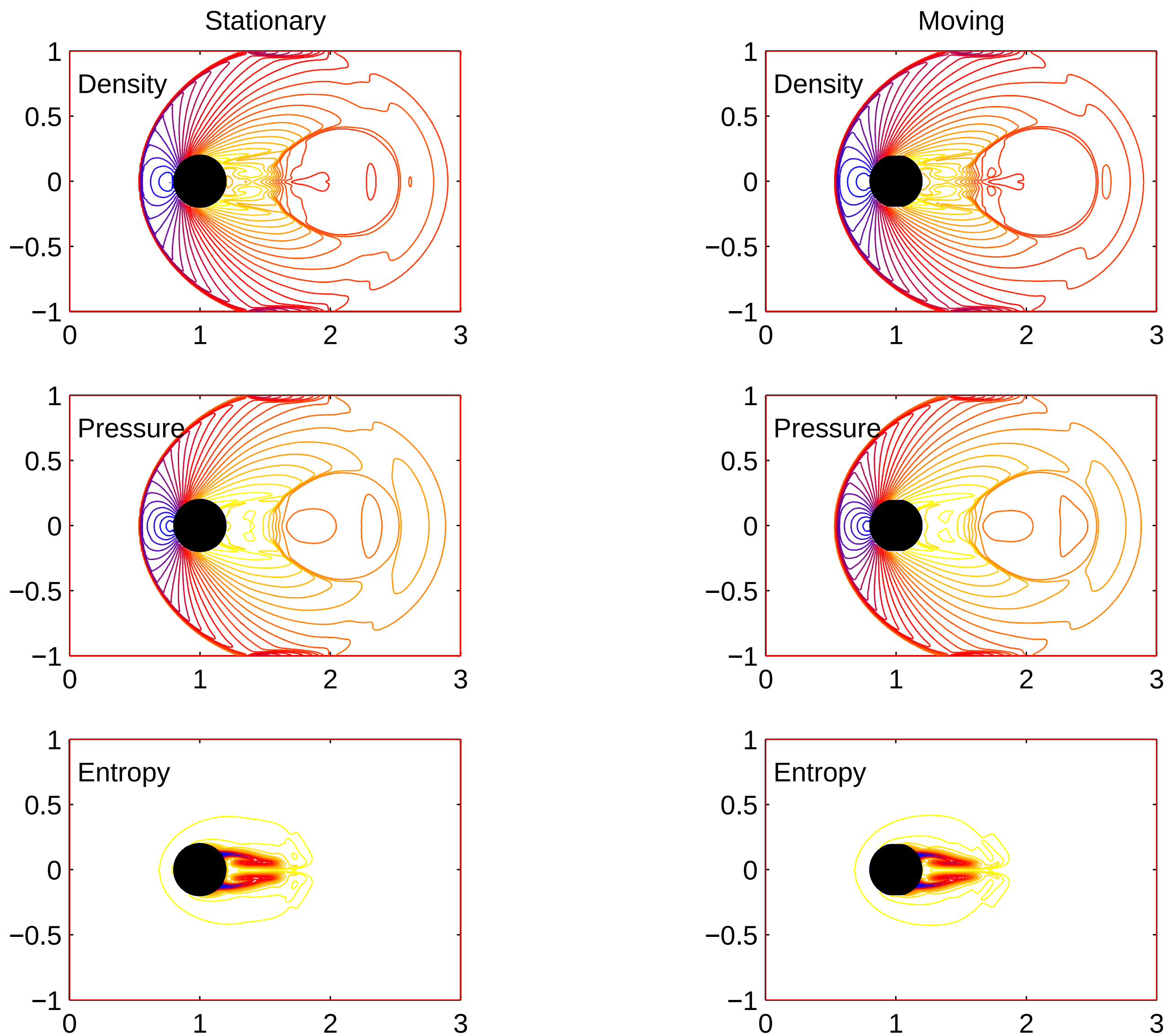
$$\frac{\Delta t \ \max_{p,q}\left(\lambda_p, \mu_q\right)}{\min(\Delta x, \Delta y)} \leq 1,$$

  - λ_p, μ_q: speed of p-wave, q-wave from Riemann problem solution in normal-, transverse-directions
- Use large time step method of LeVeque (*i.e.*, wave interactions are assumed to behave in linear manner) to maintain stability of method even in the presence of small Cartesian cut cells
- Apply interpolation operator (such as, h-box approach of Berger *et al.*) locally for cell averages in irregular cells

References

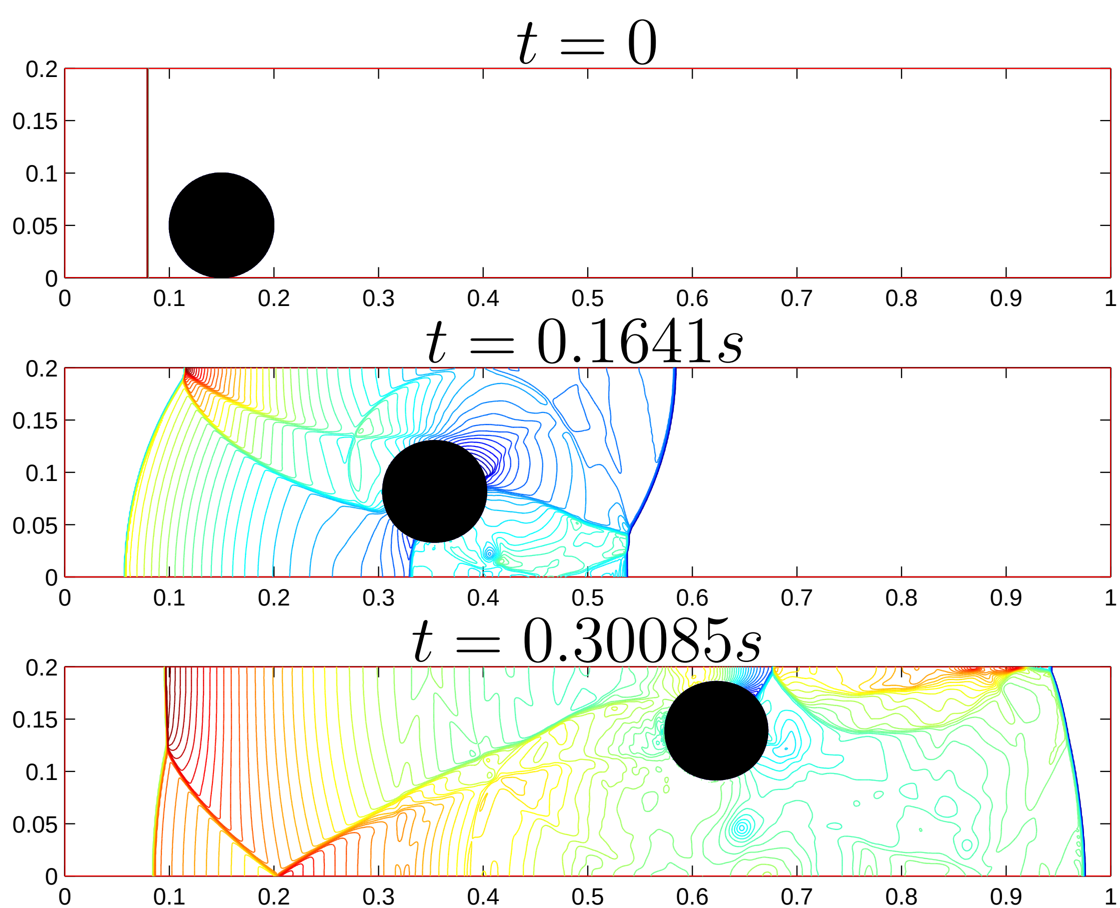
- (JCP 1998) An efficient shock-capturing algorithm for compressible multicomponent problems
- (JCP 1999, 2001) A fluid-mixture type algorithm for compressible multicomponent flow with van der Waals (Mie-Grüneisen) equation of state
- (JCP 2004) A fluid-mixture type algorithm for barotropic two-fluid flow Problems
- (JCP 2006) A wave-propagation based volume tracking method for compressible multicomponent flow in two space dimensions
- (Shock Waves 2006) A volume-fraction based algorithm for hybrid barotropic & non-barotropic two-fluid flow problems

Flying Projectile Problem



Cylinder lift-off Problem

- Moving speed of cylinder is governed by Newton's law
- Pressure contours are shown with a 1000×200 grid



Cylinder lift-off Problem

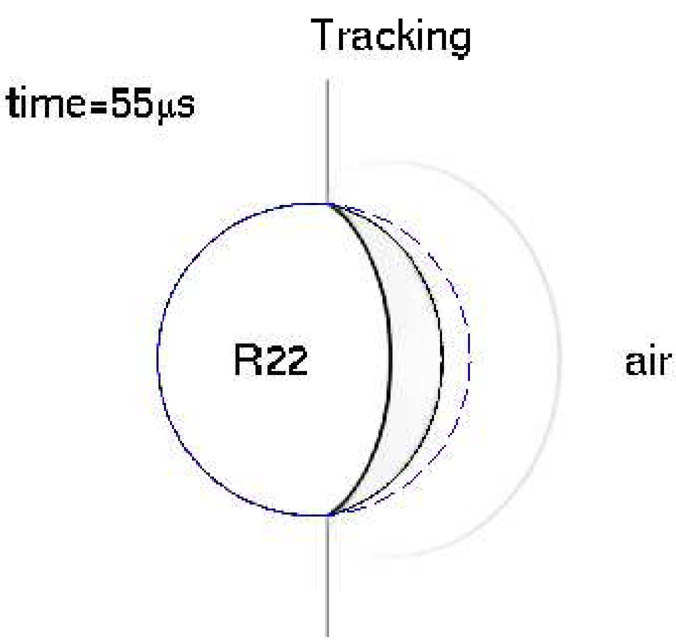
- A convergence study of center of cylinder & relative mass loss for at final stopping time $t = 0.30085s$

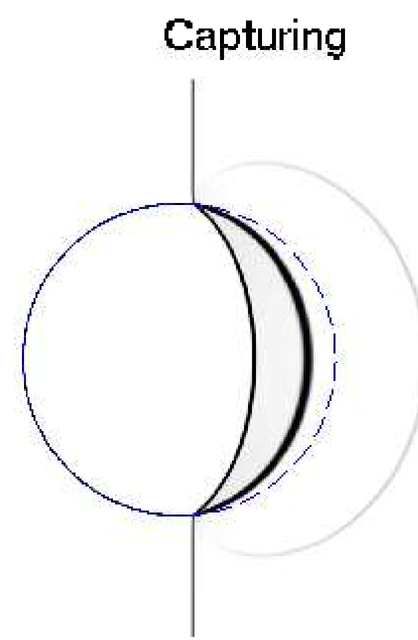
Mesh size	Center of cylinder	Relative mass loss
250×50	$(0.618181, 0.134456)$	-0.257528
500×100	$(0.620266, 0.136807)$	-0.131474
1000×200	$(0.623075, 0.138929)$	-0.066984

- Results are comparable with numerical appeared in literature

Shock in Air & R22 Bubble Interaction

- Leftward-going Mach 1.22 shock wave in air over heavier R22 bubble
- Numerical schlieren images for density





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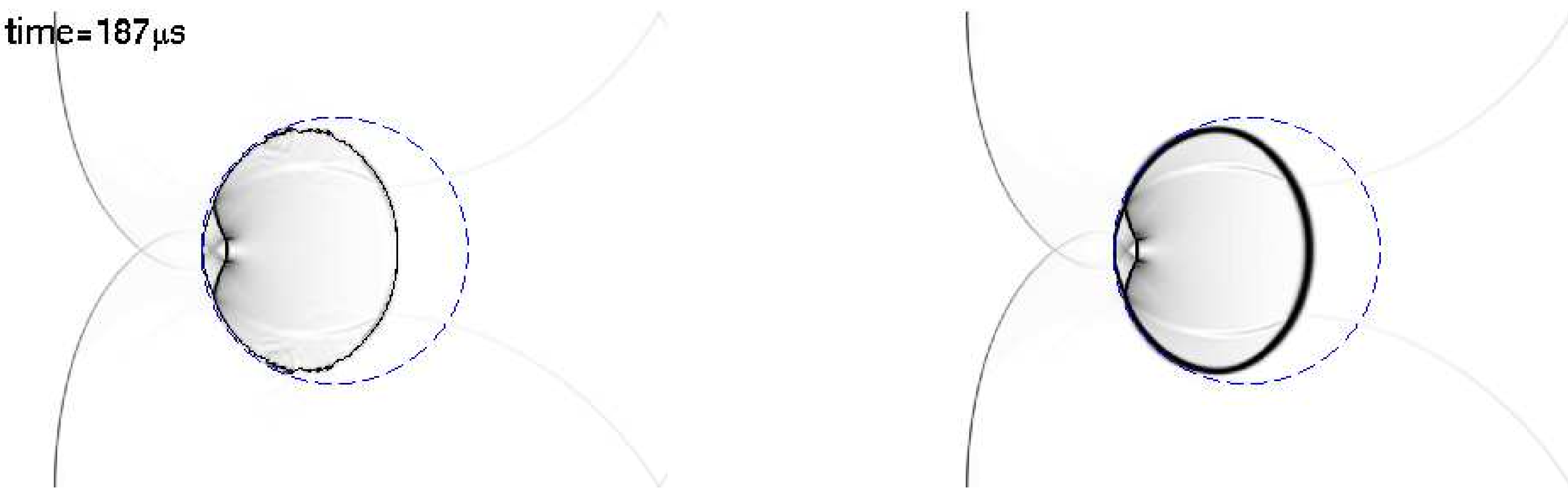

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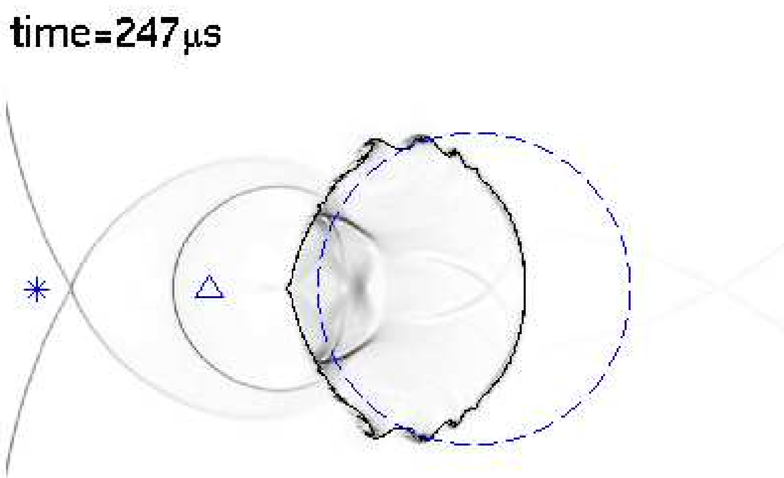

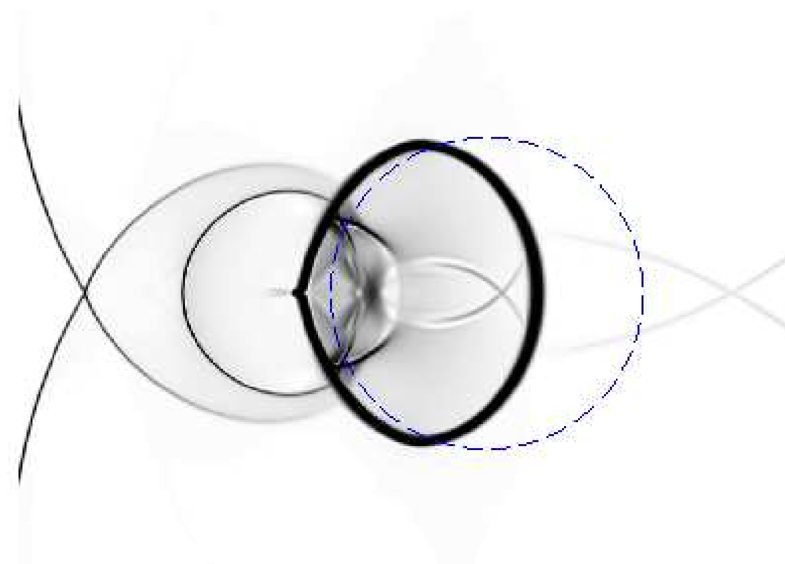

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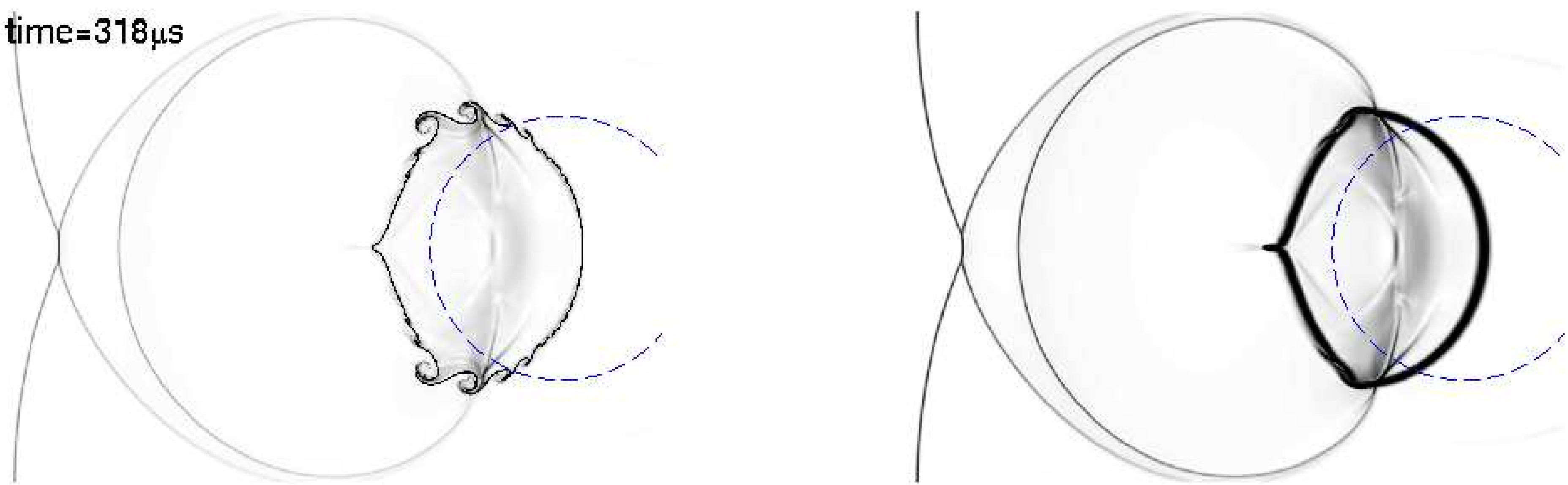

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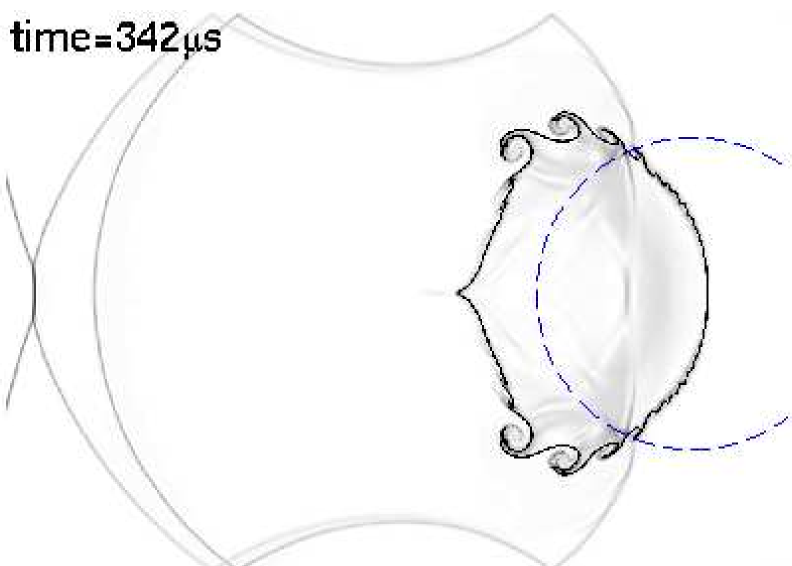

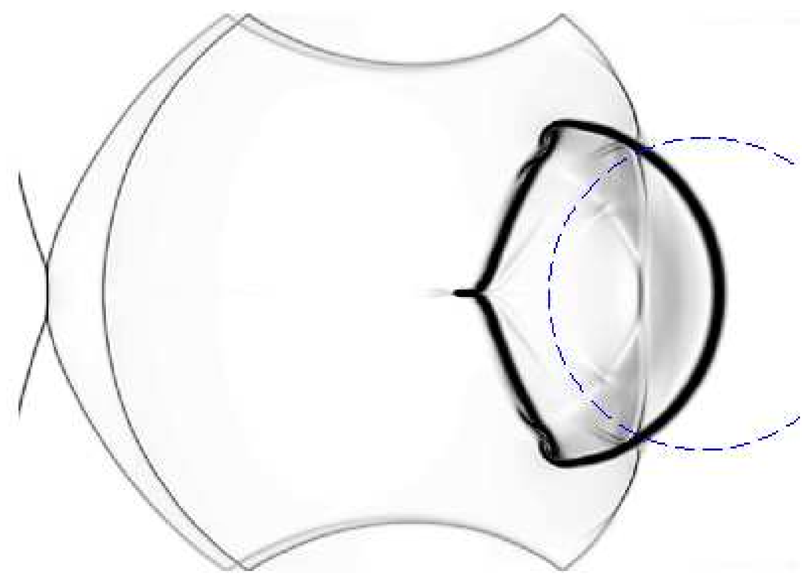

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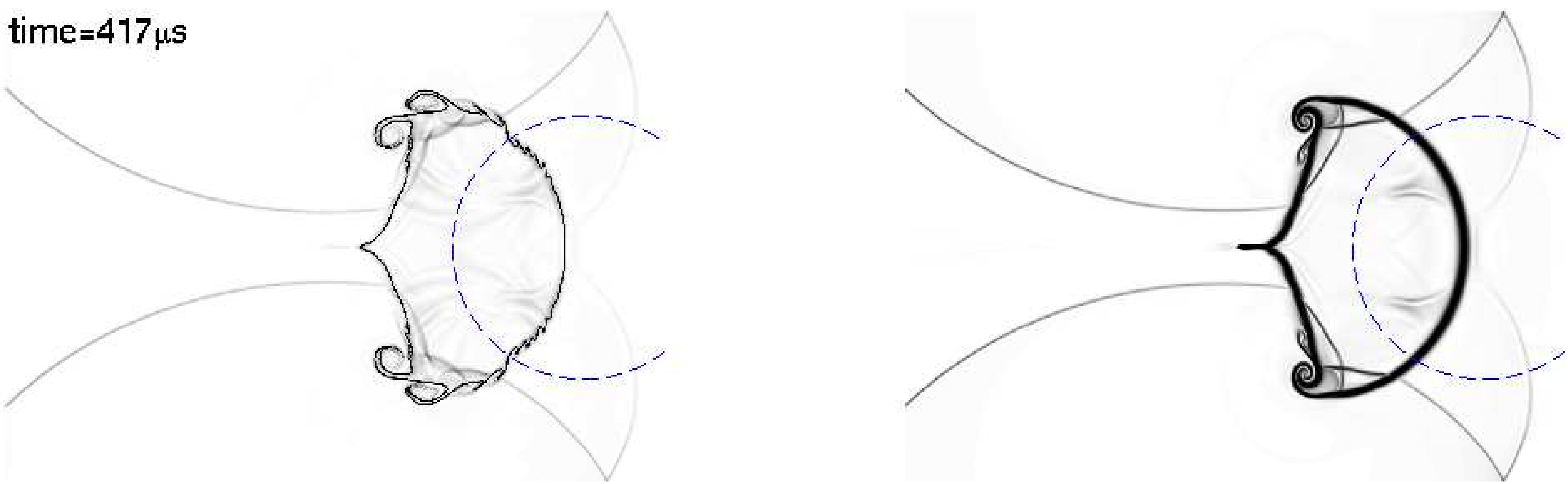

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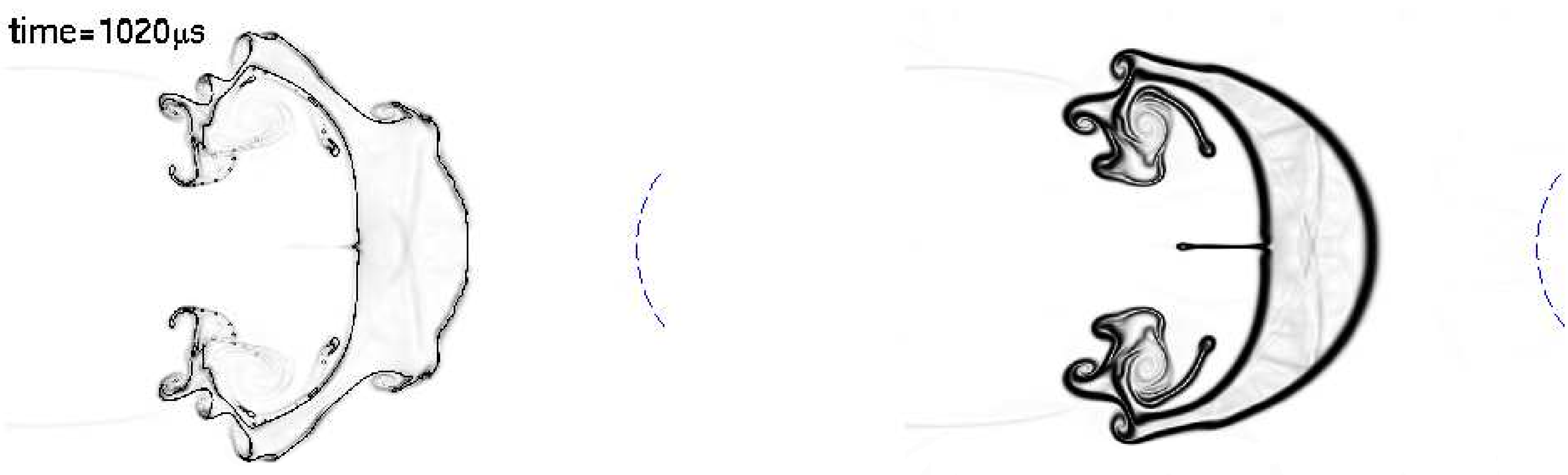
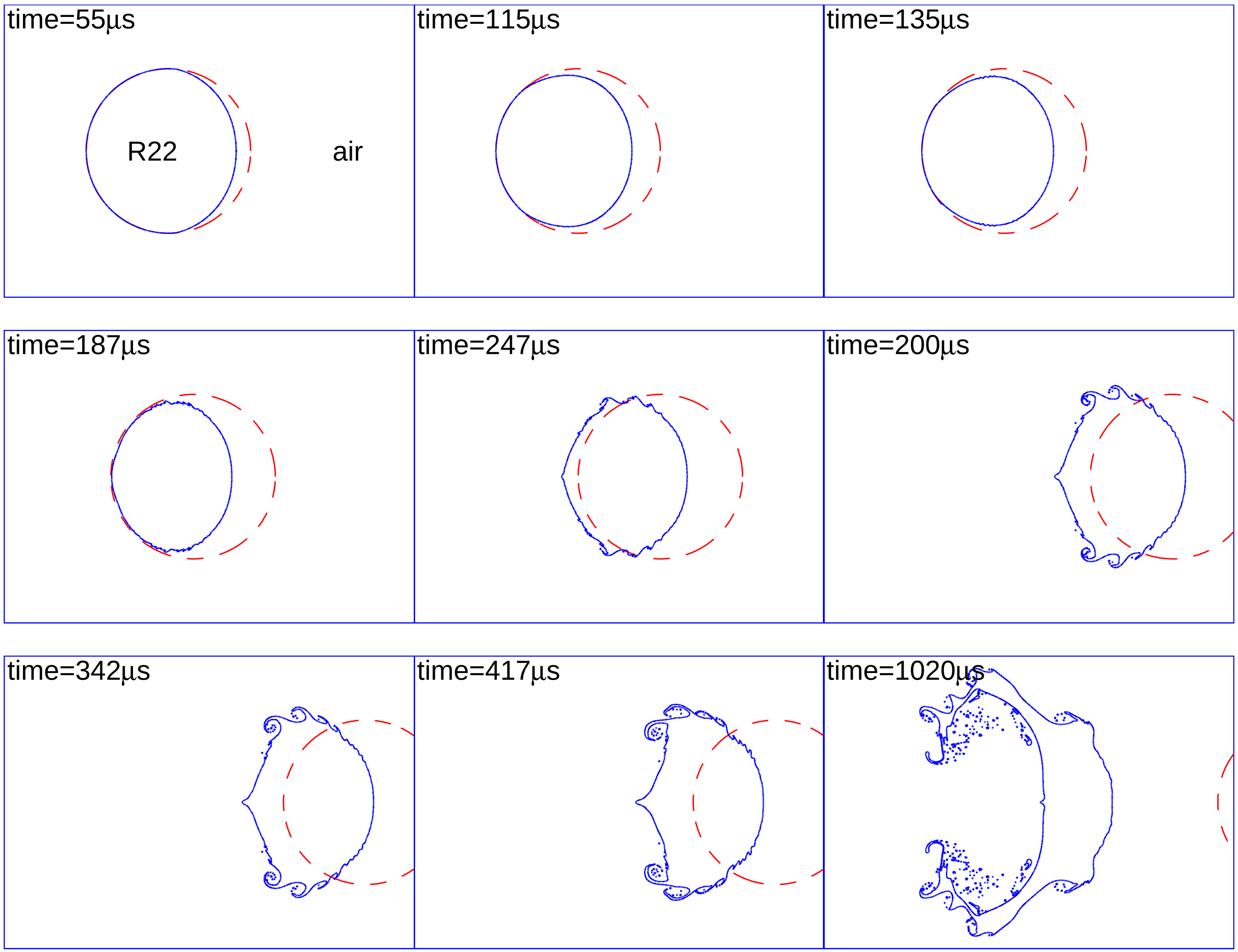


Shock-Bubble Interaction (cont.)

- Approximate locations of interfaces



Shock-Bubble Interaction (cont.)

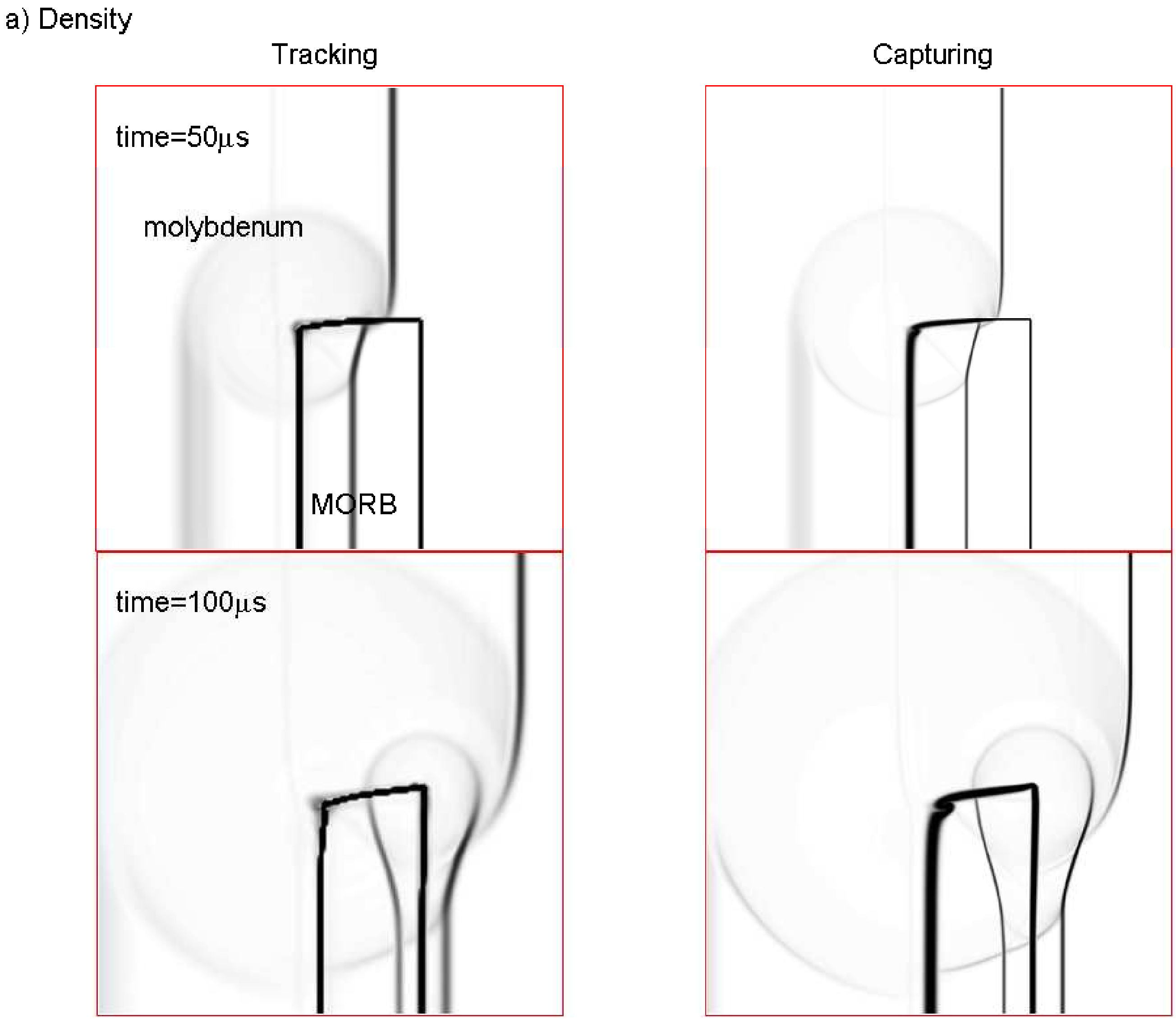
- Quantitative assessment of prominent flow velocities:

Velocity (m/s)	V_s	V_R	V_T	V_{ui}	V_{uf}	V_{di}	V_{df}
Haas & Sturtevant	415	240	540	73	90	78	78
Quirk & Karni	420	254	560	74	90	116	82
Our result (tracking)	411	243	538	64	87	82	60
Our result (capturing)	411	244	534	65	86	98	76

- V_s (V_R, V_T) Incident (refracted, transmitted) shock speed $t \in [0, 250]\mu$s ($t \in [0, 202]\mu$s, $t \in [202, 250]\mu$s)
- V_{ui} (V_{uf}) Initial (final) upstream bubble wall speed $t \in [0, 400]\mu$s ($t \in [400, 1000]\mu$s)
- V_{di} (V_{df}) Initial (final) downstream bubble wall speed $t \in [200, 400]\mu$s ($t \in [400, 1000]\mu$s)

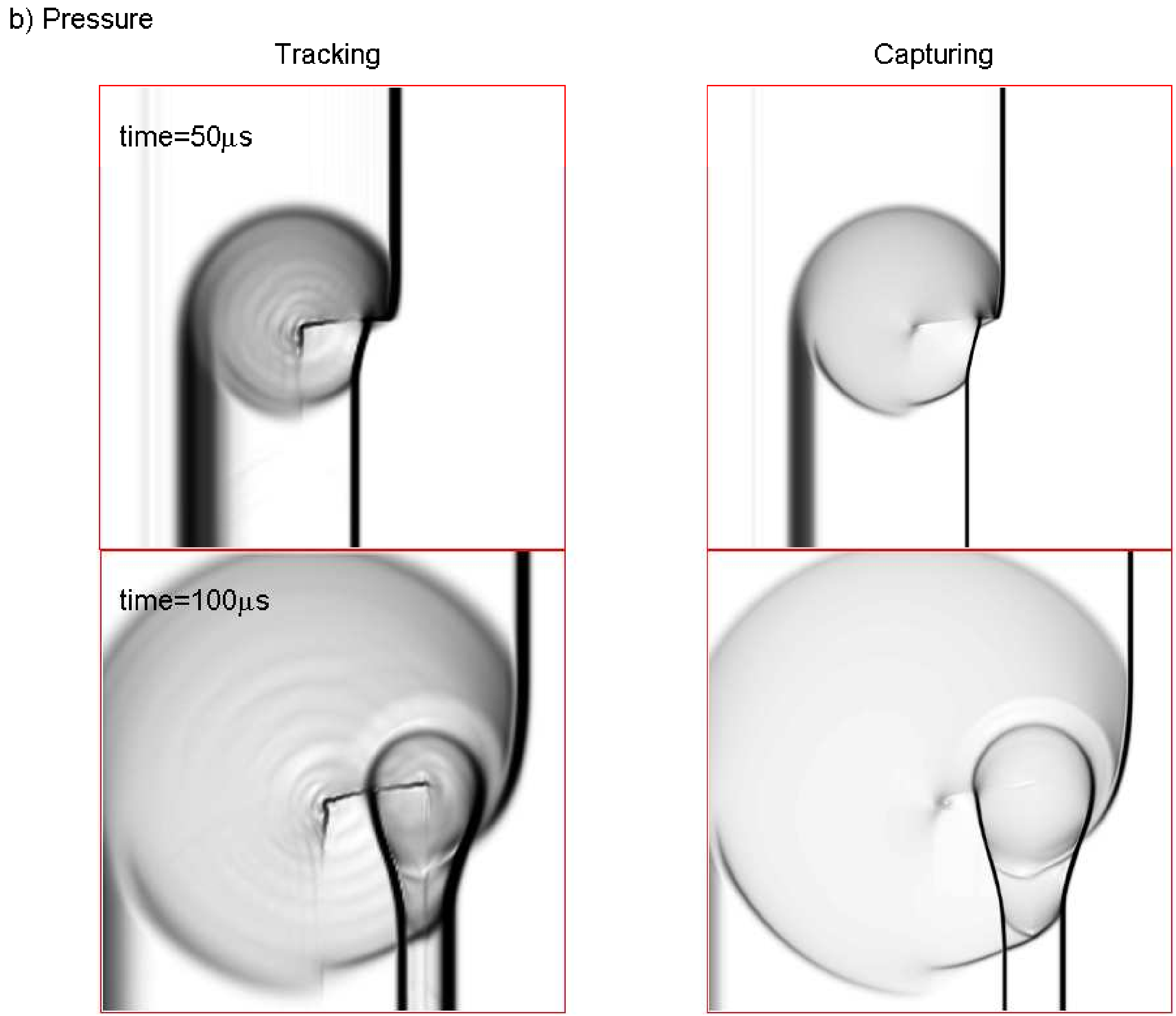
Shock wave in molybdenum over MORB

- Numerical schlieren images for density



Shock-MORB Interaction (cont.)

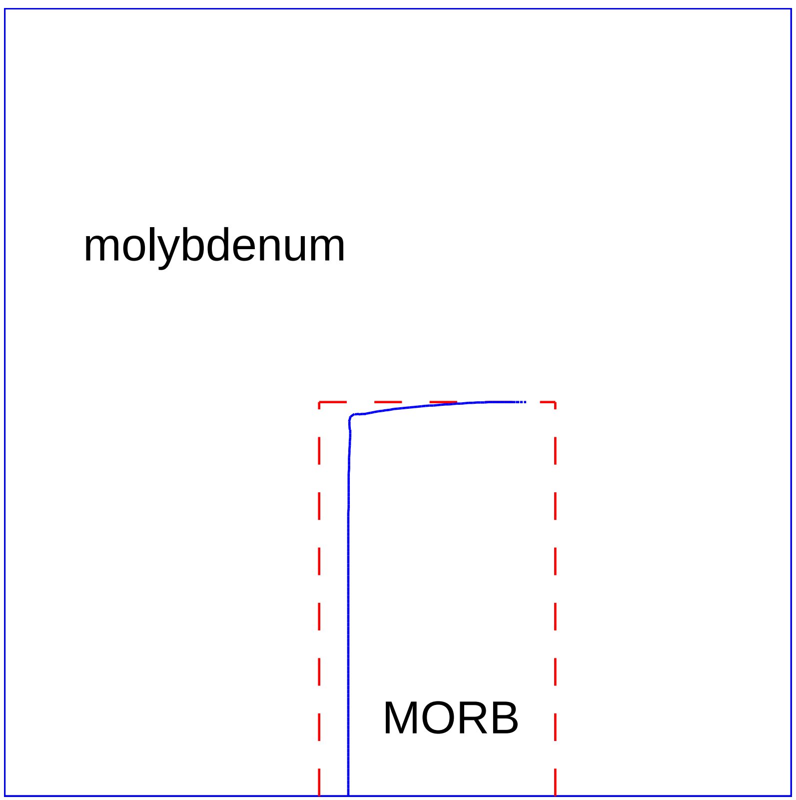
- Numerical schlieren images for pressure



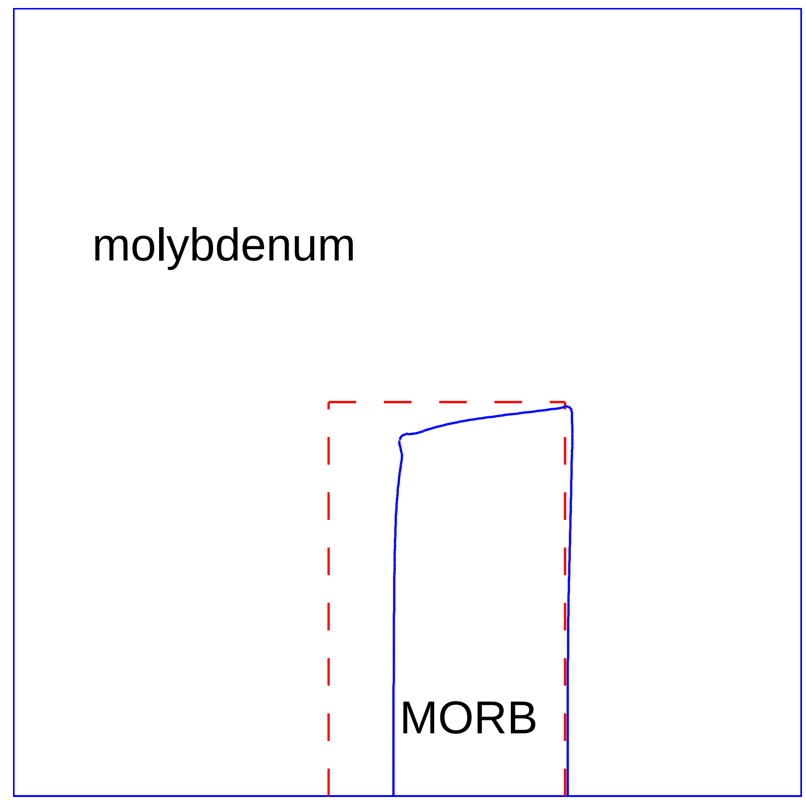
Shock-MORB Interaction (cont.)

- Approximate locations of interfaces

time = 50μs



time = 100μs



Future Work

- Extension to low Mach number flow
  - Remove sound-speed stiffness by preconditioning techniques or pressure-based method
- Extension to include more physics towards real applications
  - Such as capillary, diffusion, or elastic-plastic effect
- Extension to 3D volume tracking method
  - Surface reconstruction
  - Finite volume method with moving interfaces
  - Stability in presence of small cut cells
- Extension to unified coordinates of W.-H. Hui

Thank You