Wave-propagation based methods for compressible homogeneous two-phase flow

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Outline

- Eulerian formulation
  - Mathematical models
  - Wave-propagation based volume tracking method
  - Sample examples
- Generalized Lagrangian formulation
  - Mathematical models
  - Flux-based wave decomposition method
  - Sample examples
- Future work

Two-Phase Flow Model (I)

- Baer & Nunziato (J. Multiphase Flow 1986)

$$(\alpha_1\rho_1)_t + \nabla\cdot(\alpha_1\rho_1\vec{u}_1) = 0$$

$$(\alpha_1\rho_1\vec{u}_1)_t + \nabla\cdot(\alpha_1\rho_1\vec{u}_1\otimes\vec{u}_1) + \nabla(\alpha_1 p_1) = p_0\nabla\alpha_1 + \lambda(\vec{u}_2-\vec{u}_1)$$

$$(\alpha_1\rho_1 E_1)_t + \nabla\cdot(\alpha_1\rho_1 E_1\vec{u}_1 + \alpha_1 p_1\vec{u}_1) = p_0\,(\alpha_2)_t + \lambda\vec{u}_0\cdot(\vec{u}_2-\vec{u}_1)$$

$$(\alpha_2\rho_2)_t + \nabla\cdot(\alpha_2\rho_2\vec{u}_2) = 0$$

$$(\alpha_2\rho_2\vec{u}_2)_t + \nabla\cdot(\alpha_2\rho_2\vec{u}_2\otimes\vec{u}_2) + \nabla(\alpha_2 p_2) = p_0\nabla\alpha_2 - \lambda(\vec{u}_2-\vec{u}_1)$$

$$(\alpha_2\rho_2 E_2)_t + \nabla\cdot(\alpha_2\rho_2 E_2\vec{u}_2 + \alpha_2 p_2\vec{u}_2) = -p_0\,(\alpha_2)_t - \lambda\vec{u}_0\cdot(\vec{u}_2-\vec{u}_1)$$

$$(\alpha_2)_t + \vec{u}_0\cdot\nabla\alpha_2 = \mu\,(p_2-p_1)$$

$\alpha_k = V_k/V$: volume fraction for phase k ($\alpha_1+\alpha_2=1$)
z_k: global state for phase k, z_0: local interface state
λ: velocity relaxation parameter, μ: pressure relaxation

Two-Phase Flow Model (II)

- Saurel & Gallouet (1998)

$$(\alpha_1\rho_1)_t + \nabla\cdot(\alpha_1\rho_1\vec{u}_1) = \dot{m}$$

$$(\alpha_1\rho_1\vec{u}_1)_t + \nabla\cdot(\alpha_1\rho_1\vec{u}_1\otimes\vec{u}_1) + \nabla(\alpha_1 p_1) = p_0\nabla\alpha_1 + \dot{m}\vec{u}_0 + F_d$$

$$(\alpha_1\rho_1 E_1)_t + \nabla\cdot(\alpha_1\rho_1 E_1\vec{u}_1 + \alpha_1 p_1\vec{u}_1) = p_0\,(\alpha_2)_t + \dot{m}E_0 + F_d\vec{u}_0 + Q$$

$$(\alpha_2\rho_2)_t + \nabla\cdot(\alpha_2\rho_2\vec{u}_2) = -\dot{m}$$

$$(\alpha_2\rho_2\vec{u}_2)_t + \nabla\cdot(\alpha_2\rho_2\vec{u}_2\otimes\vec{u}_2) + \nabla(\alpha_2 p_2) = p_0\nabla\alpha_2 - \dot{m}\vec{u}_0 - F_d$$

$$(\alpha_2\rho_2 E_2)_t + \nabla\cdot(\alpha_2\rho_2 E_2\vec{u}_2 + \alpha_2 p_2\vec{u}_2) = -p_0\,(\alpha_2)_t - \dot{m}E_0 - F_d\vec{u}_0 -$$

$$(\alpha_2)_t + \vec{u}_0\cdot\nabla\alpha_2 = \mu\,(p_2 - p_1)$$

$\dot{m}$: mass transfer, F_d: drag force

Q_0: convective heat exchange

Two-Phase Flow Model (cont.)

p_0 & $\vec{u}_0$: interfacial pressure & velocity

- Baer & Nunziato (1986)
  - $p_0 = p_2, \quad \vec{u}_0 = \vec{u}_1$
- Saurel & Abgrall (1999)
  - $p_0 = \sum_{k=1}^{2} \alpha_k p_k, \quad \vec{u}_0 = \sum_{k=1}^{2} \alpha_k \rho_k \vec{u}_k \Big/ \sum_{k=1}^{2} \alpha_k \rho_k$

λ & μ (> 0): relaxation parameters that determine rates at which velocities and pressures of two phases reach equilibrium

Two-Phase Flow Model: Derivation

- Standard way to derive these equations is 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 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

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

this leads to mass averaged equation for phase k

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

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

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

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

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

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

Note: existence of various interfacial source terms

Mathematical as well as numerical modelling of these terms are important (but difficult) for general multiphase flow problems

Reduced Two-Phase Flow Model

- Murrone & Guillard (JCP 2005)
  - Assume $\lambda = \lambda^{'}/\varepsilon$ & $\mu = \mu^{'}/\varepsilon$, $\lambda^{'} = O(1)$ & $\mu^{'} = O(1)$
  - Apply formal asymptotic analysis to Baer & Nunziato's model, as $\varepsilon \to 0$, gives leading order approximation

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

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

$$(\rho\vec{u})_t + \nabla \cdot (\rho\vec{u} \otimes \vec{u}) + \nabla p = 0 \qquad \text{(mixture momentum)}$$

$$(\rho E)_t + \nabla \cdot (\rho E\vec{u} + p\vec{u}) = 0 \qquad \text{(mixture total energy)}$$

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

Reduced Two-Phase Model (cont.)

Remarks:

1. In this case, $p_1 \to p_2$ & $\vec{u}_1 \to \vec{u}_2$, as $\varepsilon \to 0$, which means the flow is homogeneous (1-pressure & 1-velocity) with $p_\iota = p$ & $\vec{u}_\iota = \vec{u}$, $\iota = 0, 1, 2$, across interfaces
2. Mixture equation of state: $p = p(\alpha_2,\ \alpha_1\rho_1,\ \alpha_2\rho_2,\ \rho e)$
3. Isobaric closure: $p_1 = p_2 = p$
   - For some EOS, explicit formula for p is available (examples are given next)
   - For some other EOS, p is found by solving coupled equations

$$p_1(\rho_1, \rho_1 e_1) = p_2(\rho_2, \rho_2 e_2) \quad \& \quad \alpha_1\rho_1 e_1 + \alpha_2\rho_2 e_2 = \rho e$$

Reduced Two-Phase Model (cont.)

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

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

$$p = \rho e \Bigg/ \sum_{k=1}^{2} \frac{\alpha_k}{\gamma_k - 1}$$

Reduced Two-Phase Model (cont.)

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

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

$$p = \rho e \bigg/ \sum_{k=1}^{2} \frac{\alpha_k}{\gamma_k - 1}$$

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

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

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

Reduced Two-Phase 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

$$\begin{aligned}
\rho e = \sum_{k=1}^{2} \alpha_k \rho_k e_k &= \sum_{k=1}^{2} \alpha_k \left[\left(\frac{\rho_k R_k T_k}{\gamma_k - 1} \right) + \frac{\rho_k R_k T_{\text{vib},k}}{\exp\left(T_{\text{vib},k}/T_k\right) - 1} \right] \\
&= \sum_{k=1}^{2} \alpha_k \left[\left(\frac{p}{\gamma_k - 1} \right) + \frac{p_{\text{vib},k}}{\exp\left(p_{\text{vib},k}/p\right) - 1} \right] \quad \text{(Nonlinear eq.)}
\end{aligned}$$

Reduced Model: Remarks

4. It can be shown entropy of each phase $\mathcal{S}_k$ now satisfies

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

5. Model system is hyperbolic under suitable thermodynamic stability condition
6. When $\alpha_k = 0$, ρ_k can not be recovered from α_k & $\alpha_k \rho_k$, and so take $\alpha_k \in [\varepsilon, 1-\varepsilon]$, $\varepsilon \ll 1$
7. Other model systems exist in the literature that are more robust for homogeneous flow (examples)
8. When individual pressure law differs in form (see below), new mixture pressure law should be devised first & construct model equations based on that

Barotropic & Non-Barotropic Flow

- Fluid component 1: Tait EOS

$$p(\rho) = (p_0 + \mathcal{B}) \left(\frac{\rho}{\rho_0}\right)^{\gamma} - \mathcal{B}$$

- Fluid component 2: Noble-Abel EOS

$$p(\rho, e) = \left(\frac{\gamma - 1}{1 - b\rho}\right) \rho e$$

- Mixture pressure law (Shyue, Shock Waves 2006)

$$p = \begin{cases} (p_0 + \mathcal{B}) \left(\dfrac{\rho}{\rho_0}\right)^{\gamma} - \mathcal{B} & \text{if} \quad \alpha = 1 \\ \left(\dfrac{\gamma - 1}{1 - b\rho}\right) (\rho e - \mathcal{B}) - \mathcal{B} & \text{if} \quad \alpha \neq 1 \end{cases}$$

Barotropic Two-Phase Flow

- Fluid component ι: Tait EOS

$$p(\rho) = (p_{0\iota} + \mathcal{B}_\iota) \left(\frac{\rho}{\rho_{0\iota}} \right)^{\gamma_\iota} - \mathcal{B}_\iota, \quad \iota = 1, 2$$

- Mixture pressure law (Shyue, JCP 2004)

$$p = \begin{cases} (p_{0\iota} + \mathcal{B}_\iota) \left(\dfrac{\rho}{\rho_{0\iota}} \right)^{\gamma_\iota} - \mathcal{B}_\iota & \text{if} \quad \alpha = \alpha_\iota \ (0 \text{ or } 1) \\ (\gamma - 1)\, \rho \left(e + \dfrac{\mathcal{B}}{\rho_0} \right) - \gamma \mathcal{B} & \text{if} \quad \alpha \in (0, 1) \end{cases}$$

Homogeneous Two-Phase Model

In summary, mathematical model for compressible homogeneous two-phase flow:

- Equations of motion

$$
\begin{aligned}
&(\alpha_1\rho_1)_t + \nabla\cdot(\alpha_1\rho_1\vec{u}) = 0 \\
&(\alpha_2\rho_2)_t + \nabla\cdot(\alpha_2\rho_2\vec{u}) = 0 \\
&(\rho\vec{u})_t + \nabla\cdot(\rho\vec{u}\otimes\vec{u}) + \nabla p = 0 \\
&(\rho E)_t + \nabla\cdot(\rho E\vec{u} + p\vec{u}) = 0 \\
&(\alpha_2)_t + \vec{u}\cdot\nabla\alpha_2 = \alpha_1\alpha_2\left(\frac{\rho_1 c_1^2 - \rho_2 c_2^2}{\sum_{k=1}^{2}\alpha_k\rho_k c_k^2}\right)\nabla\cdot\vec{u}
\end{aligned}
$$

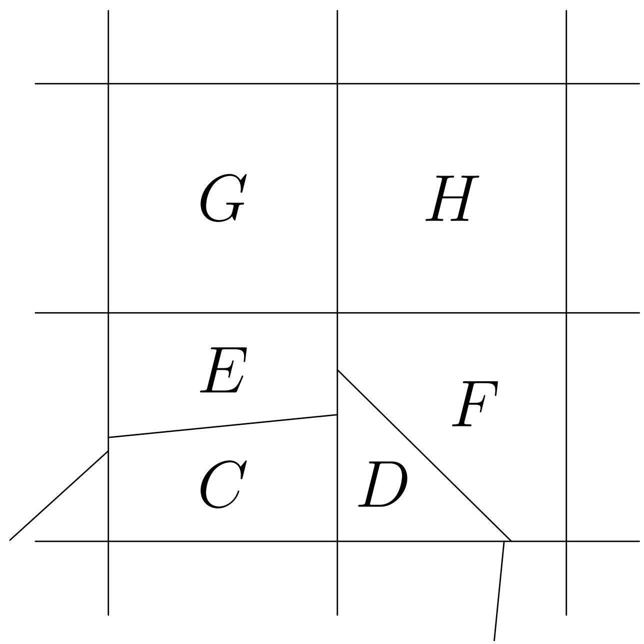
- Mixture equation of state: $p = p(\alpha_2,\ \alpha_1\rho_1,\ \alpha_2\rho_2,\ \rho e)$

Wave Propagation Method

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

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

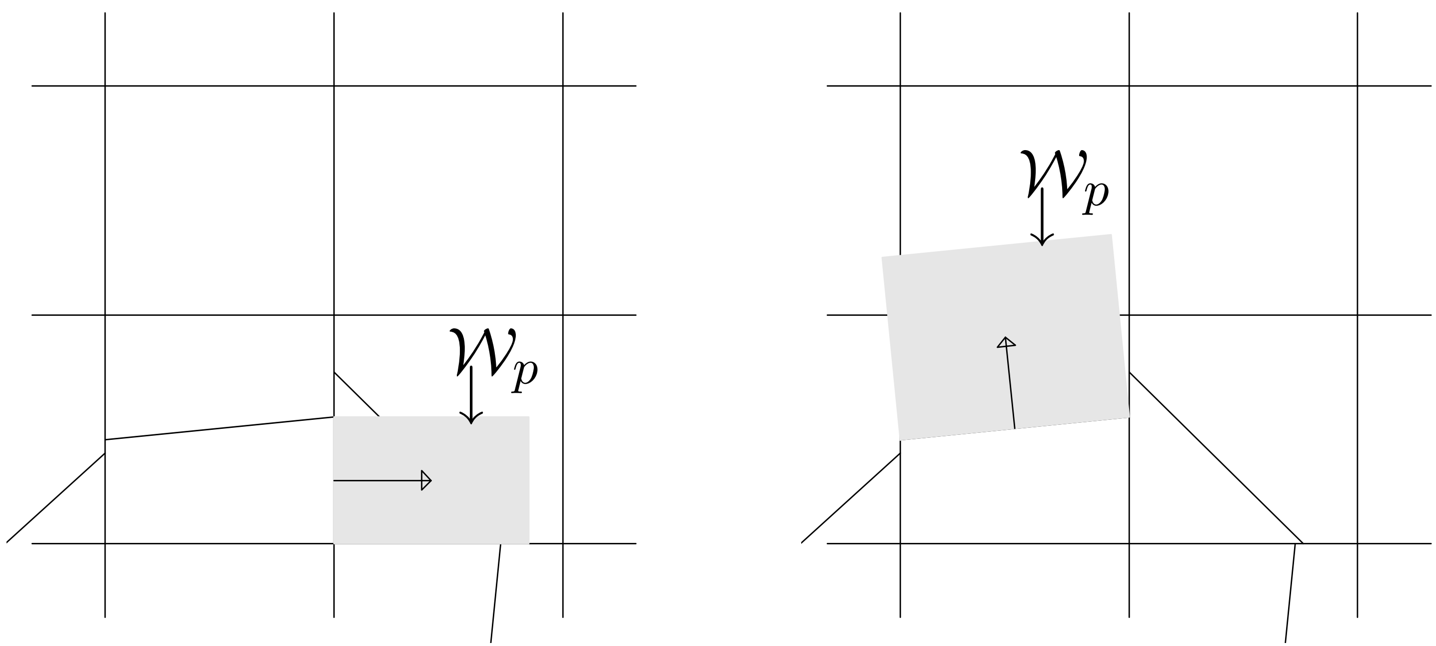
$\mathcal{M}(S)$: measure (area in 2D or volume in 3D) of cell S



Wave Propagation Method (cont.)

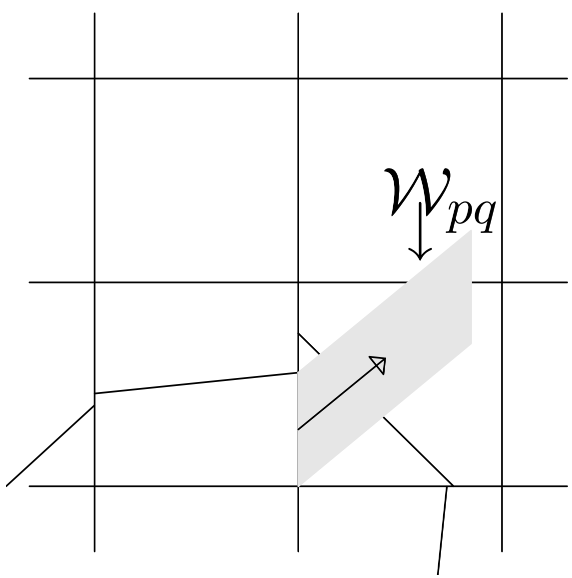
- First order version: Piecewise constant wave update
  - Godunov-type method: Solve Riemann problem at each cell interface in normal direction & use resulting waves to update cell averages

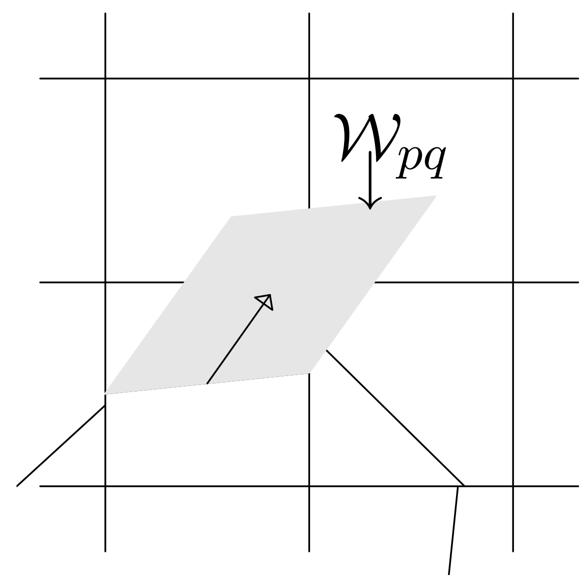
$$Q_S^{n+1} := Q_S^{n+1} - \frac{\mathcal{M}\left(\mathcal{W}_p \cap S\right)}{\mathcal{M}(S)} R_p, \qquad R_p \text{ being jump from RP}$$



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

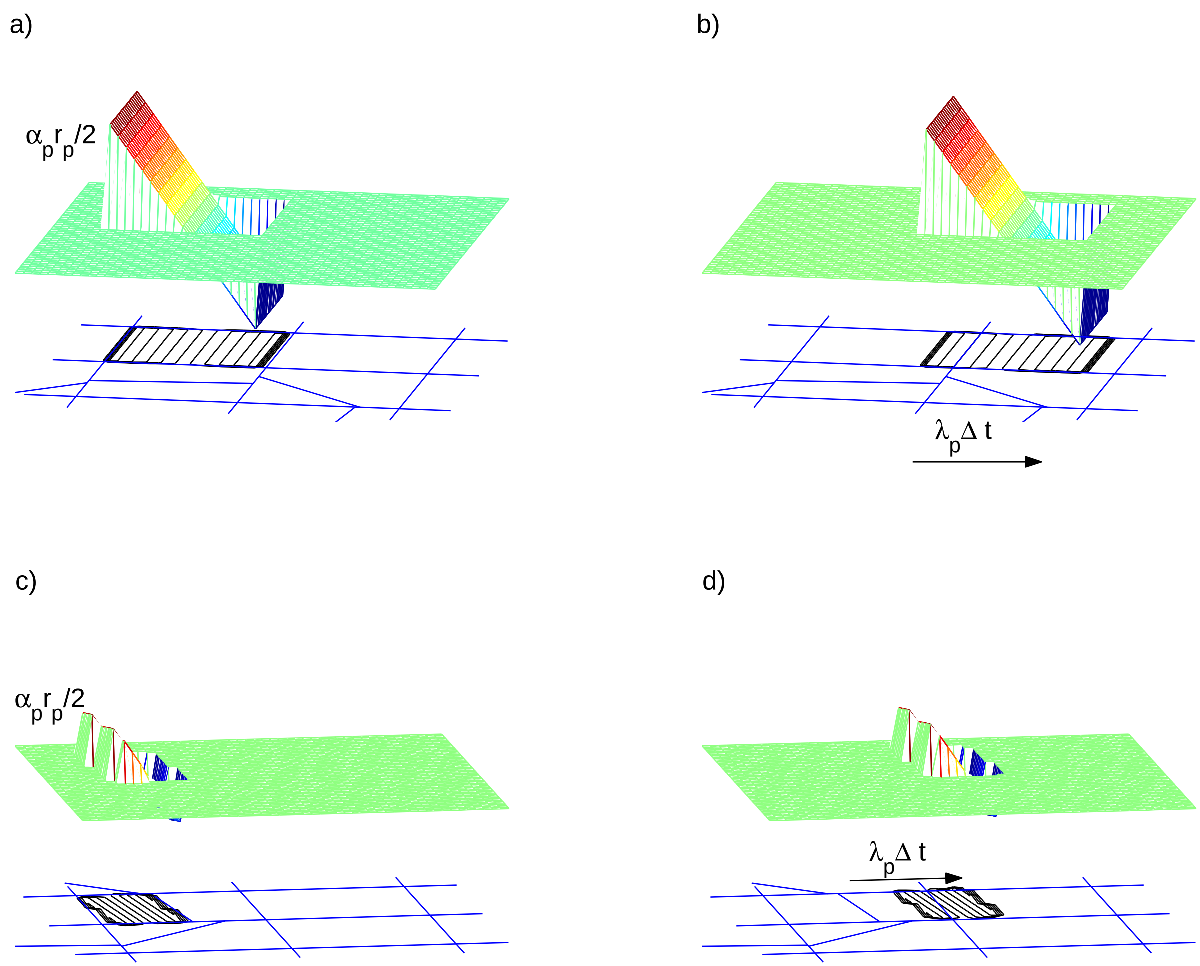




Wave Propagation Method (cont.)

- 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

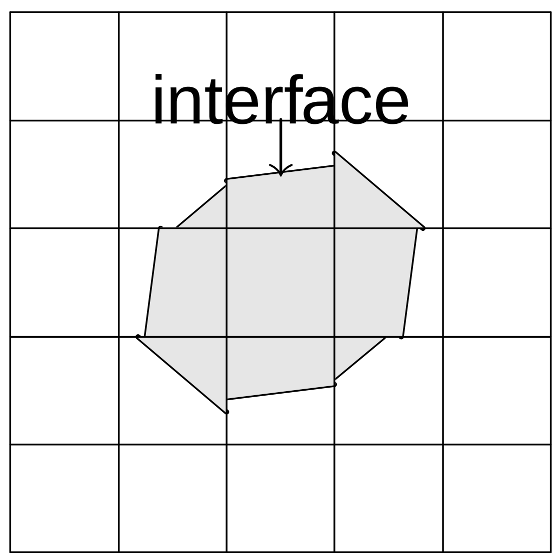
Given volume fractions on current grid, piecewise linear interface reconstruction (PLIC) method does:

1. Compute interface normal
   - Gradient method of Parker & Youngs
   - Least squares method of Puckett
2. Determine interface location by iterative bisection

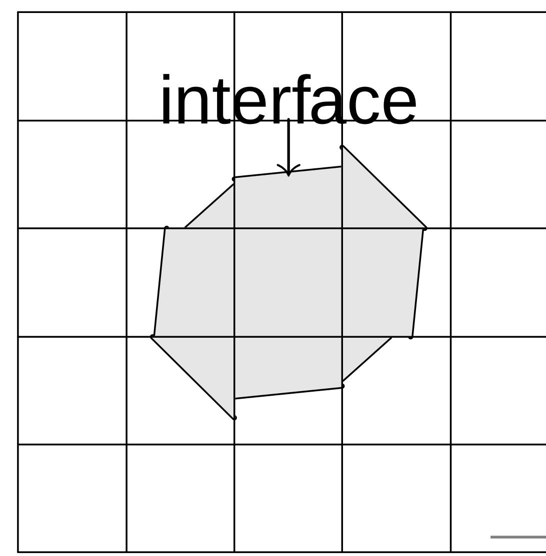
Data set

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

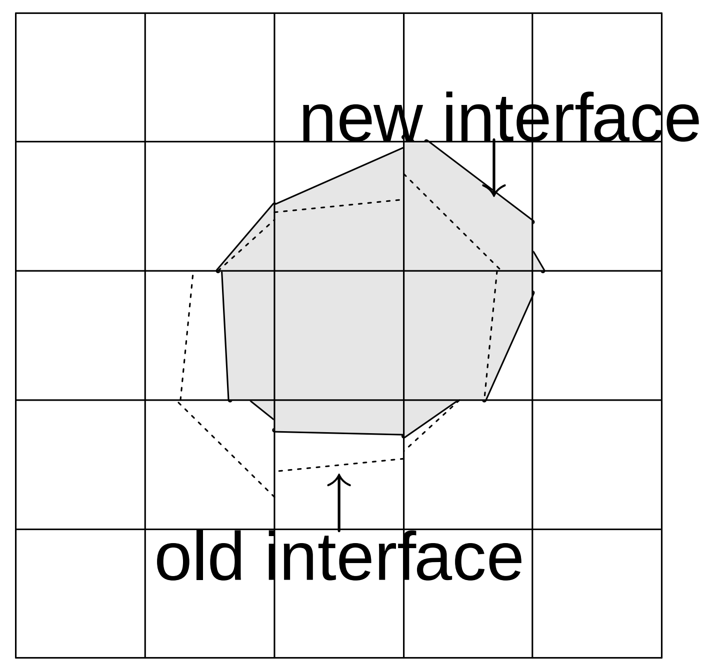
(a) Volume fractions given in previous slide are updated with uniform $(u, v) = (1, 1)$ over $\Delta t = 0.06$

(b) New interface location is reconstructed

(a)

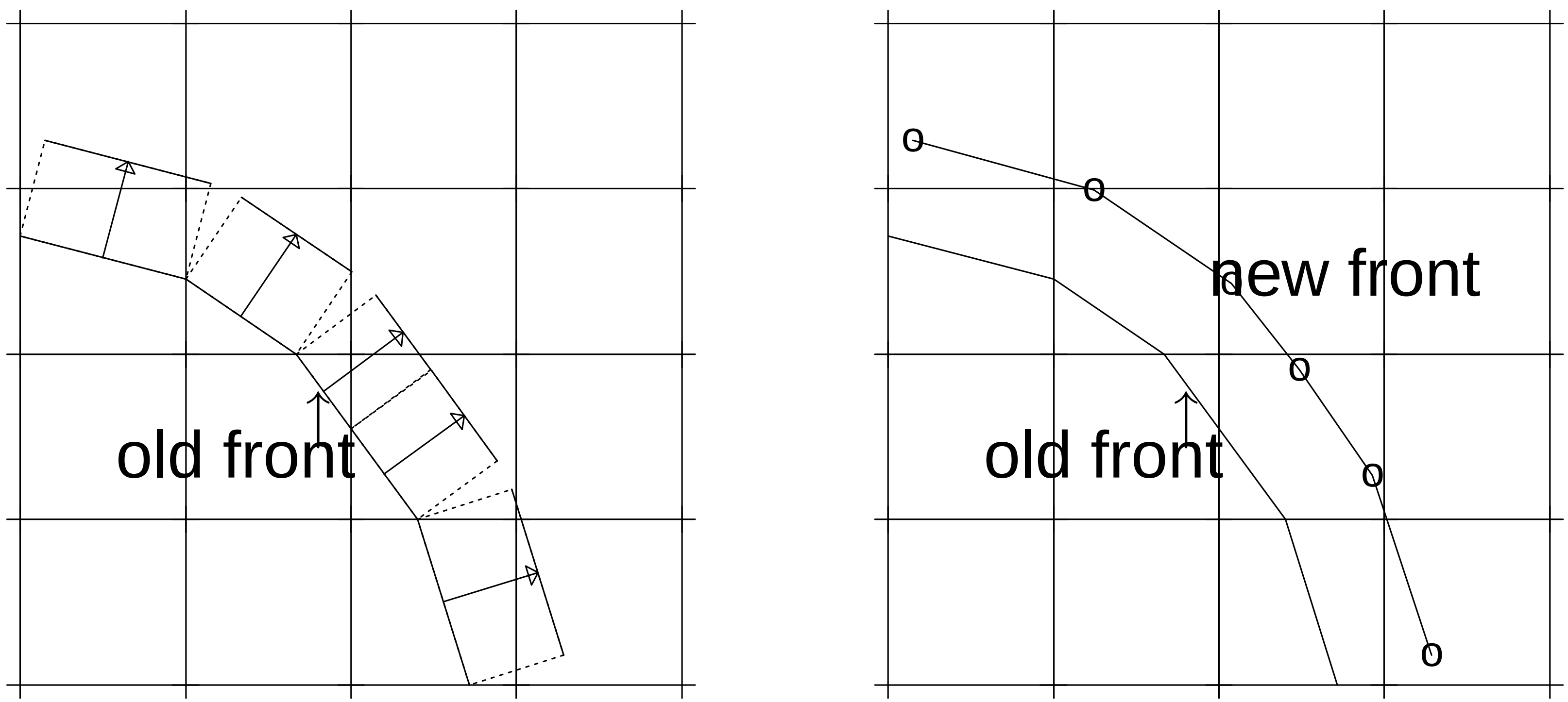
0	0	0	$1(-3)$	0
0	0.11	0.72	0.74	$5(-3)$
0	0.38	1	0.85	0
0	0.01	0.25	0.06	0
0	0	0	0	0

(b)



Surface Moving Procedure

Solve Riemann problem at tracked interfaces & use resulting wave speed of the tracked wave family over Δt to find new location of interface at the next time step



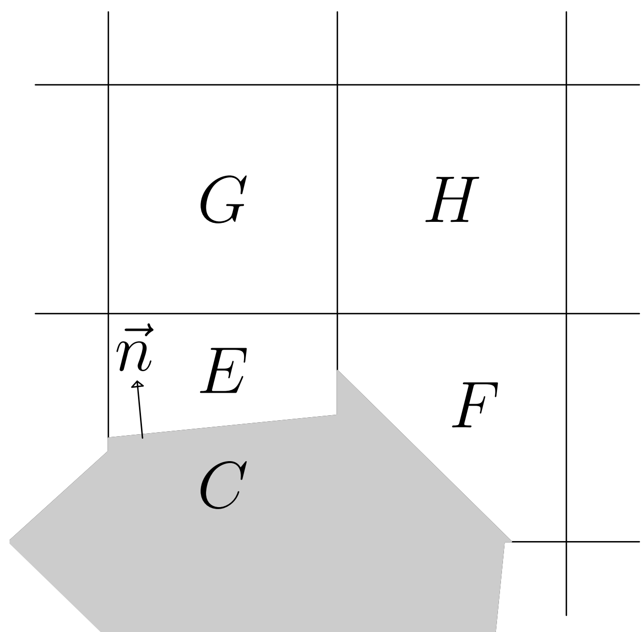
Boundary Conditions

For tracked segments representing rigid (solid wall) boundary (stationary or moving), reflection principle is used to assign states for fictitious subcells in each time step:

$$z_C := z_E \qquad (z = \rho, p, \alpha)$$

$$\vec{u}_C := \vec{u}_E - 2(\vec{u}_E \cdot \vec{n})\vec{n} + 2(\vec{u}_0 \cdot \vec{n})$$

$\vec{u}_0$: moving boundary velocity



Interface Conditions

For tracked segments representing material interfaces, pressure equilibrium as well as velocity continuity conditions across interfaces are fulfilled by

1. Devise of the wave-propagation method
2. Choice of Riemann solver used in the method

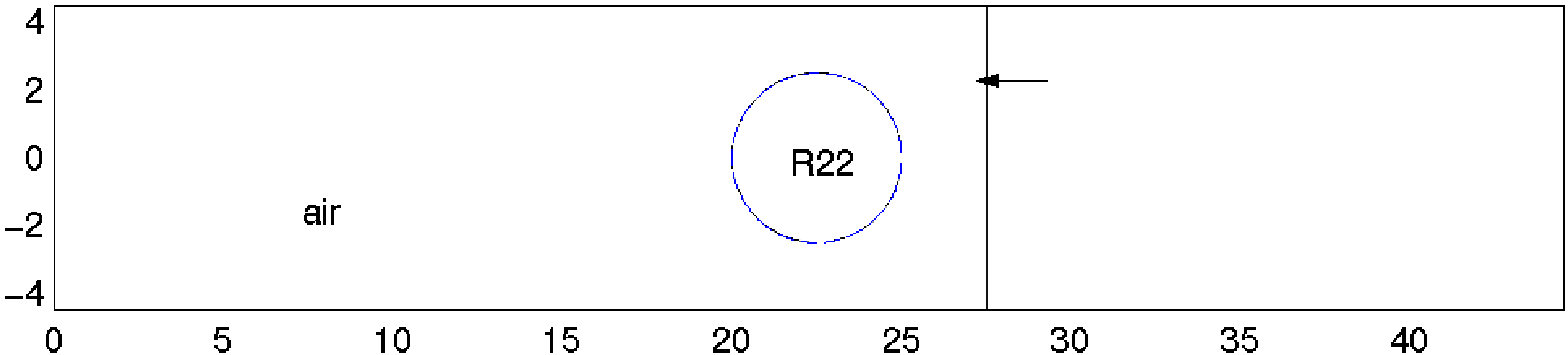
Stability Issues

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

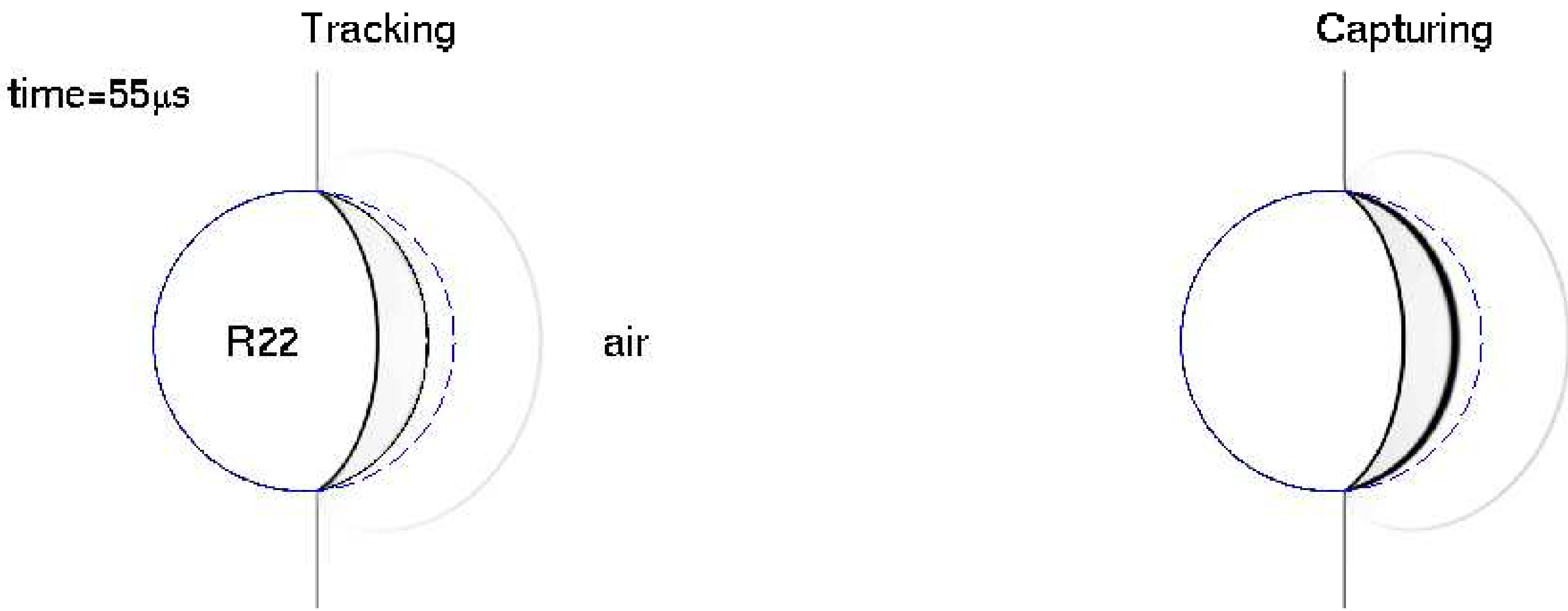
$$\frac{\Delta t \ \max_{p,q}\left(\lambda_p, \mu_q\right)}{\min(\Delta x, \Delta y)} \le 1,$$

  - 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 smoothing operator (such as, h-box approach of Berger *et al.*) locally for cell averages in irregular cells

Shock-Bubble Interaction



Shock-Bubble Interaction



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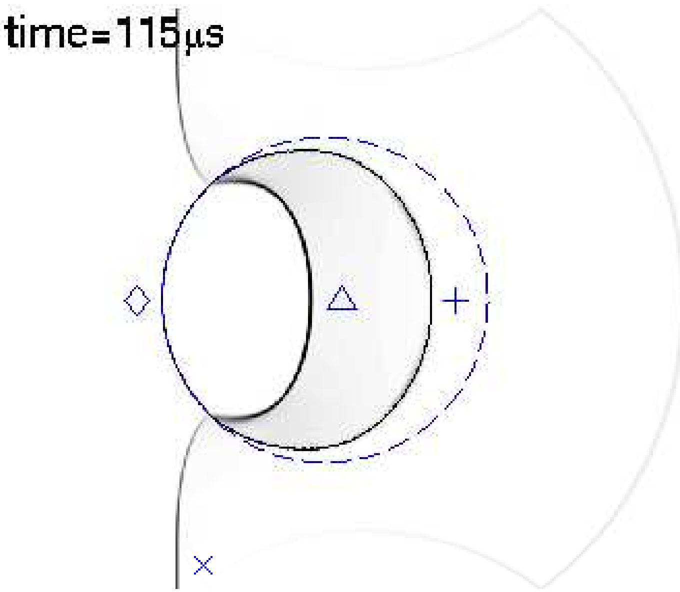

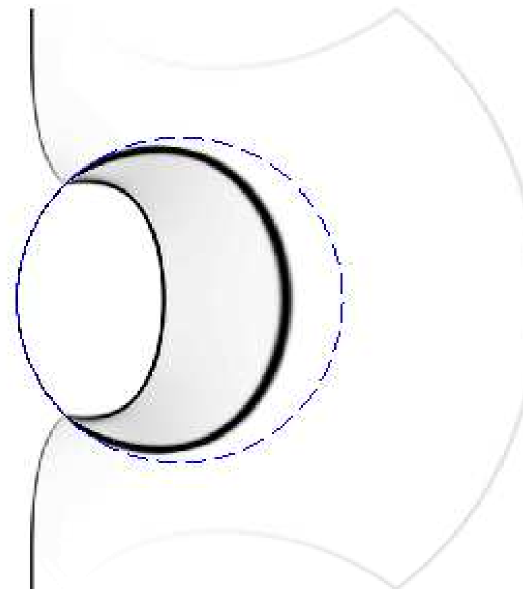

Shock-Bubble Interaction

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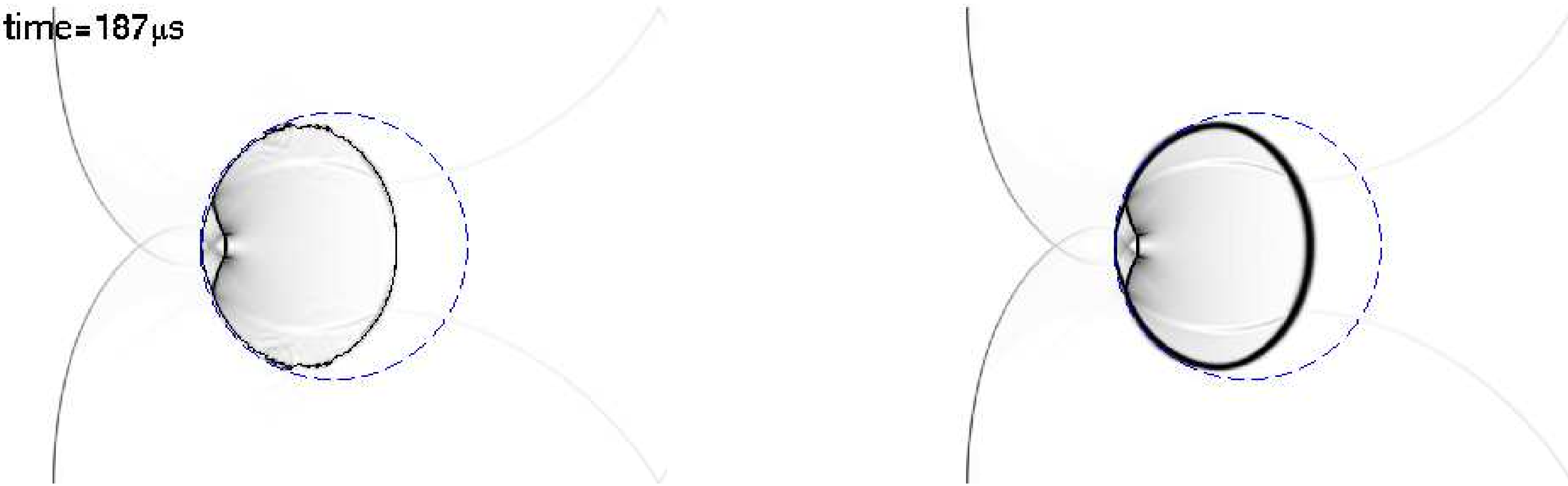

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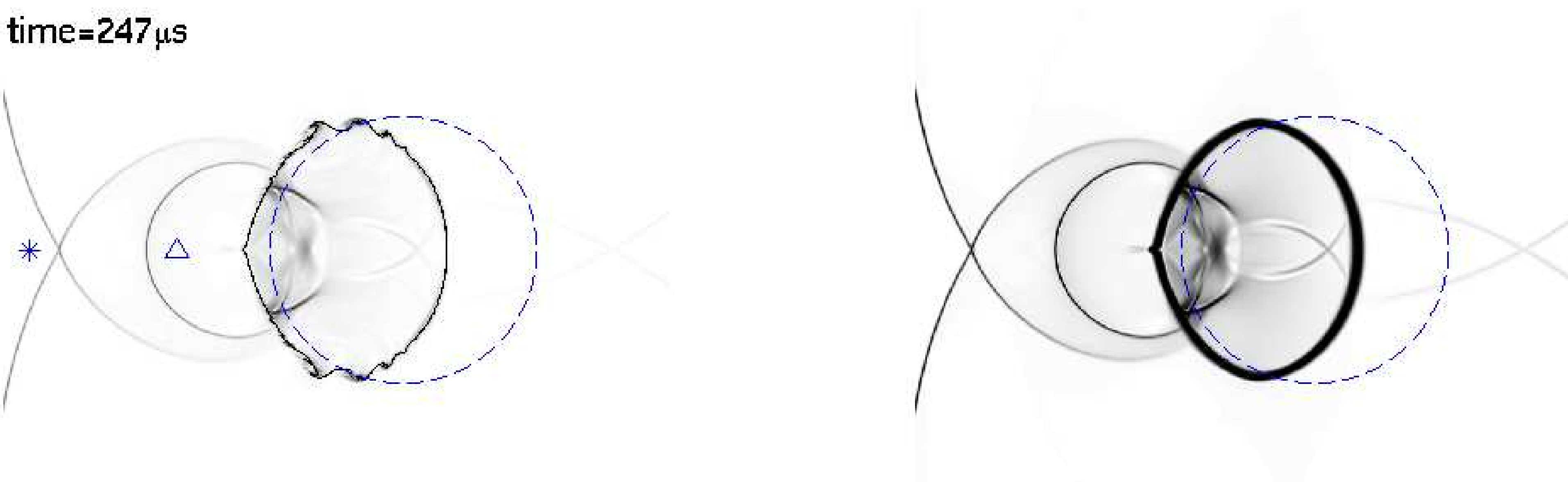

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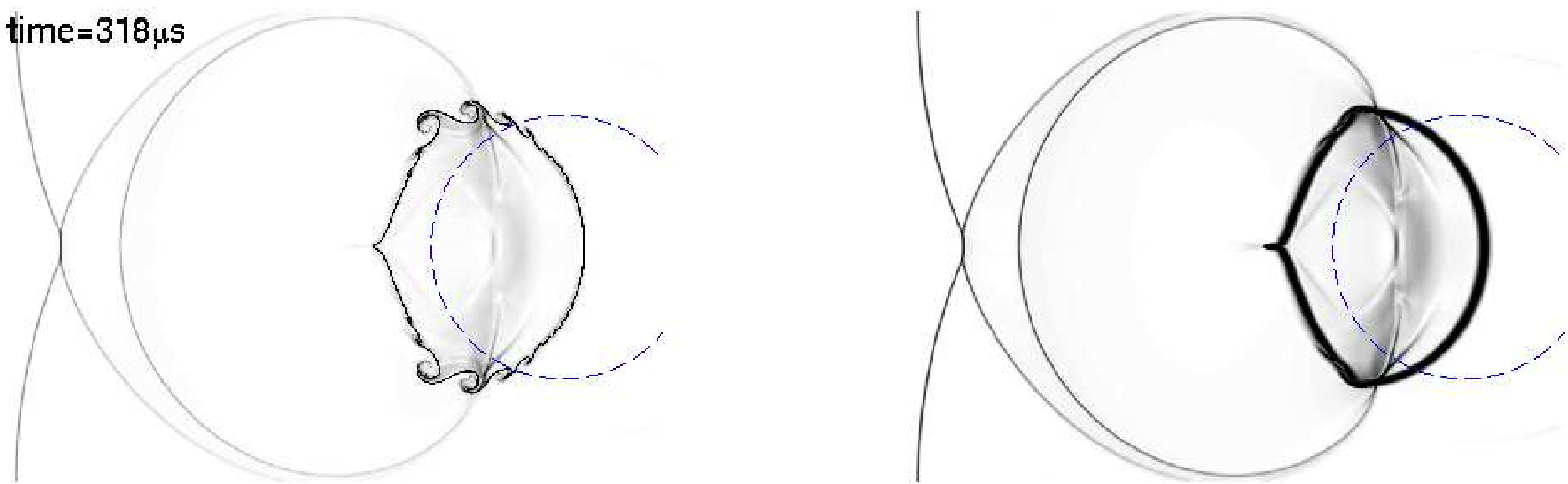

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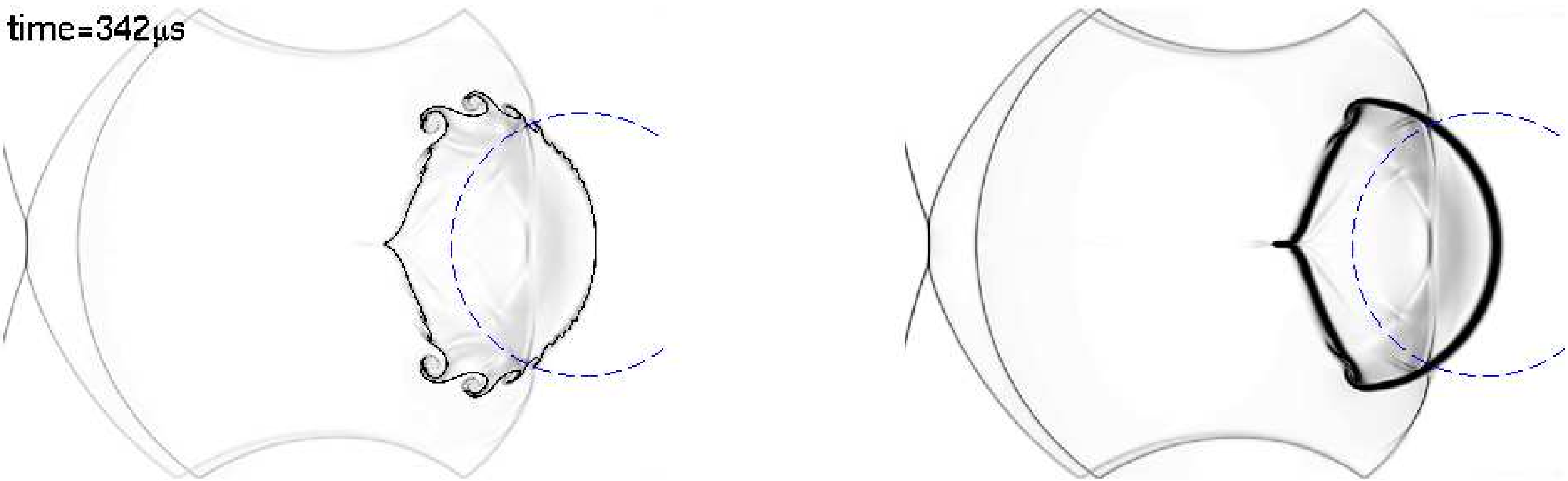

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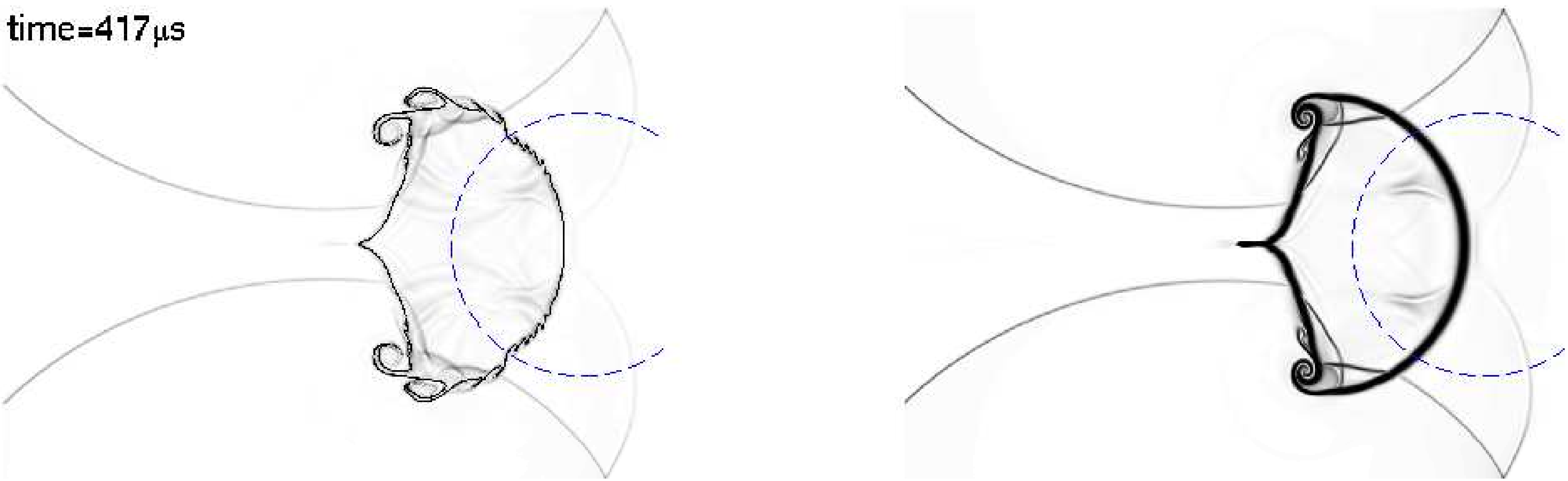
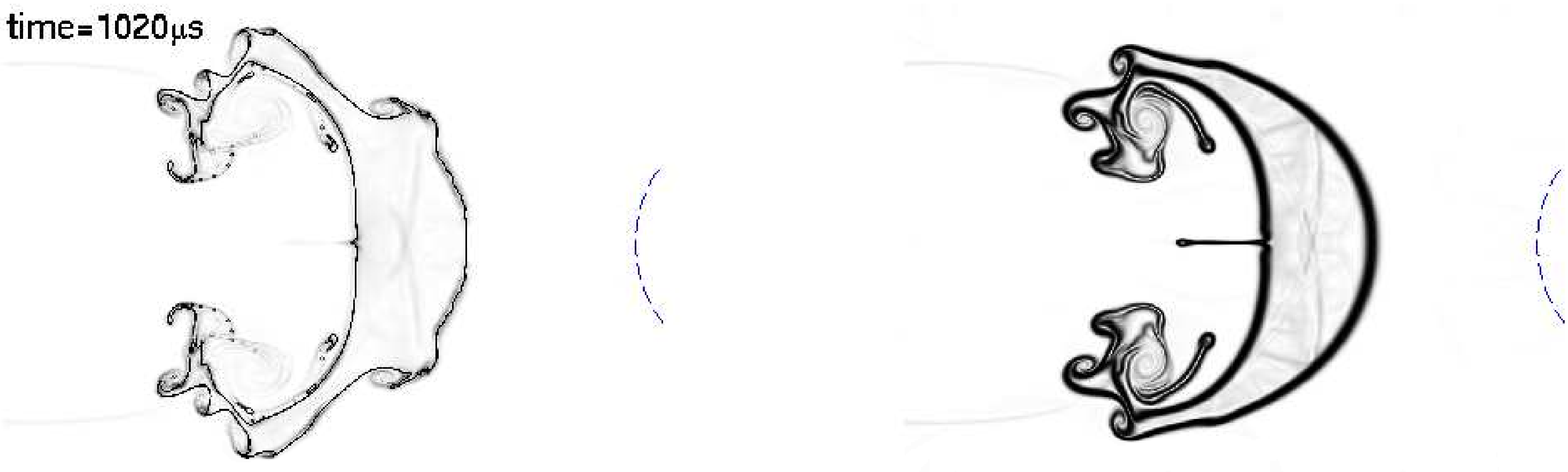
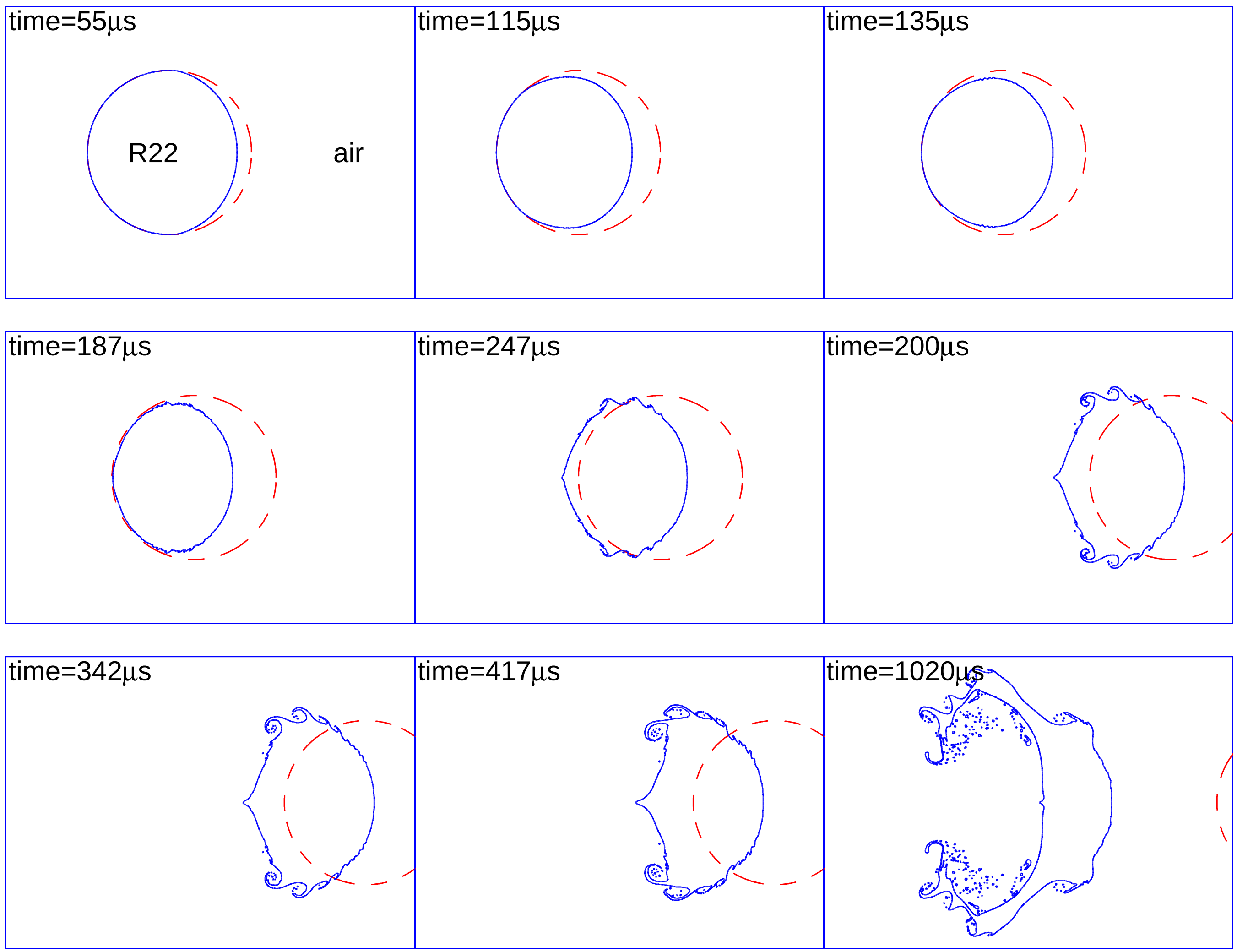


Shock-Bubble Interaction



Shock-Bubble Interaction (cont.)

- Approximate locations of interfaces



Shock-Bubble Interaction (cont.)

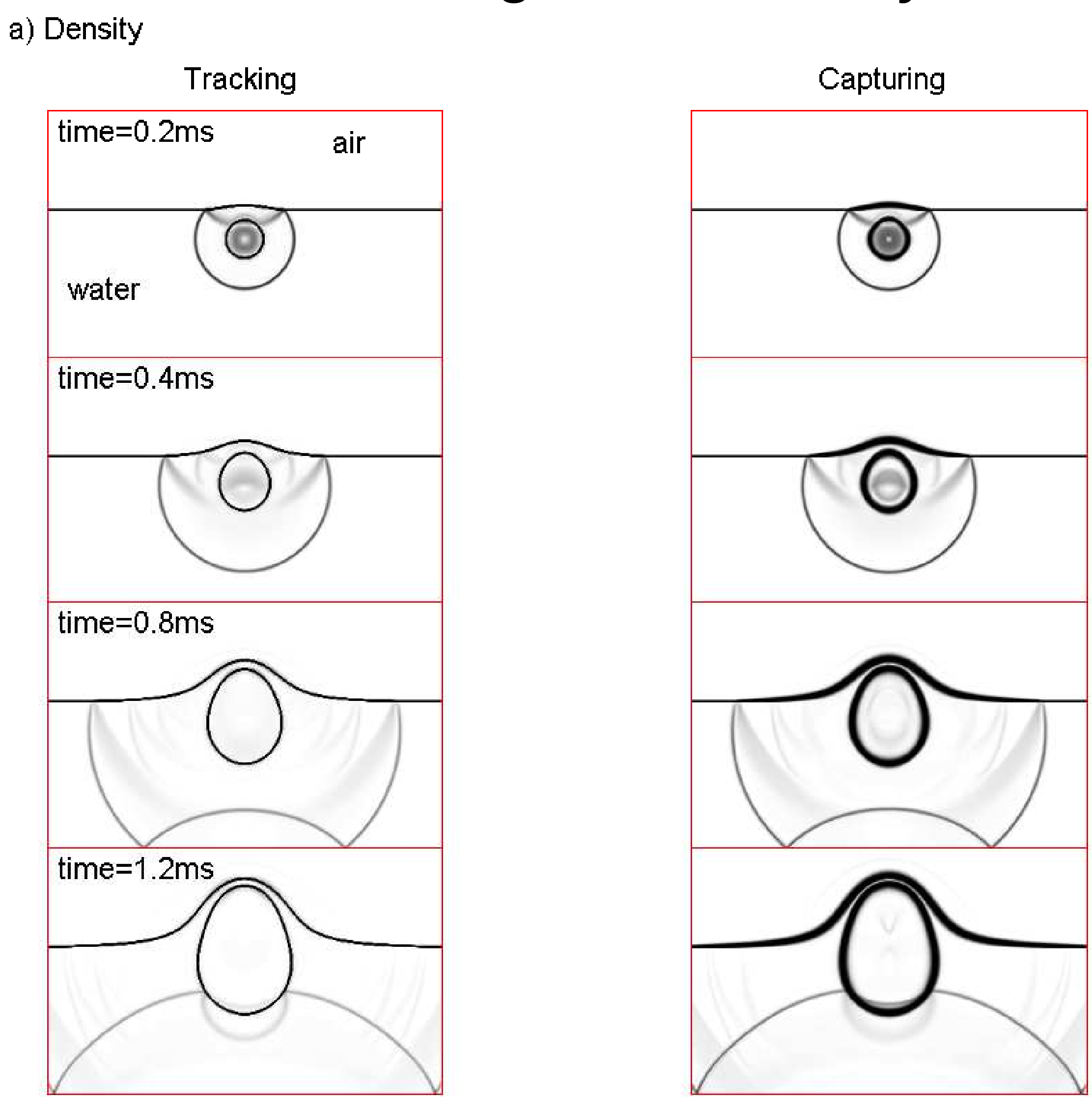
- Quantitative assessment of prominent flow velocities:

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)

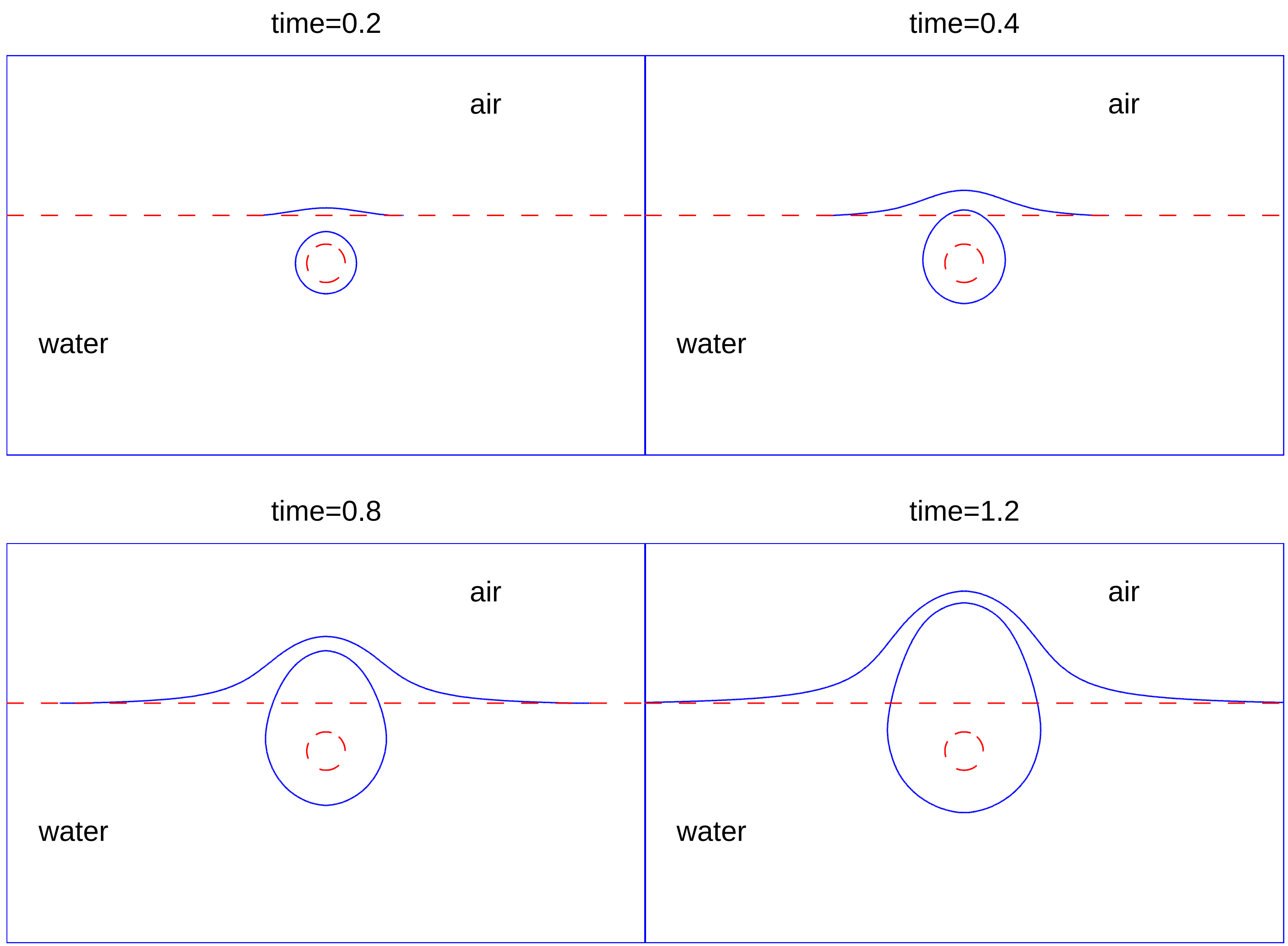
Underwater Explosions

- Numerical schlieren images for density

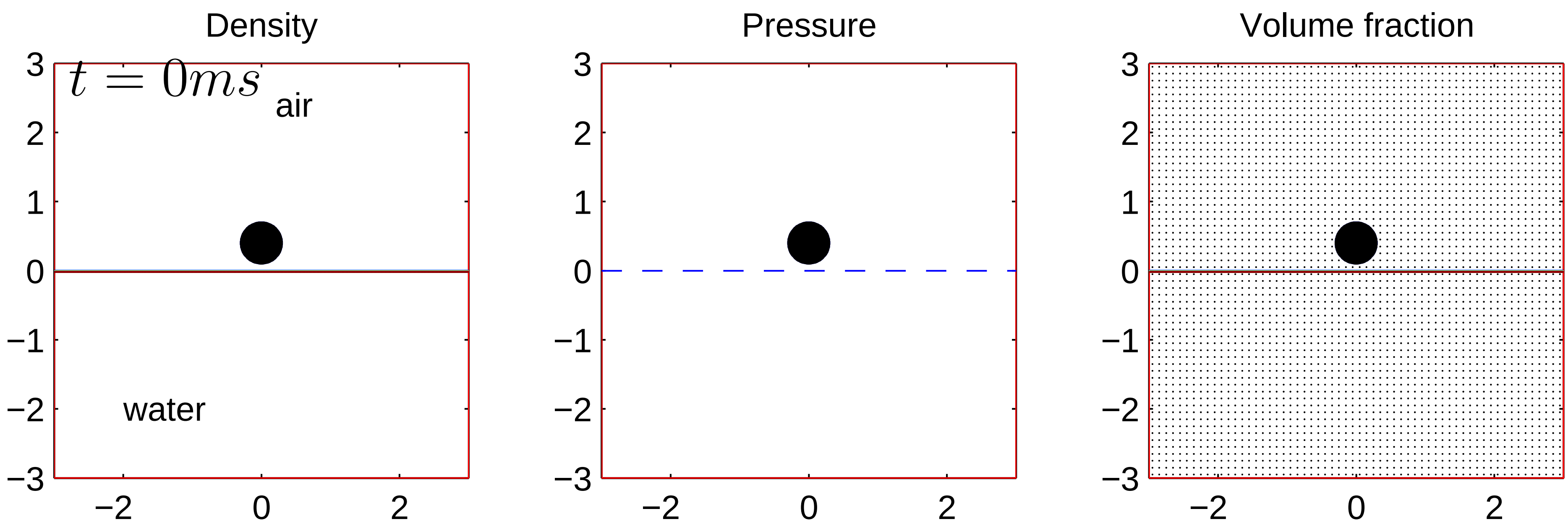


Underwater Explosions (cont.)

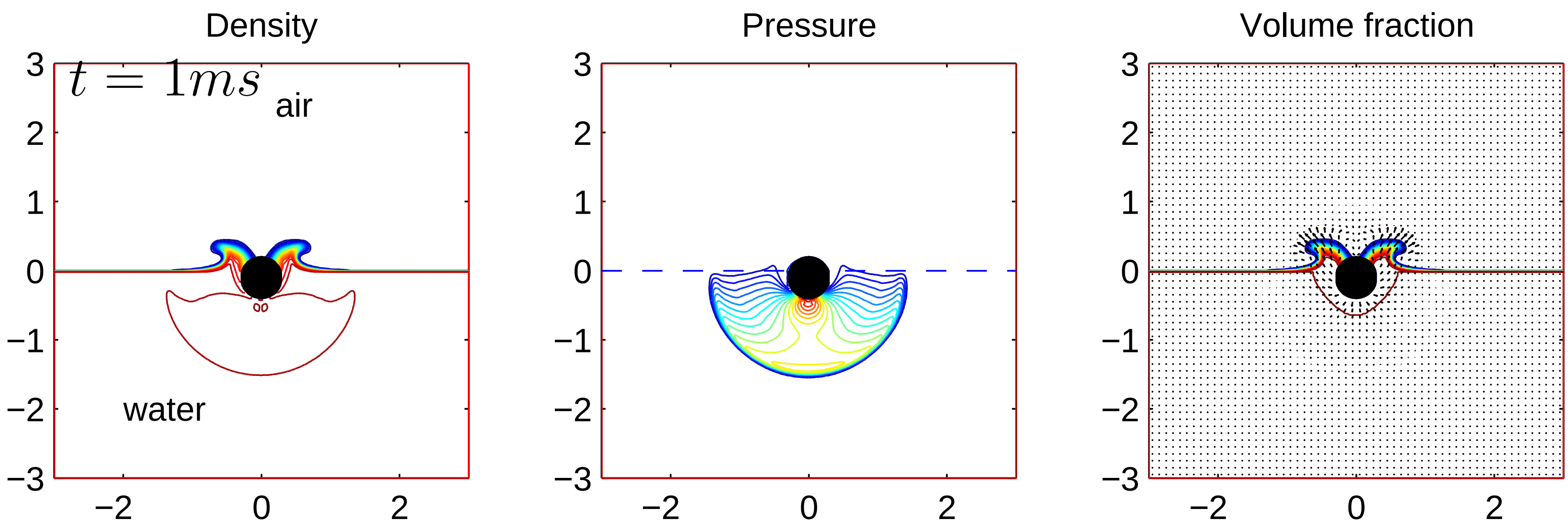
- Approximate locations of interfaces



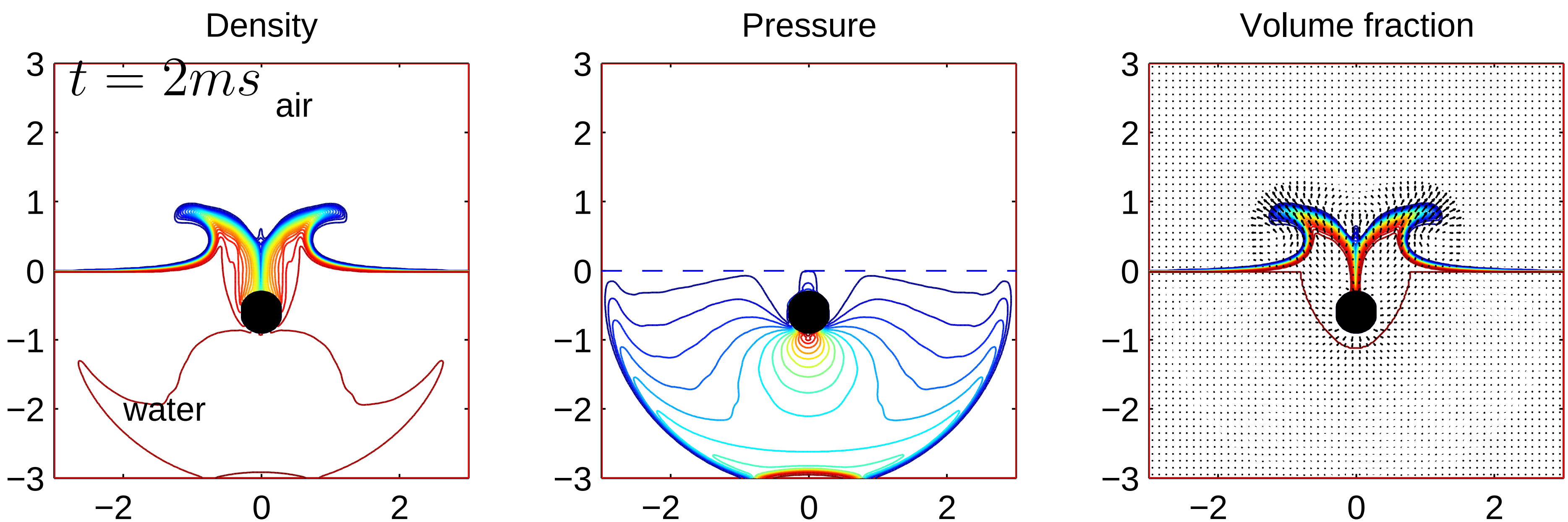
Falling Rigid Object in Water Tank



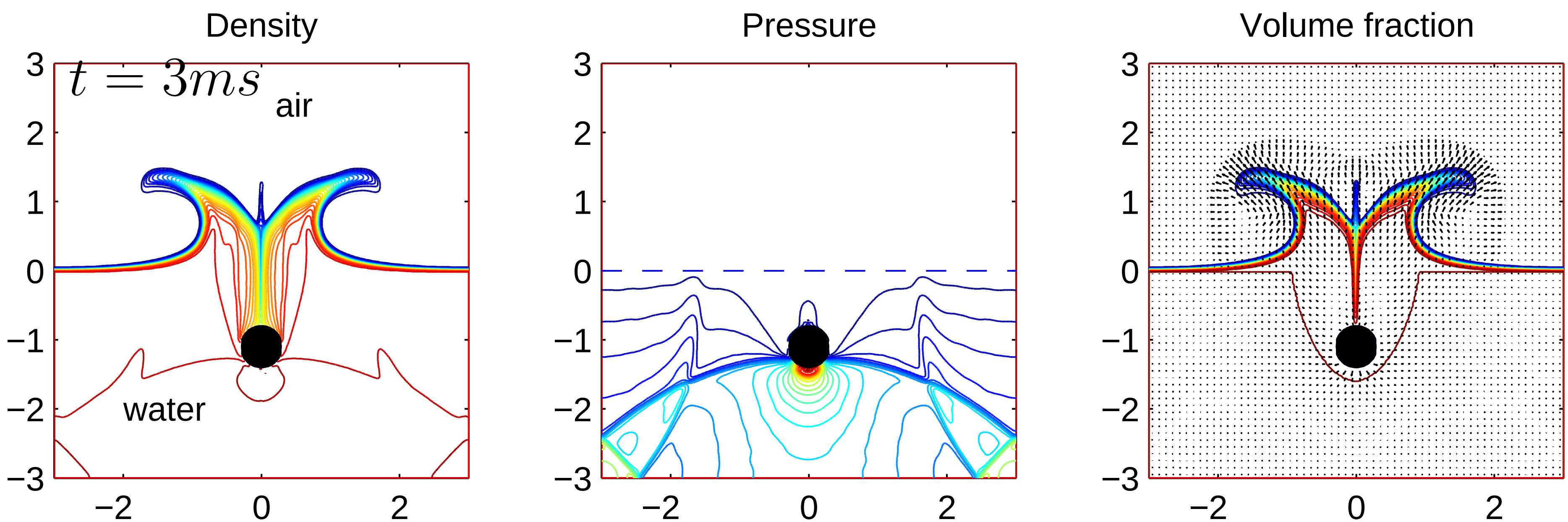
Falling Rigid Object in Water Tank



Falling Rigid Object in Water Tank



Falling Rigid Object in Water Tank



Generalized Lagrangian Model

- Introduce transformation $(t,\ x,\ y) \leftrightarrow (\tau,\ \xi,\ \eta)$ via

$$\begin{pmatrix} dt \\ dx \\ dy \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ x_\tau & x_\xi & x_\eta \\ y_\tau & y_\xi & y_\eta \end{pmatrix} \begin{pmatrix} d\tau \\ d\xi \\ d\eta \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} d\tau \\ d\xi \\ d\eta \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \xi_t & \xi_x & \xi_y \\ \eta_t & \eta_x & \eta_y \end{pmatrix} \begin{pmatrix} dt \\ dx \\ dy \end{pmatrix}$$

- Basic grid-metric relations:

$$\begin{pmatrix} 1 & 0 & 0 \\ \xi_t & \xi_x & \xi_y \\ \eta_t & \eta_x & \eta_y \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ x_\tau & x_\xi & x_\eta \\ y_\tau & y_\xi & y_\eta \end{pmatrix}^{-1} = \frac{1}{J} \begin{bmatrix} x_\xi y_\eta - x_\eta y_\xi & 0 & 0 \\ -x_\tau y_\eta + y_\tau x_\eta & y_\eta & -x_\eta \\ x_\tau y_\xi - y_\tau x_\xi & -y_\xi & x_\xi \end{bmatrix}$$

  - $J = x_\xi y_\eta - x_\eta y_\xi$: grid Jacobian

G. Lagrangian Model (cont.)

Homogeneous two-phase model in N_d generalized coord.:

$$\frac{\partial}{\partial \tau}\left(\alpha_1 \rho_1 J\right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial \xi_j}\left(\alpha_1 \rho_1 J U_j\right) = 0,$$

$$\frac{\partial}{\partial \tau}\left(\alpha_2 \rho_2 J\right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial \xi_j}\left(\alpha_2 \rho_2 J U_j\right) = 0,$$

$$\frac{\partial}{\partial \tau}\left(\rho J u_i\right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial \xi_j} J\left(\rho u_i U_j + p\frac{\partial \xi_j}{\partial x_i}\right) = 0 \qquad \text{for} \quad i = 1, 2, \ldots, N_d,$$

$$\frac{\partial}{\partial \tau}\left(J E\right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial \xi_j} J\left(E U_j + p U_j - p\frac{\partial \xi_j}{\partial t}\right) = 0,$$

$$\frac{\partial \alpha_2}{\partial \tau} + \sum_{j=1}^{N_d} U_j \frac{\partial \alpha_2}{\partial \xi_j} = 0, \qquad U_j = \partial_t \xi_j + \sum_{i=1}^{N_d} u_i \partial_{x_i} \xi_j$$

G. Lagrangian Model (cont.)

Continuity on mixed derivatives of grid coordinates gives geometrical conservation laws

$$\frac{\partial}{\partial \tau}\begin{pmatrix} x_\xi \\ y_\xi \\ x_\eta \\ y_\eta \end{pmatrix} + \frac{\partial}{\partial \xi}\begin{pmatrix} -x_\tau \\ -y_\tau \\ 0 \\ 0 \end{pmatrix} + \frac{\partial}{\partial \eta}\begin{pmatrix} 0 \\ 0 \\ -x_\tau \\ -y_\tau \end{pmatrix} = 0$$

with (x_τ, y_τ) to be specified as, for example,

- Eulerian case: $(x_\tau, y_\tau) = \vec{0}$
- Lagrangian case: $(x_\tau, y_\tau) = (u, v)$
- Lagrangian-like case: $(x_\tau, y_\tau) = h_0(u, v)$ or $(h_0 u, k_0 v)$
  - $h_0 \in [0, 1]$ & $k_0 \in [0, 1]$ (fixed piecewise const.)

G. Lagrangian Model (cont.)

- General 1-parameter case: $(x_\tau, y_\tau) = h(u,v)$, $\quad h \in [0,1]$

  At given time instance, h can be chosen based on

  - Grid-angle preserving condition (Hui *et al.* JCP 1999)

$$\frac{\partial}{\partial \tau}\cos^{-1}\left(\frac{\nabla\xi}{|\nabla\xi|}\cdot\frac{\nabla\eta}{|\nabla\eta|}\right) = \frac{\partial}{\partial \tau}\cos^{-1}\left(\frac{-y_\eta x_\eta - y_\xi x_\xi}{\sqrt{y_\xi^2 + y_\eta^2}\sqrt{x_\xi^2 + x_\eta^2}}\right)$$

$$= \cdots$$

$$= \mathcal{A}h_\xi + \mathcal{B}h_\eta + \mathcal{C}h = 0 \quad \text{(1st order PDE)}$$

  with

$$\mathcal{A} = \sqrt{x_\eta^2 + y_\eta^2}\,(vx_\xi - uy_\xi)\,, \quad \mathcal{B} = \sqrt{x_\xi^2 + y_\xi^2}\,(uy_\eta - vx_\eta)$$

$$\mathcal{C} = \sqrt{x_\xi^2 + y_\xi^2}\,(u_\eta y_\eta - v_\eta x_\eta) - \sqrt{x_\eta^2 + y_\eta^2}\,(u_\xi y_\xi - v_\xi x_\xi)$$

G. Lagrangian Model (cont.)

- General 1-parameter case: $(x_\tau, y_\tau) = h(u, v)$, $\quad h \in [0, 1]$

  Or alternatively, based on
  - Mesh-area preserving condition

$$\begin{aligned}\frac{\partial J}{\partial \tau} &= \frac{\partial}{\partial \tau}\left(x_\xi y_\eta - x_\eta y_\xi\right) \\ &= x_{\xi\tau}\, y_\eta + x_\xi\, y_{\eta\tau} - x_{\eta\tau}\, y_\xi - x_\eta\, y_{\xi\tau} \\ &= \cdots \\ &= \mathcal{A} h_\xi + \mathcal{B} h_\eta + \mathcal{C} h = 0 \quad \text{(1st order PDE)}\end{aligned}$$

  with

$$\mathcal{A} = u y_\eta - v x_\eta, \quad \mathcal{B} = v x_\xi - u y_\xi, \quad \mathcal{C} = u_\xi y_\eta + v_\eta x_\xi - u_\eta y_\xi - v_\xi x_\eta$$

G. Lagrangian Model (cont.)

- Numerics: h- or $\tilde{h}$-equation constraint geometrical laws

$$\frac{\partial}{\partial \tau}\begin{pmatrix} x_\xi \\ y_\xi \\ x_\eta \\ y_\eta \end{pmatrix} - \frac{\partial}{\partial \xi}\begin{pmatrix} hu \\ hv \\ 0 \\ 0 \end{pmatrix} - \frac{\partial}{\partial \eta}\begin{pmatrix} 0 \\ 0 \\ hu \\ hv \end{pmatrix} = 0$$

- Usability: Mesh-area evolution equation

$$\frac{\partial J}{\partial \tau} - \frac{\partial}{\partial \xi}\left[h\left(u y_\eta - v x_\eta\right)\right] - \frac{\partial}{\partial \eta}\left[h\left(v x_\xi - u y_\xi\right)\right] = 0$$

- Initial & boundary conditions for h- or $\tilde{h}$-equation ?

G. Lagrangian Model (cont.)

In summary, with $(x_\tau, y_\tau) = h_0(u,v)$ & EOS, model system for homogeneous two-phase flow reads

$$\frac{\partial}{\partial \tau}\begin{pmatrix} J\alpha_1\rho_1 \\ J\alpha_2\rho_2 \\ J\rho u \\ J\rho v \\ JE \\ x_\xi \\ y_\xi \\ x_\eta \\ y_\eta \end{pmatrix} + \frac{\partial}{\partial \xi}\begin{pmatrix} J\alpha_1\rho_1 U \\ J\alpha_2\rho_2 U \\ J\rho u U + y_\eta p \\ J\rho v U - x_\eta p \\ JEU + (y_\eta u - x_\eta v)p \\ -h_0 u \\ -h_0 v \\ 0 \\ 0 \end{pmatrix} + \frac{\partial}{\partial \eta}\begin{pmatrix} J\alpha_1\rho_1 V \\ J\alpha_2\rho_2 V \\ J\rho u V - y_\xi p \\ J\rho v V + x_\xi p \\ JEV + (x_\xi v - y_\xi u)p \\ 0 \\ 0 \\ -h_0 u \\ -h_0 v \end{pmatrix} = 0$$

$$\frac{\partial \alpha_2}{\partial \tau} + U\frac{\partial \alpha_2}{\partial \xi} + V\frac{\partial \alpha_2}{\partial \eta} = 0, \quad U = (1-h_0)(y_\eta u - x_\eta v) \& V = (1-h_0)(x_\xi v - y_\xi u$$

G. Lagrangian Model (cont.)

- Under thermodyn. stability condition, our multifluid model in generalized coordinates is hyperbolic when $h_0 \neq 1$, & is weakly hyperbolic when $h_0 = 1$
- Model system is written in quasi-conservative form with spatially varying fluxes in generalized coordinates
- Grid system is a time-varying grid
- Extension of the model to general non-barotropic multifluid flow can be made in an analogous manner

Flux-based Wave Decomposition

- In 2D, equations to be solved takes the form

$$\frac{\partial q}{\partial \tau} + f_1\left(\frac{\partial}{\partial \xi}, q, \nabla\vec{\xi}\right) + f_2\left(\frac{\partial}{\partial \eta}, q, \nabla\vec{\xi}\right) = \tilde{\psi}$$

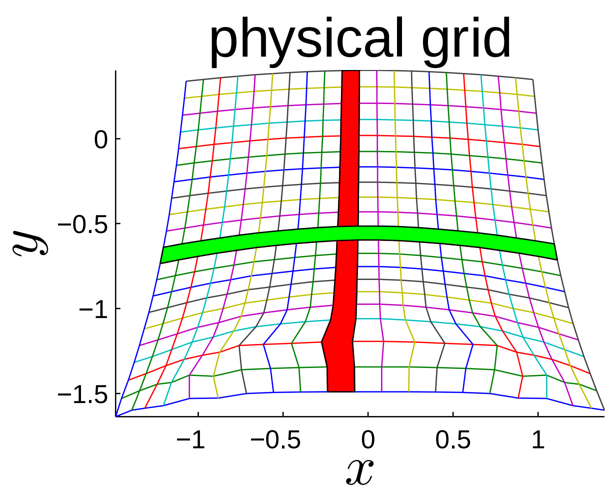
- A simple dimensional-splitting approach based on f-wave formulation of LeVeque *et al.* is used
  - Solve one-dimensional generalized Riemann problem (defined below) at each cell interfaces
  - Use resulting jumps of fluxes (decomposed into each wave family) of Riemann solution to update cell averages
  - Introduce limited jumps of fluxes to achieve high resolution

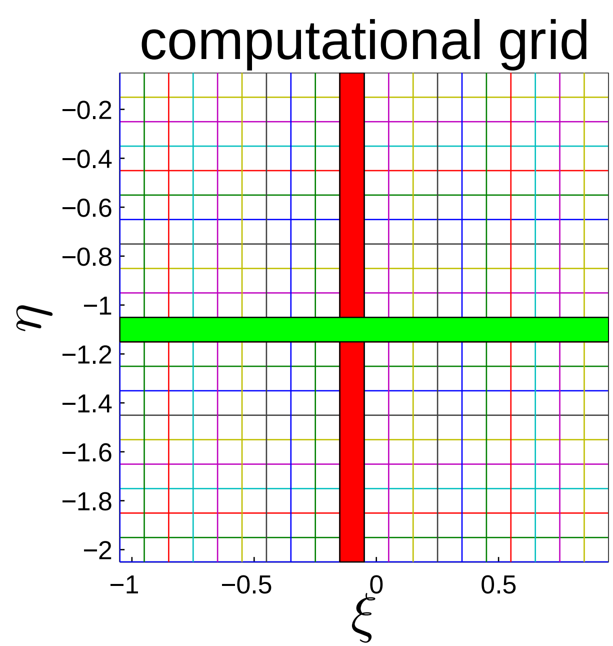
F-Waves Decomposition (cont.)

Employ finite volume formulation of numerical solution

$$Q_{ij}^{n} \approx \frac{1}{\Delta\xi\Delta\eta}\int_{C_{ij}} q(\xi,\eta,\tau_n)\,dA$$

that gives approximate value of cell average of solution q over cell $C_{ij} = [\xi_i, \xi_{i+1}] \times [\eta_j, \eta_{j+1}]$ at time τ_n





Generalized Riemann Problem

Generalized Riemann problem of our multifluid model at cell interface $\xi_{i-1/2}$ consists of the equation

$$\frac{\partial q}{\partial \tau} + F_{i-\frac{1}{2},j}\left(\partial_\xi, q, \nabla\vec{\xi}\right) = 0$$

together with flux function

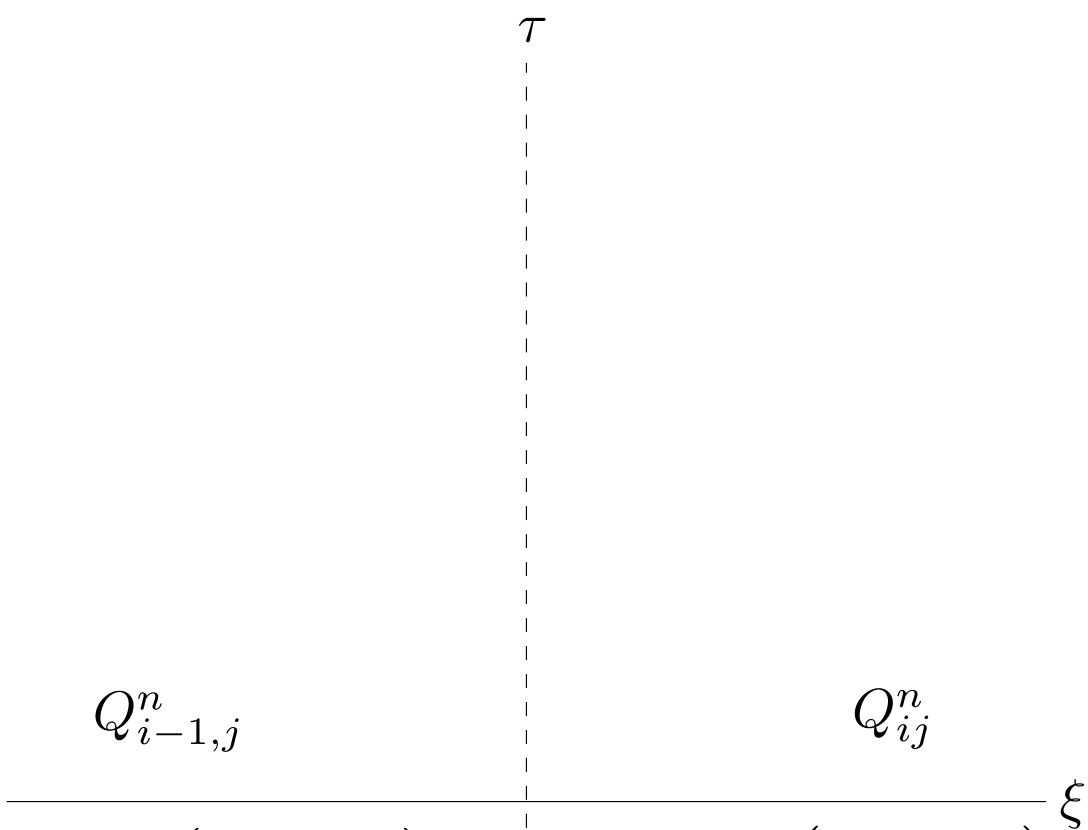
$$F_{i-\frac{1}{2},j} = \begin{cases} f_{i-1,j}\left(\partial_\xi, q, \nabla\vec{\xi}\right) & \text{for} \quad \xi < \xi_{i-1/2} \\ f_{ij}\left(\partial_\xi, q, \nabla\vec{\xi}\right) & \text{for} \quad \xi > \xi_{i-1/2} \end{cases}$$

and piecewise constant initial data

$$q(\xi, 0) = \begin{cases} Q^n_{i-1,j} & \text{for} \quad \xi < \xi_{i-1/2} \\ Q^n_{ij} & \text{for} \quad \xi > \xi_{i-1/2} \end{cases}$$

Generalized Riemann Problem

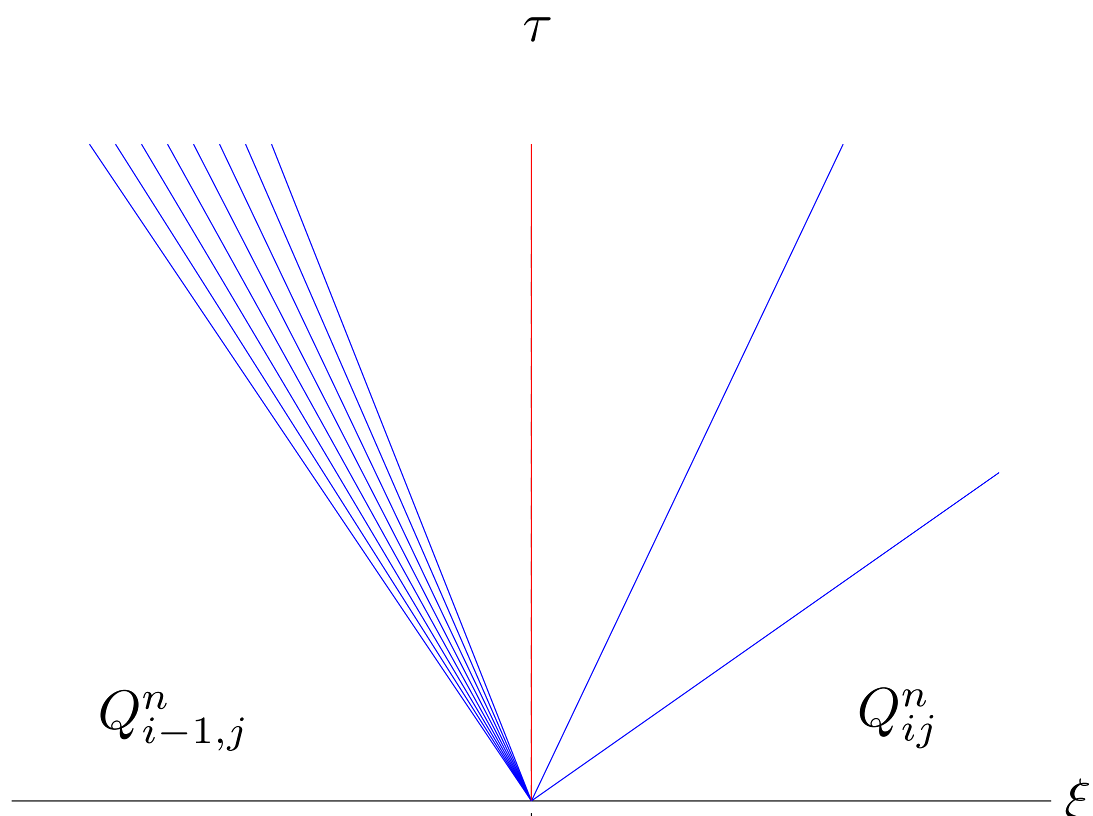
Generalized Riemann problem at time $\tau = 0$



$$q_\tau + f_{i-1,j}\left(\partial_\xi, q, \nabla\vec{\xi}\right) = 0 \qquad q_\tau + f_{i,j}\left(\partial_\xi, q, \nabla\vec{\xi}\right) = 0$$

Generalized Riemann Problem

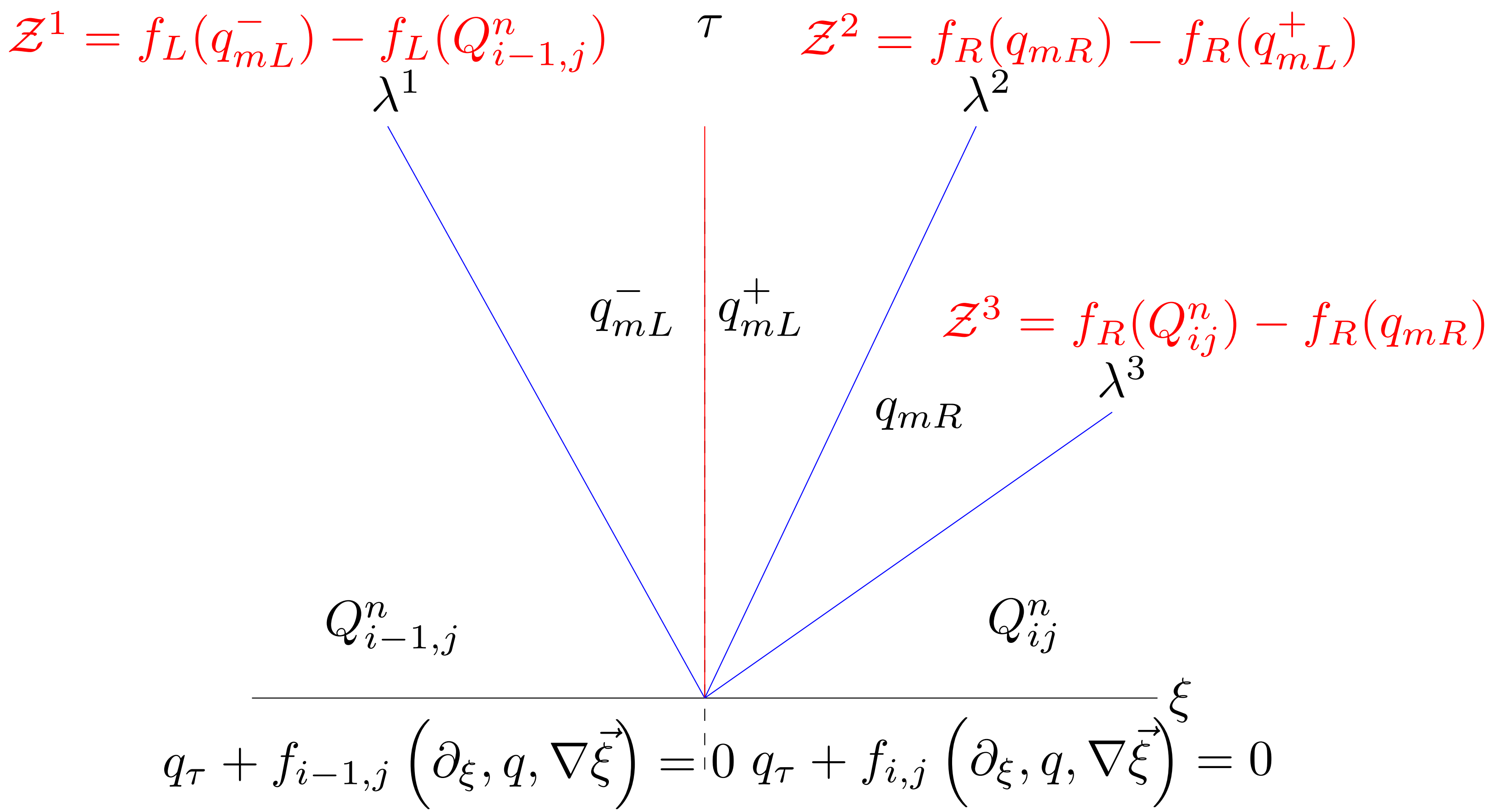
Exact generalized Riemann solution: basic structure



$$q_\tau + f_{i-1,j}\left(\partial_\xi, q, \nabla\vec{\xi}\right) = 0 \qquad q_\tau + f_{i,j}\left(\partial_\xi, q, \nabla\vec{\xi}\right) = 0$$

Generalized Riemann Problem

Shock-only approximate Riemann solution: basic structure



F-Waves Decomposition (cont.)

Basic steps of a dimensional-splitting scheme

- ξ-sweeps: solve

$$\frac{\partial q}{\partial \tau} + f_1\left(\frac{\partial}{\partial \xi}, q, \nabla\vec{\xi}\right) = 0$$

  updating Q_{ij}^n to $Q_{i,j}^*$

- η-sweeps: solve

$$\frac{\partial q}{\partial \tau} + f_2\left(\frac{\partial}{\partial \eta}, q, \nabla\vec{\xi}\right) = 0$$

  updating Q_{ij}^* to $Q_{i,j}^{n+1}$

F-Waves Decomposition (cont.)

That is to say,

- ξ-sweeps: we use

$$Q^*_{ij} = Q^n_{ij} - \frac{\Delta\tau}{\Delta\xi}\left(\mathcal{F}^-_{i+\frac{1}{2},j} - \mathcal{F}^+_{i-\frac{1}{2},j}\right) - \frac{\Delta\tau}{\Delta\xi}\left(\tilde{\mathcal{Z}}_{i+\frac{1}{2},j} - \tilde{\mathcal{Z}}_{i-\frac{1}{2},j}\right)$$

with $$\tilde{\mathcal{Z}}_{i-\frac{1}{2},j} = \frac{1}{2}\sum_{p=1}^{m_w} \text{sign}\left(\lambda^p_{i-\frac{1}{2},j}\right)\left(1 - \frac{\Delta\tau}{\Delta\xi}\left|\lambda^p_{i-\frac{1}{2},j}\right|\right)\tilde{\mathcal{Z}}^p_{i-\frac{1}{2},j}$$

- η-sweeps: we use

$$Q^{n+1}_{ij} = Q^*_{ij} - \frac{\Delta\tau}{\Delta\eta}\left(\mathcal{G}^-_{i,j+\frac{1}{2}} - \mathcal{G}^+_{i,j-\frac{1}{2}}\right) - \frac{\Delta\tau}{\Delta\eta}\left(\tilde{\mathcal{Z}}_{i,j+\frac{1}{2}} - \tilde{\mathcal{Z}}_{i,j-\frac{1}{2}}\right)$$

with $$\tilde{\mathcal{Z}}_{i,j-\frac{1}{2}} = \frac{1}{2}\sum_{p=1}^{m_w} \text{sign}\left(\lambda^p_{i,j-\frac{1}{2}}\right)\left(1 - \frac{\Delta\tau}{\Delta\eta}\left|\lambda^p_{i,j-\frac{1}{2}}\right|\right)\tilde{\mathcal{Z}}^p_{i,j-\frac{1}{2}}$$

F-Waves Decomposition (cont.)

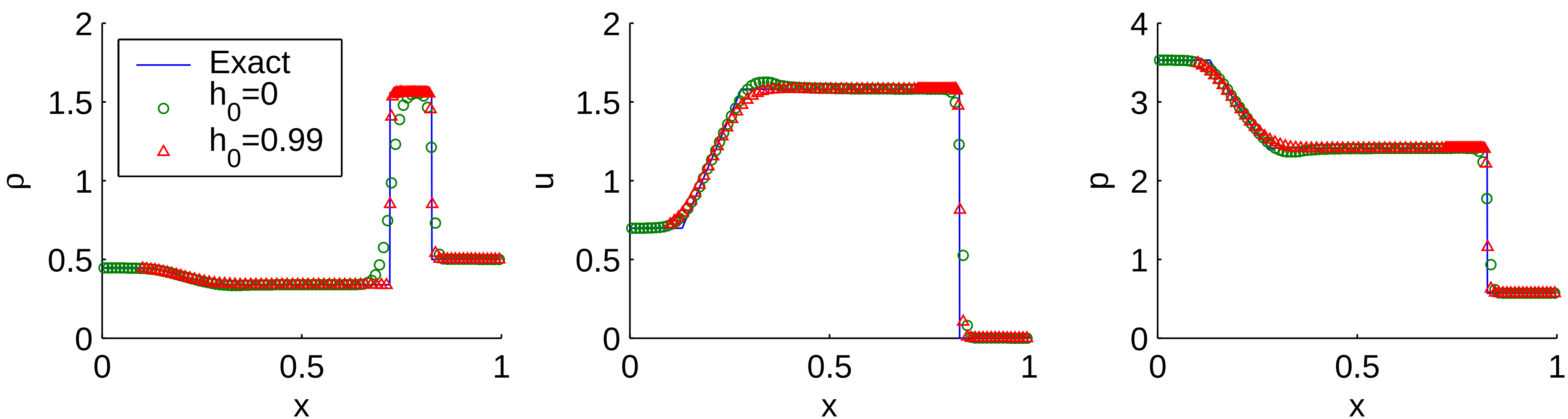
- Flux-based wave decomposition

$$f_{i,j} - f_{i-1,j} = \sum_{p=1}^{m_w} \mathcal{Z}^p_{i-1/2} = \sum_{p=1}^{m_w} \lambda^p_{i-1/2} \mathcal{W}^p_{i-1/2}$$

- Some care should be taken on the limited jump of fluxes $\tilde{\mathcal{W}}^p$, for $p = 2$ (contact wave), in particular to ensure correct pressure equilibrium across material interfaces
- MUSCL-type (slope limited) high resolution extension is not simple as one might think of for multifluid problems
- Splitting of discontinuous fluxes at cell interfaces: significance ?
- First order or high resolution method for geometric conservation laws: significance to grid uniformity ?

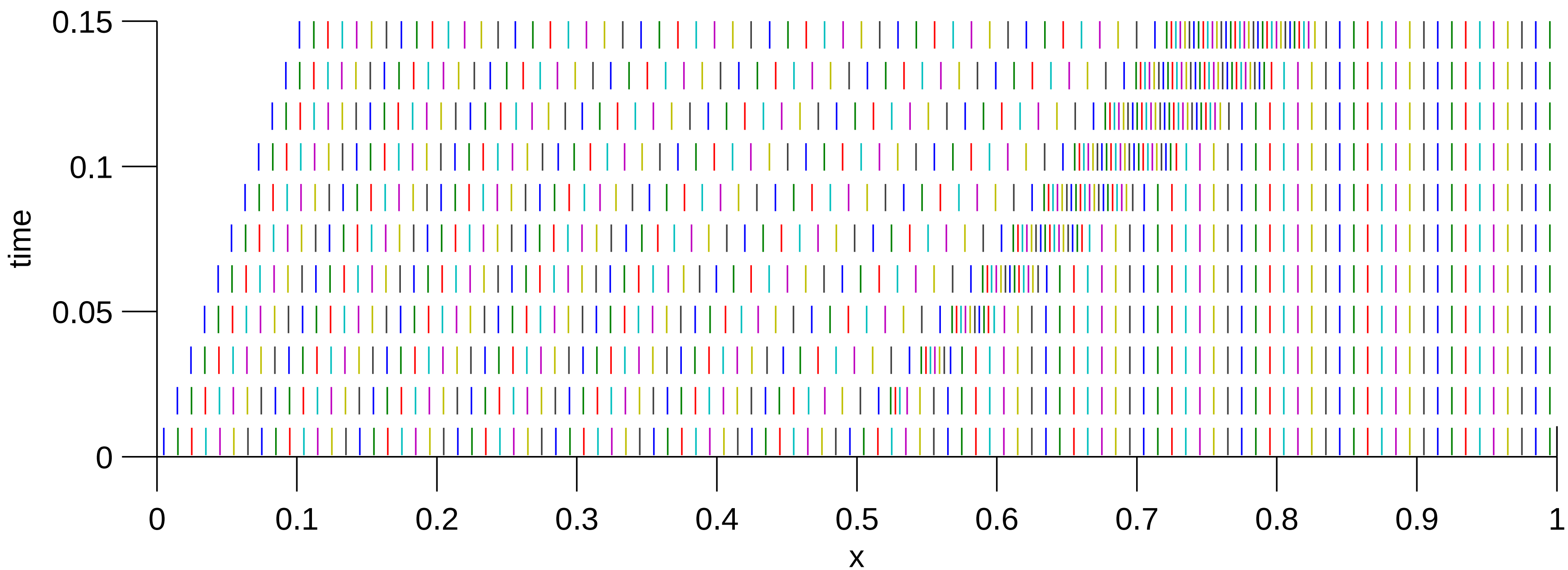
Lax's Riemann Problem

- $h_0 = 0$ Eulerian result
- $h_0 = 0.99$ Lagrangian-like result
  - sharper resolution for contact discontinuity



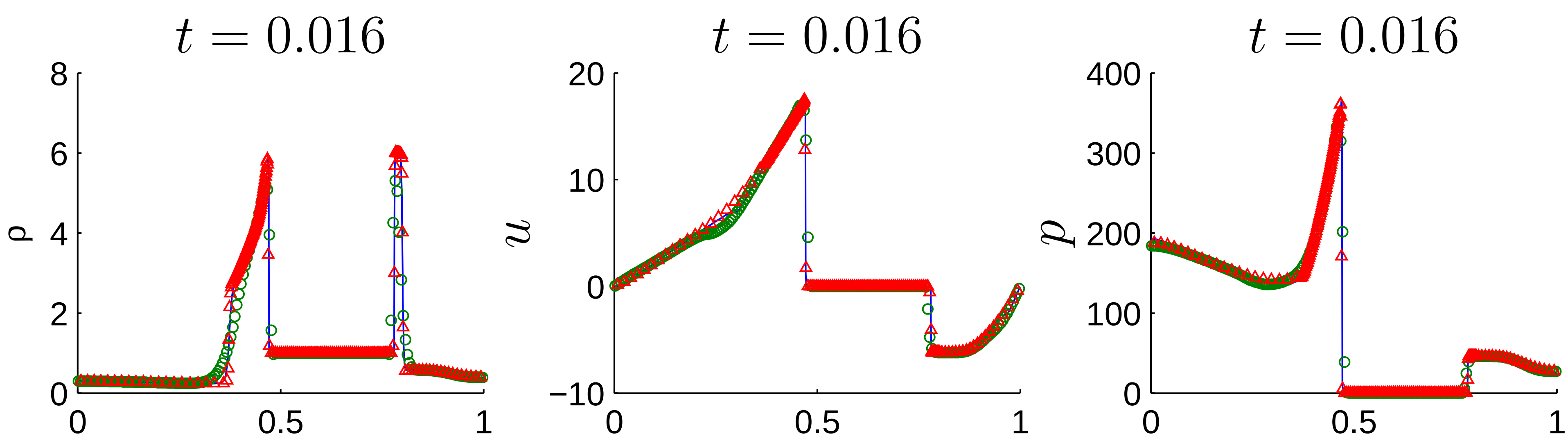
Lax's Riemann Problem

- Physical grid coordinates at selected times
  - Each little dashed line gives a cell-center location of the proposed Lagrange-like grid system



Woodward-Colella's Problem

- $h_0 = 0$ Eulerian result
- $h_0 = 0.99$ Lagrangian-like result
  - sharper resolution for contact discontinuity



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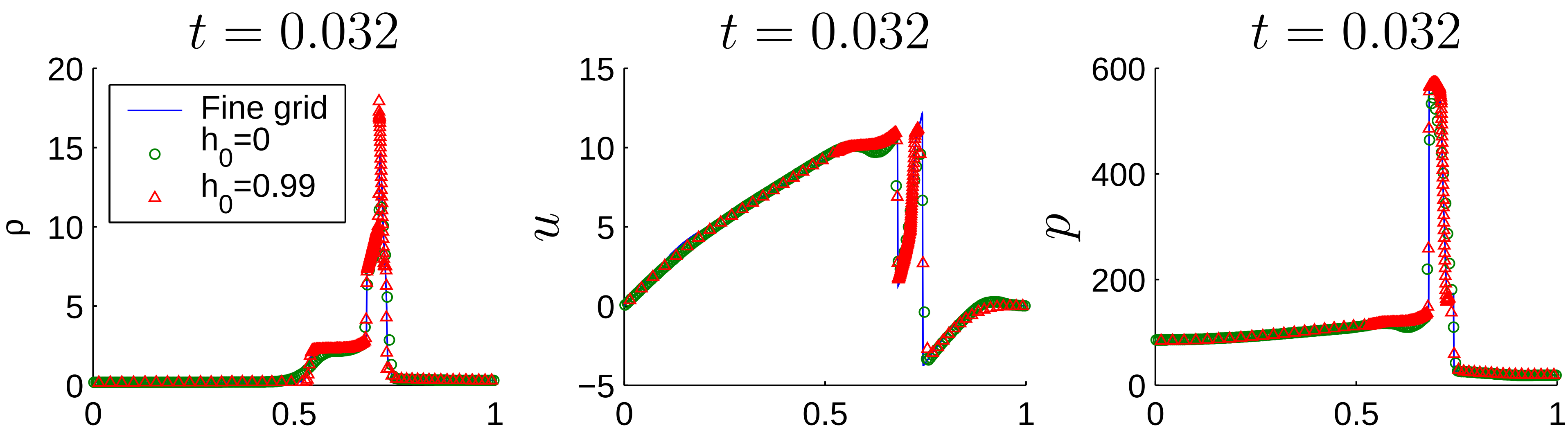

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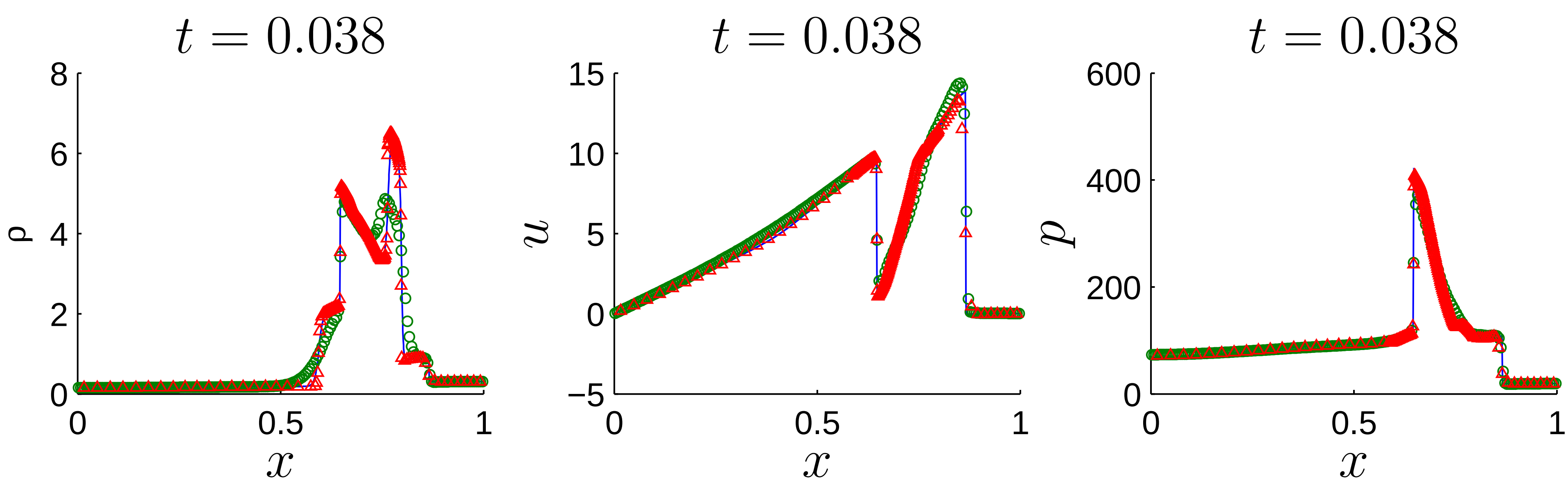

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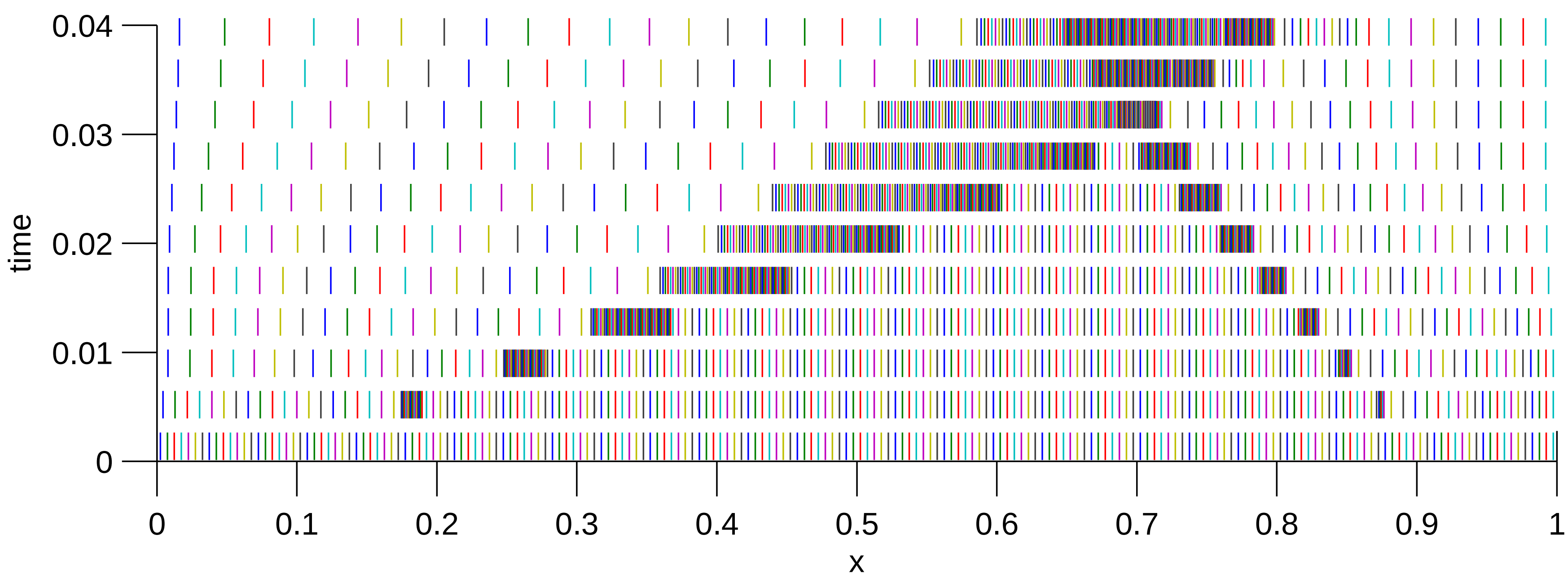
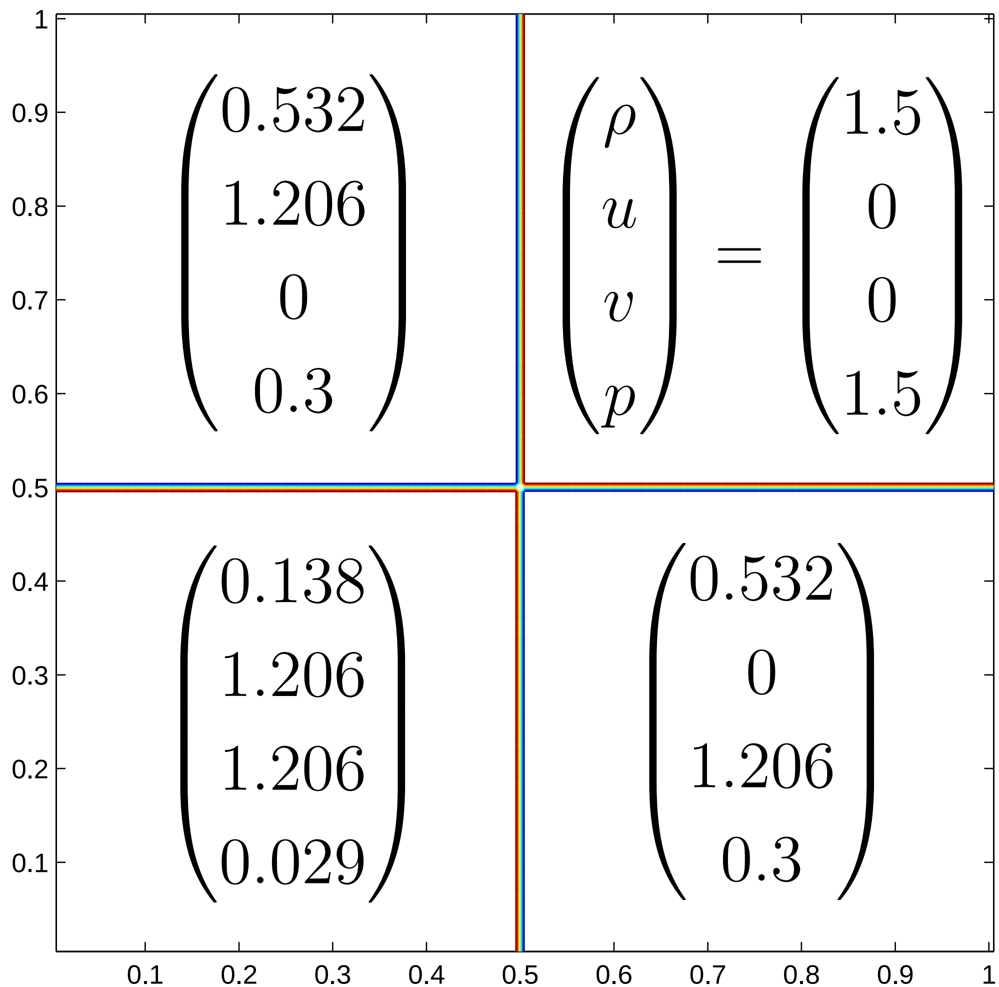


2D Riemann Problem

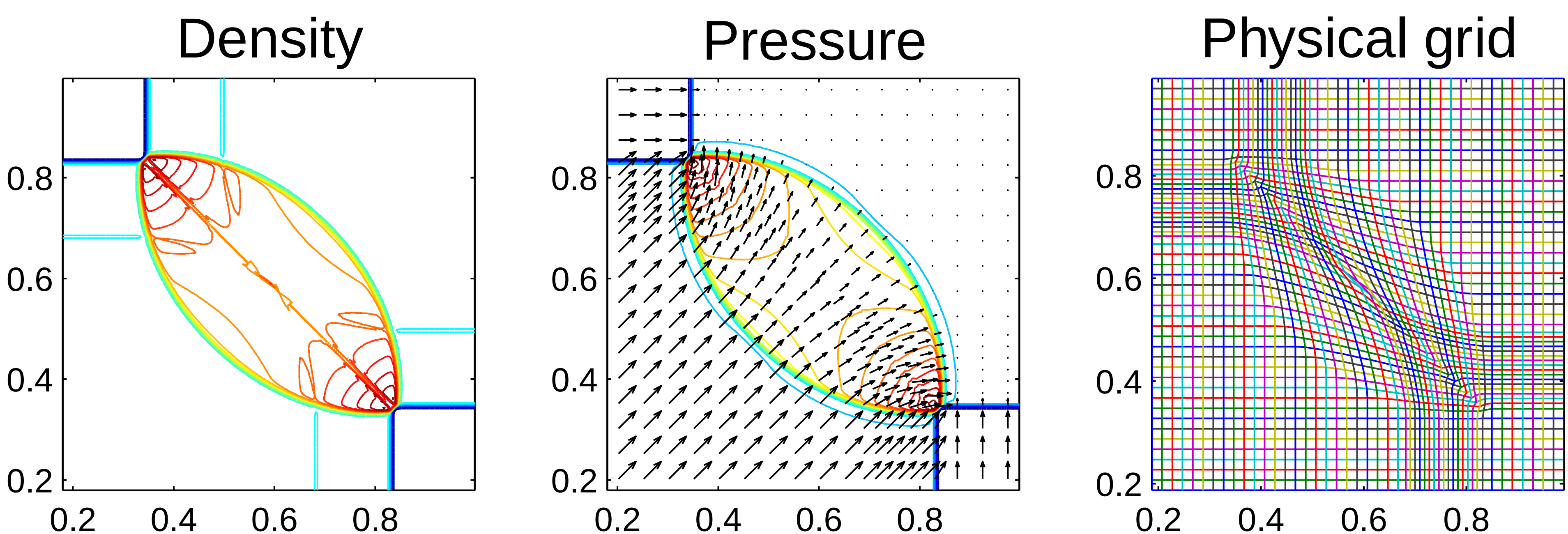
With initial 4-shock wave pattern



2D Riemann Problem

With initial 4-shock wave pattern

- Lagrange-like result
  - Occurrence of simple Mach reflection

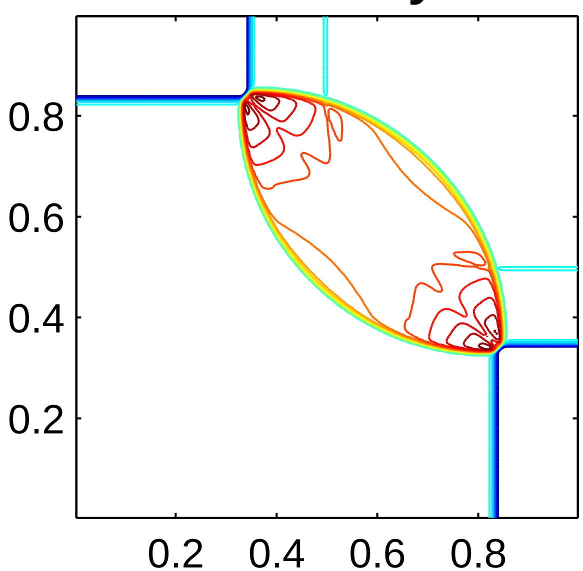


2D Riemann Problem

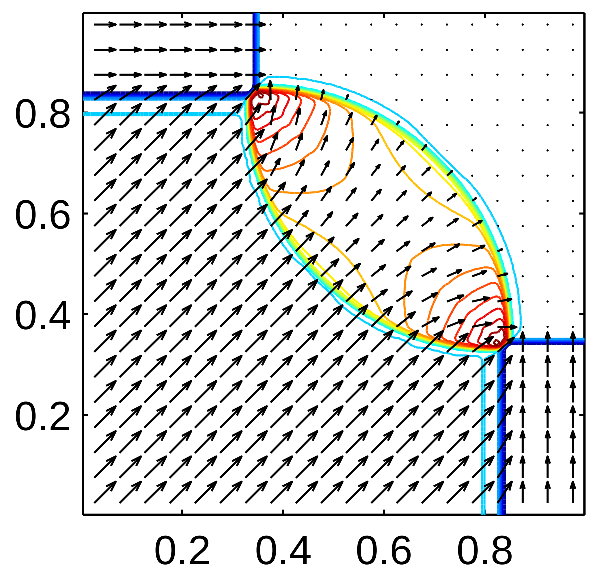
With initial 4-shock wave pattern

- Eulerian result
  - Poor resolution around simple Mach reflection

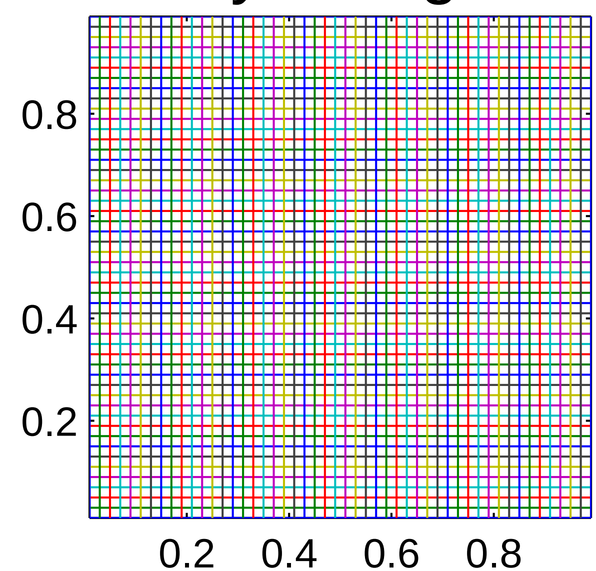
Density



Pressure



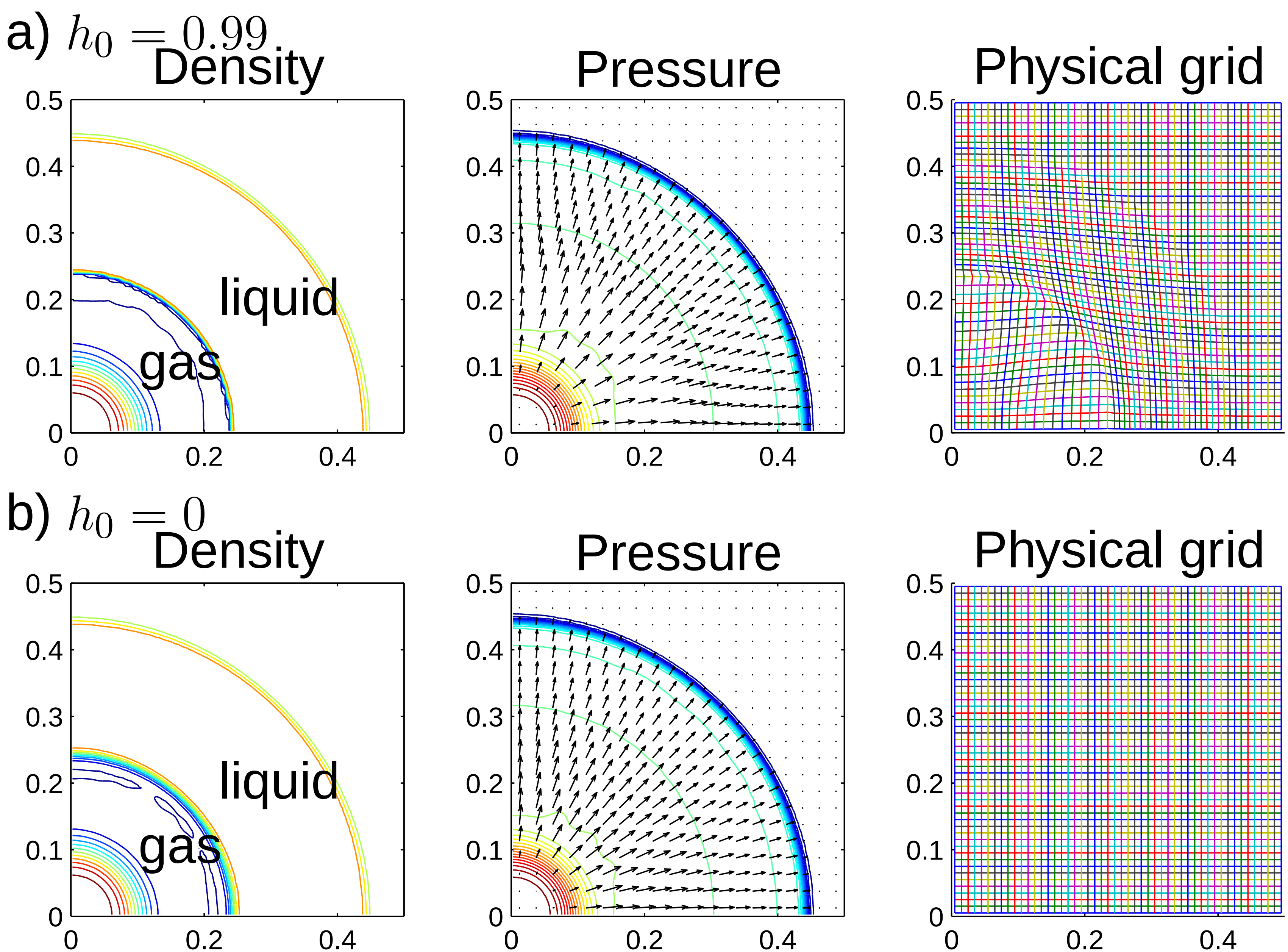
Physical grid



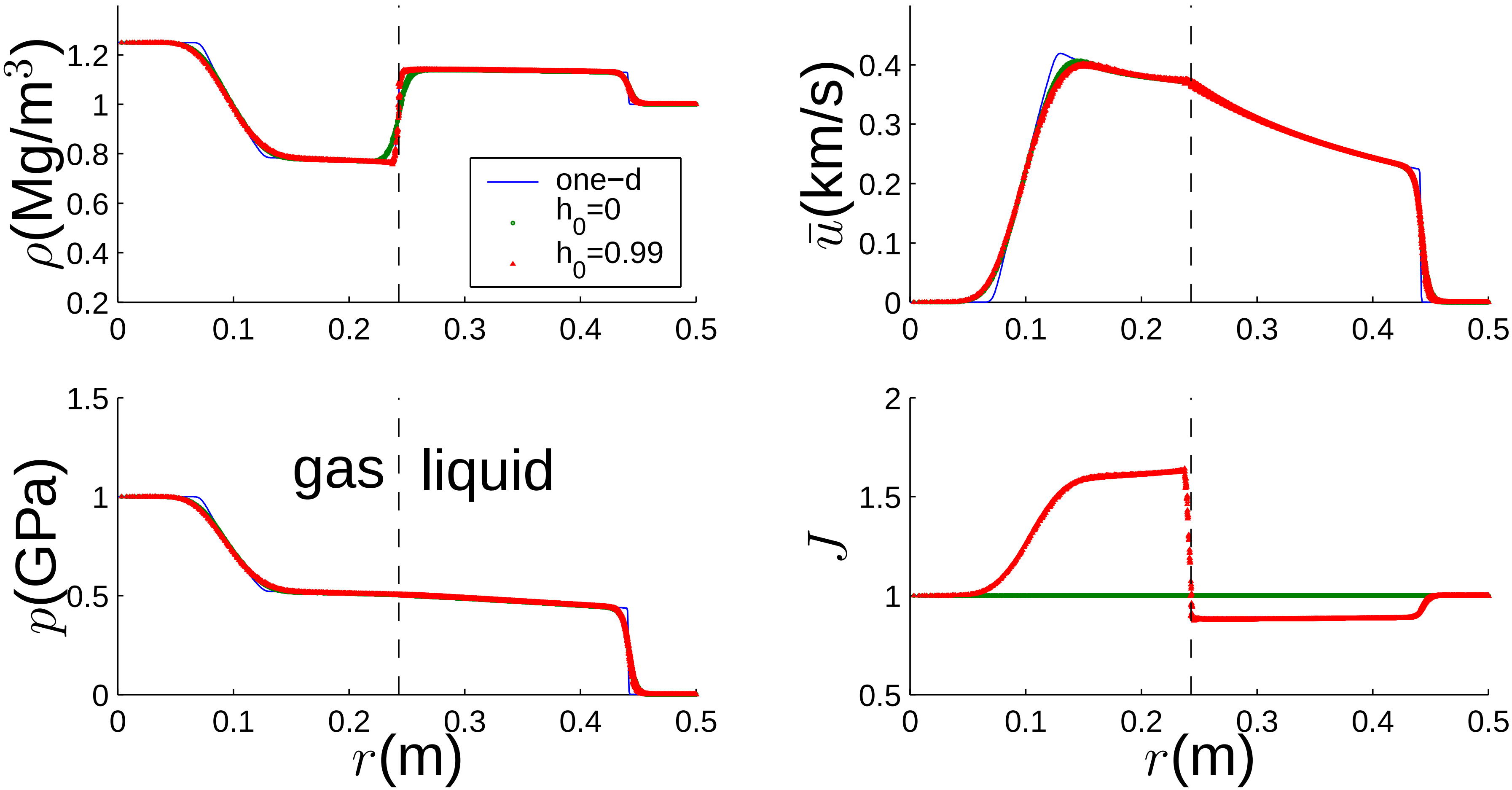
More Examples

- Two-dimensional case
  - Radially symmetric problem
  - Underwater explosion
  - Shock-bubble interaction
    - Helium bubble case
    - Refrigerant bubble case
- Three-dimensional case
  - Underwater explosion
  - Shock-bubble interaction
    - Helium bubble case
    - Refrigerant bubble case

Radially Symmetric Problem

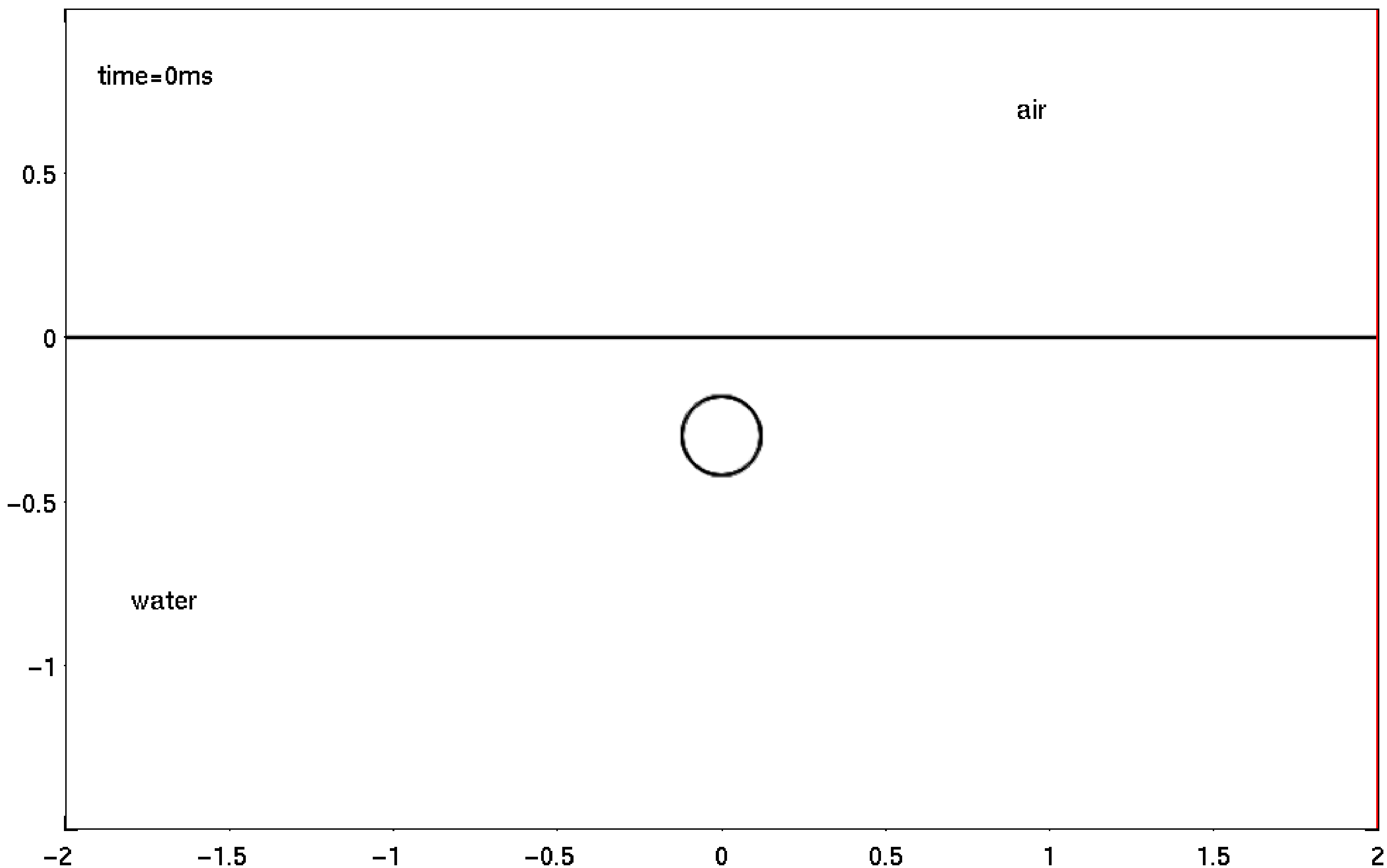


Radially Symmetric Prob. (Cont.)



Underwater Explosions

- Numerical schlieren images $h_0 = 0.9$, 800×500 grid



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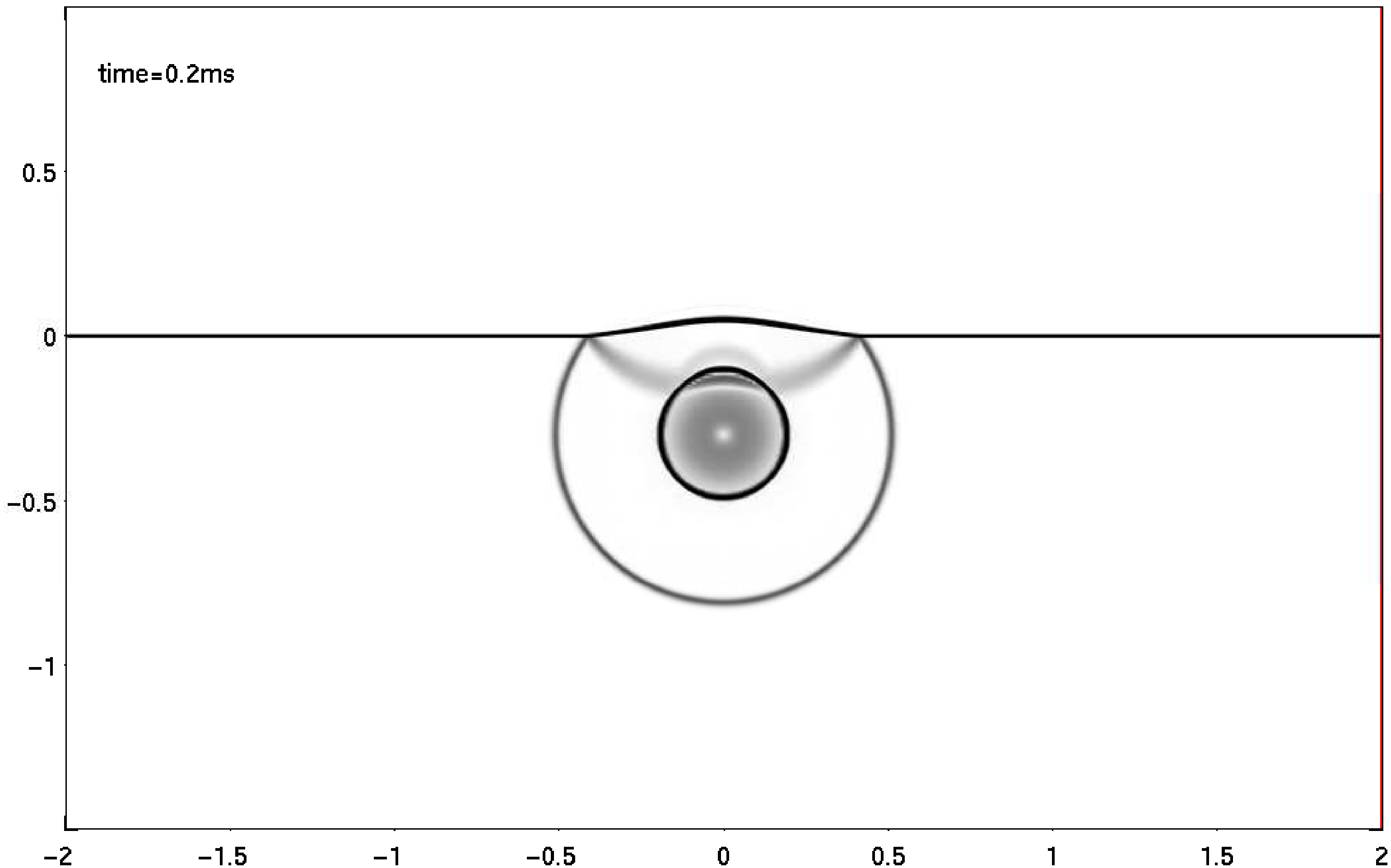

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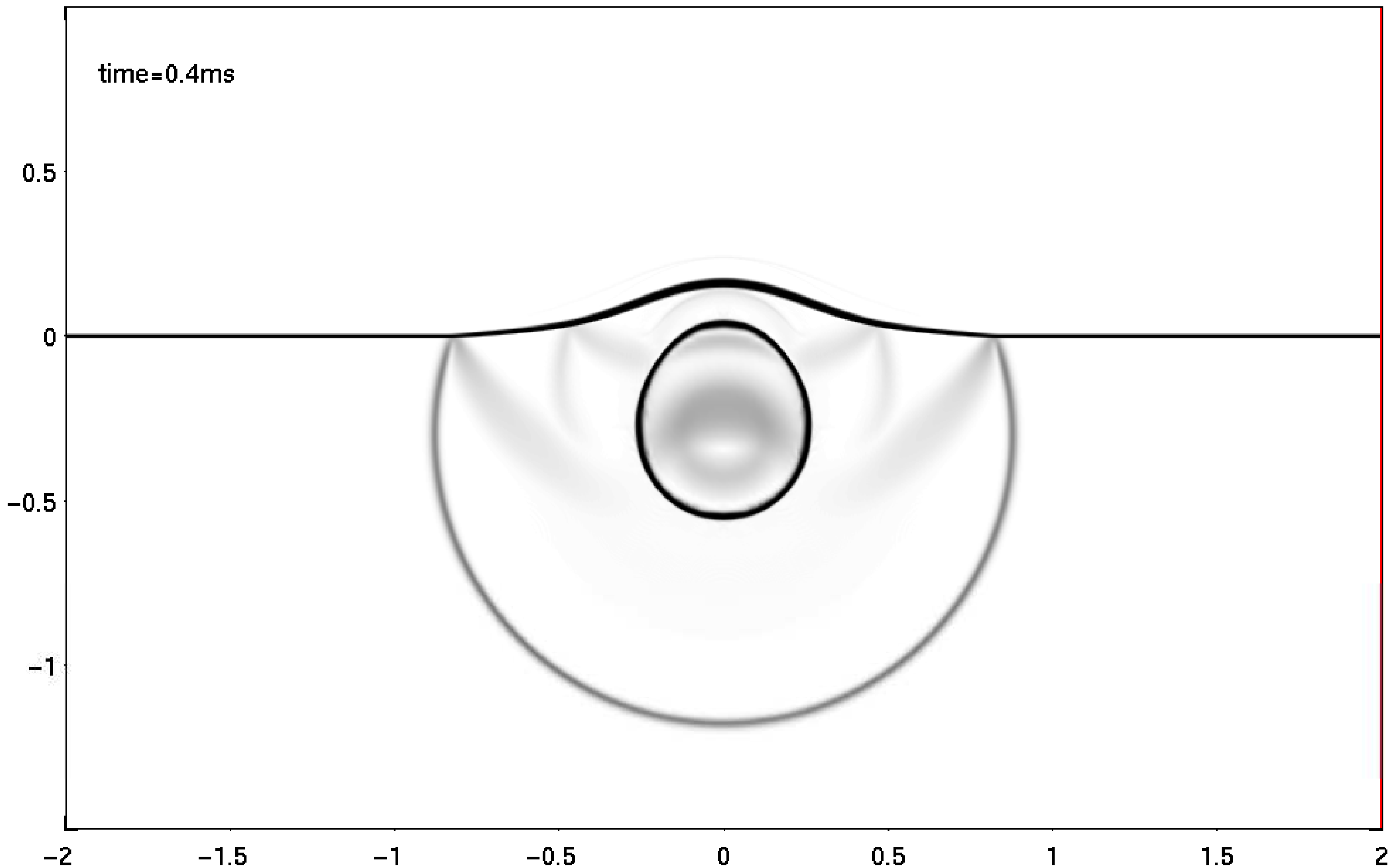

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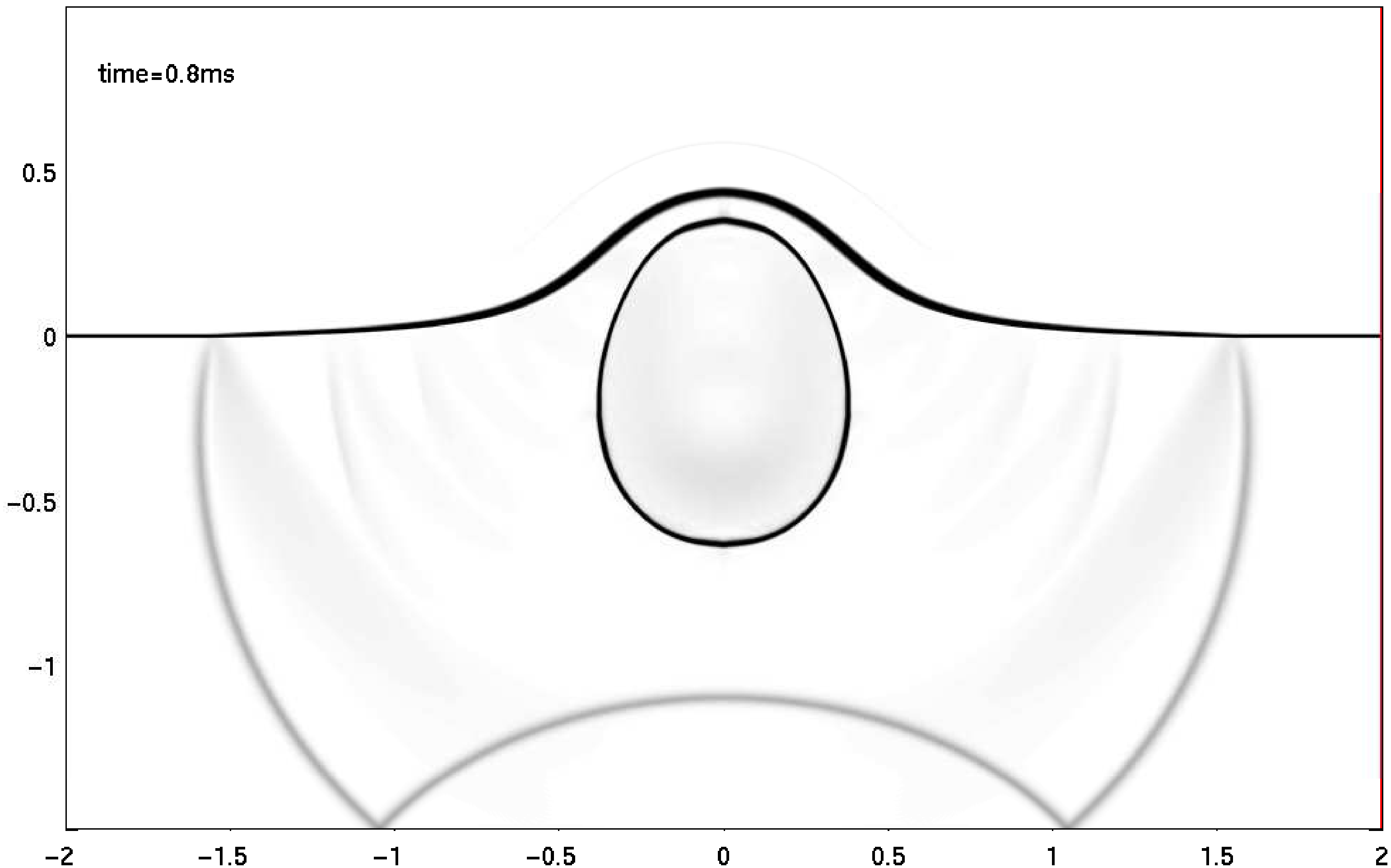

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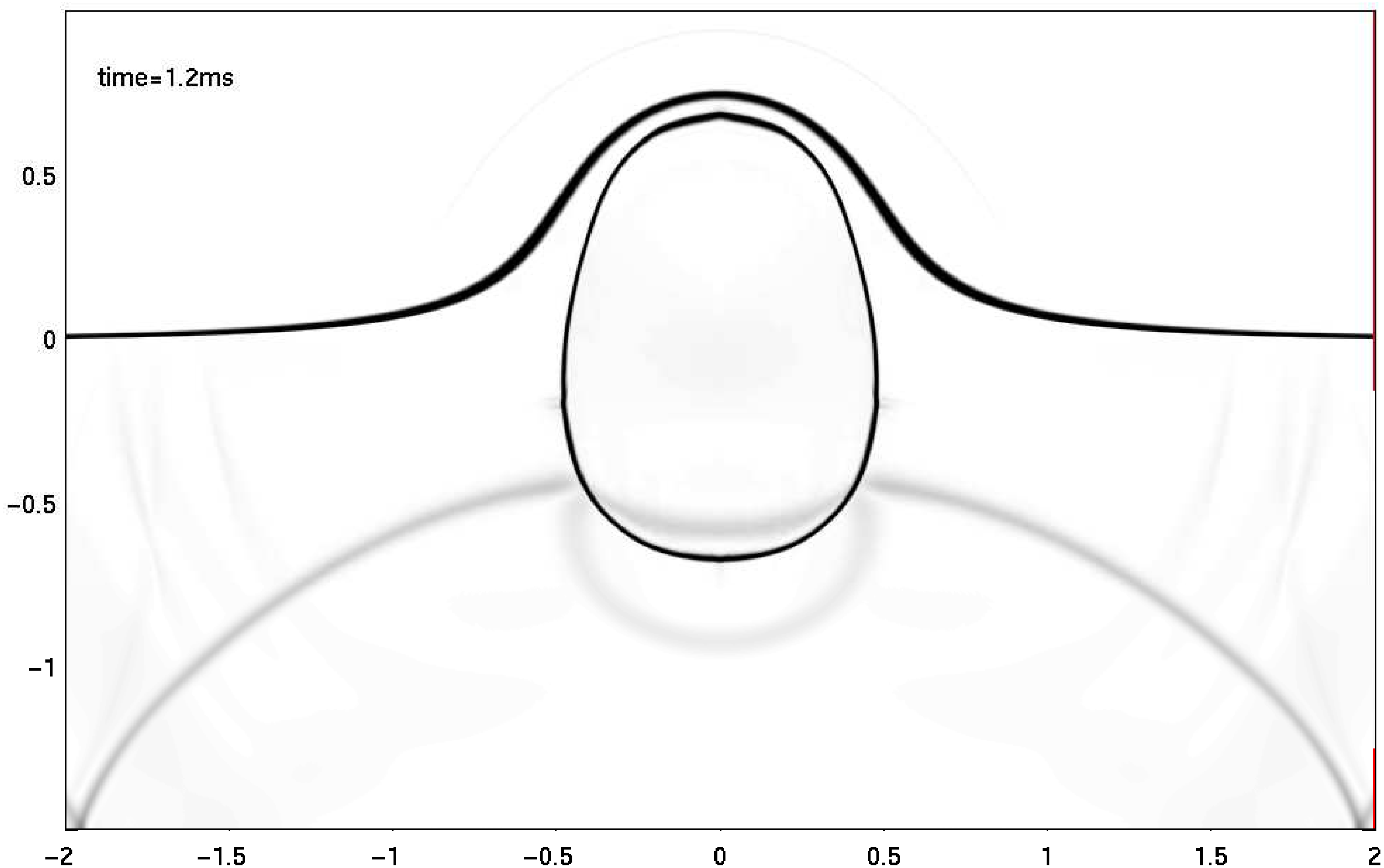
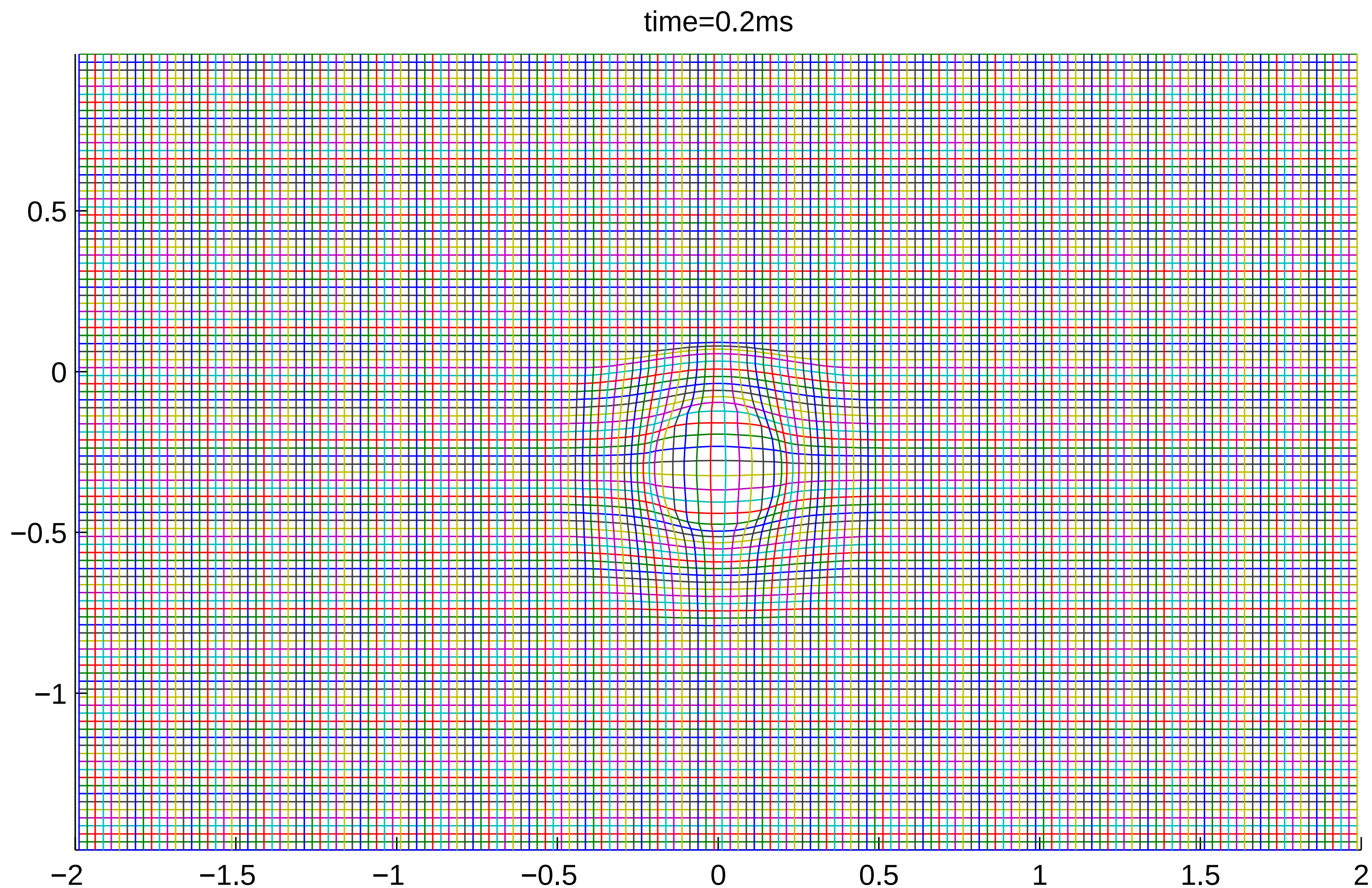


Underwater Explosions (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.9$

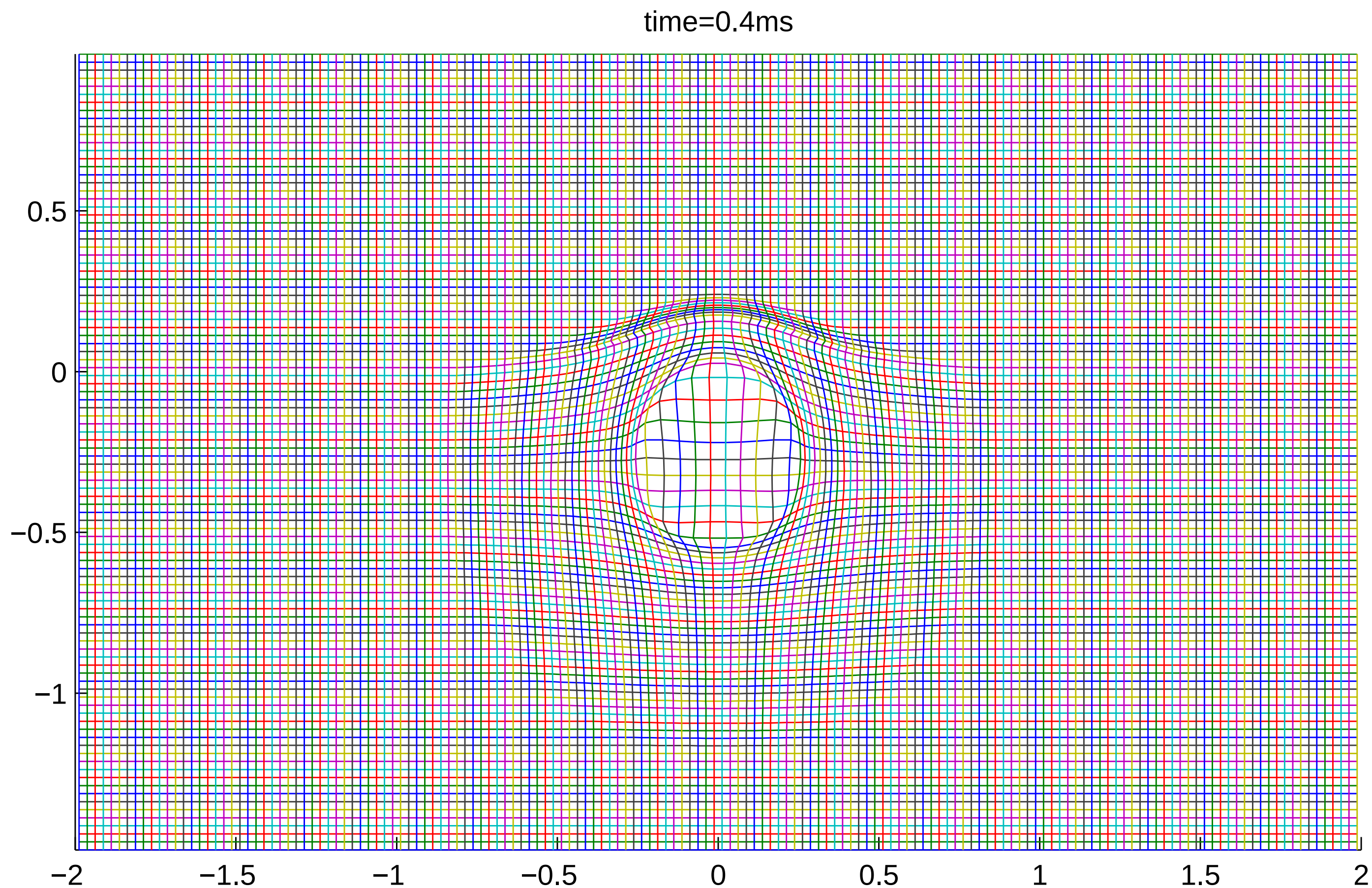
Underwater Explosions (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.9$



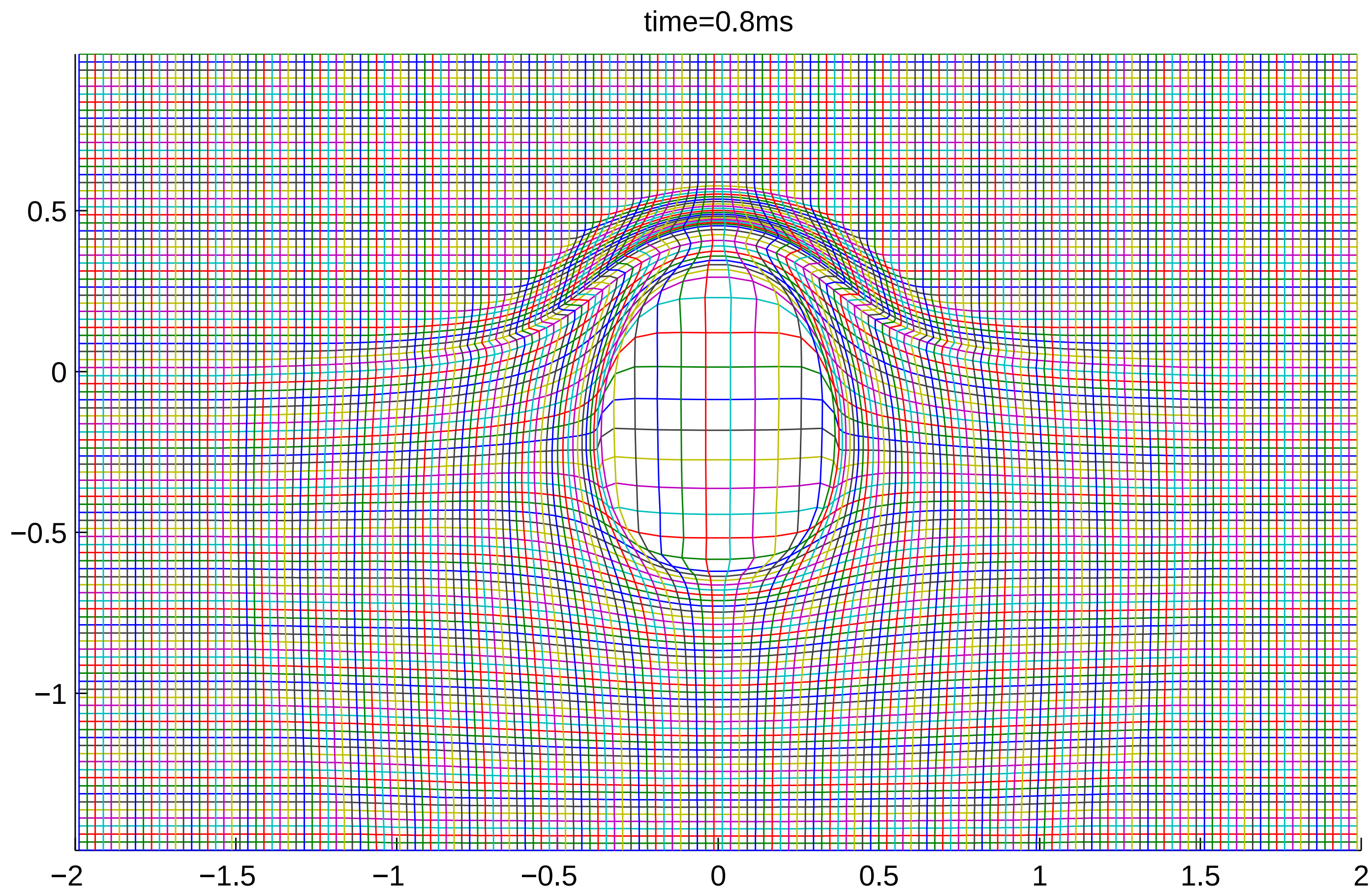
Underwater Explosions (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.9$



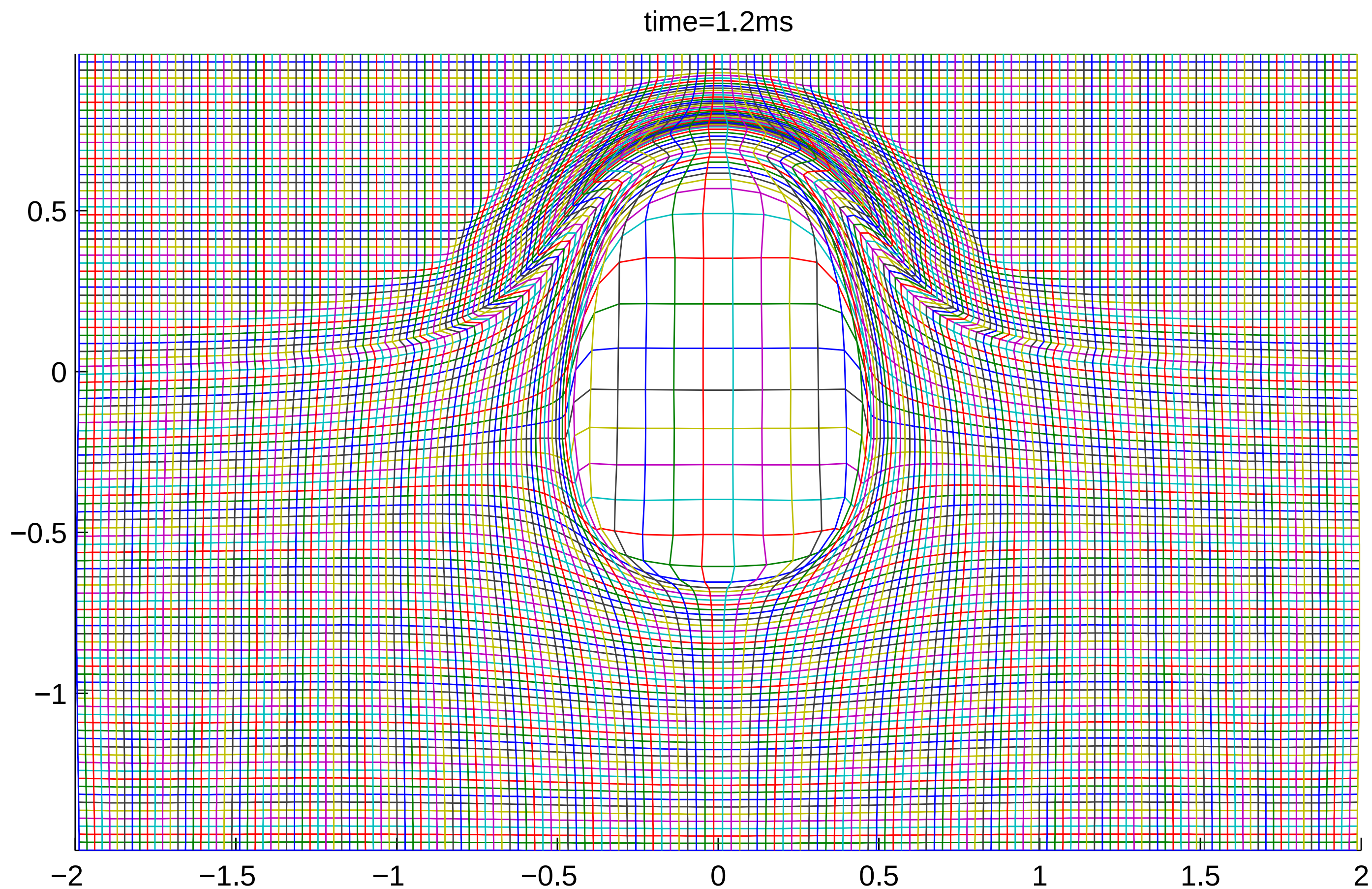
Underwater Explosions (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.9$



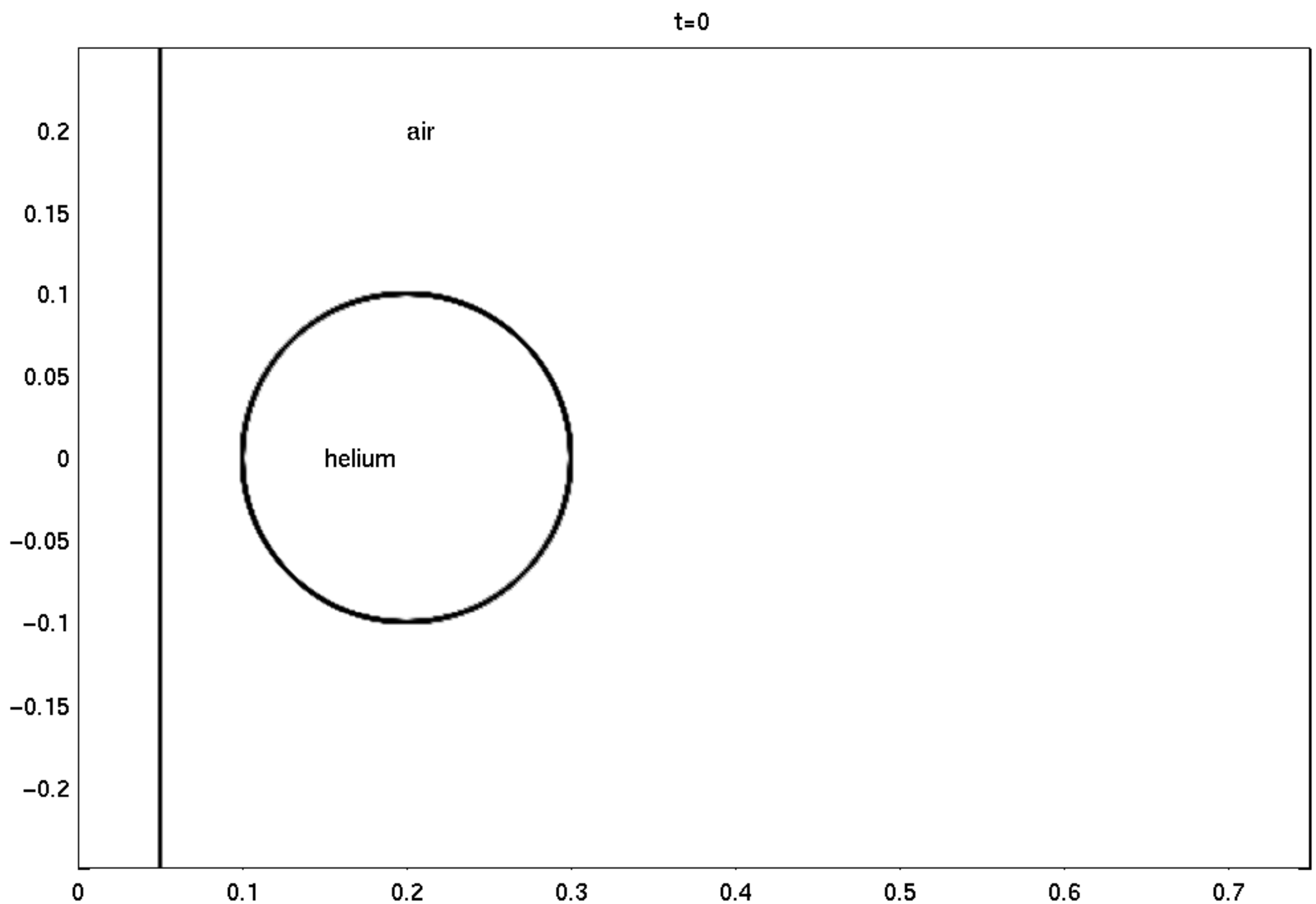
Underwater Explosions (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.9$



Shock-Bubble (Helium)

- Numerical schlieren images: $h_0 = 0.5$, 600×400 grid



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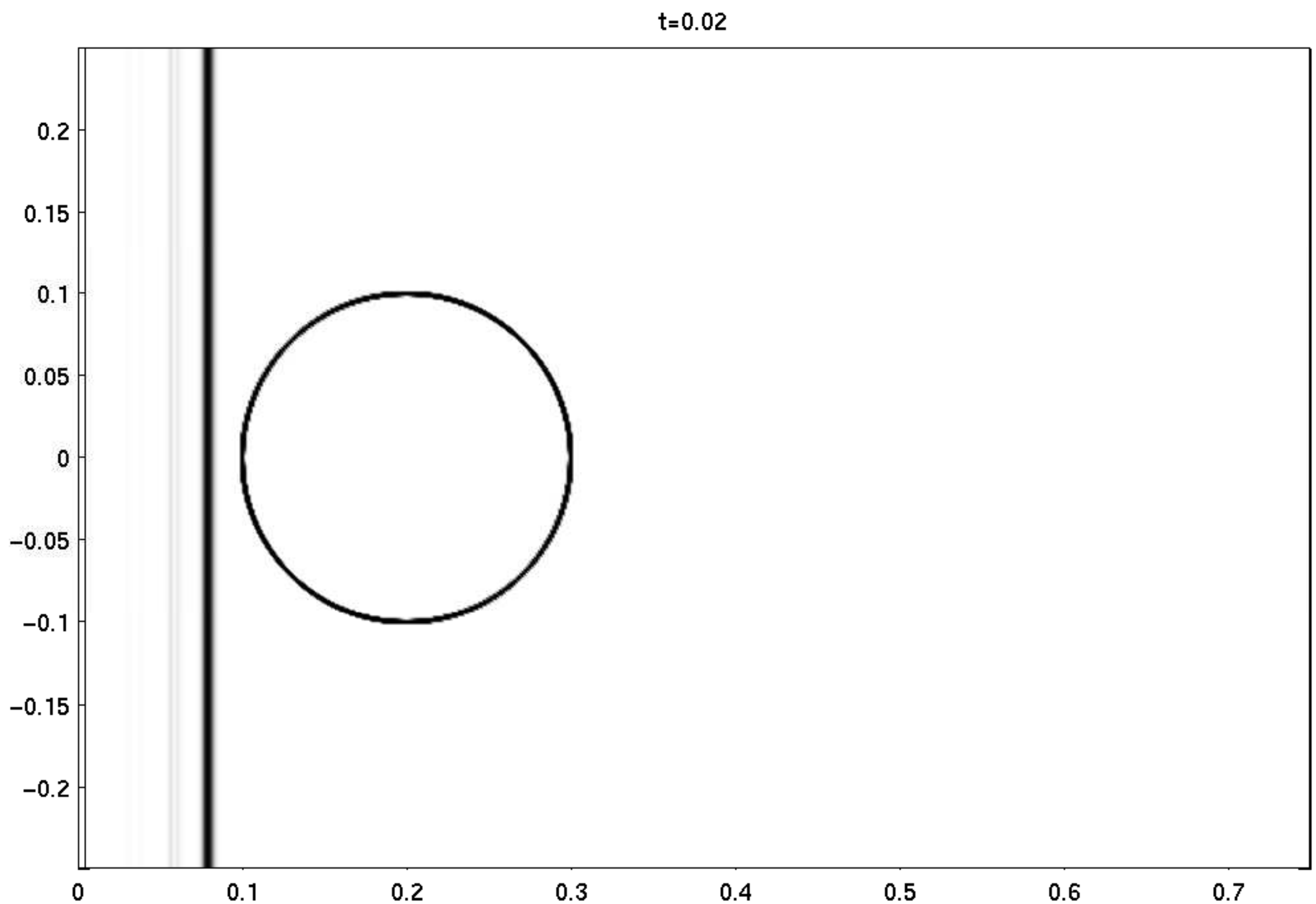

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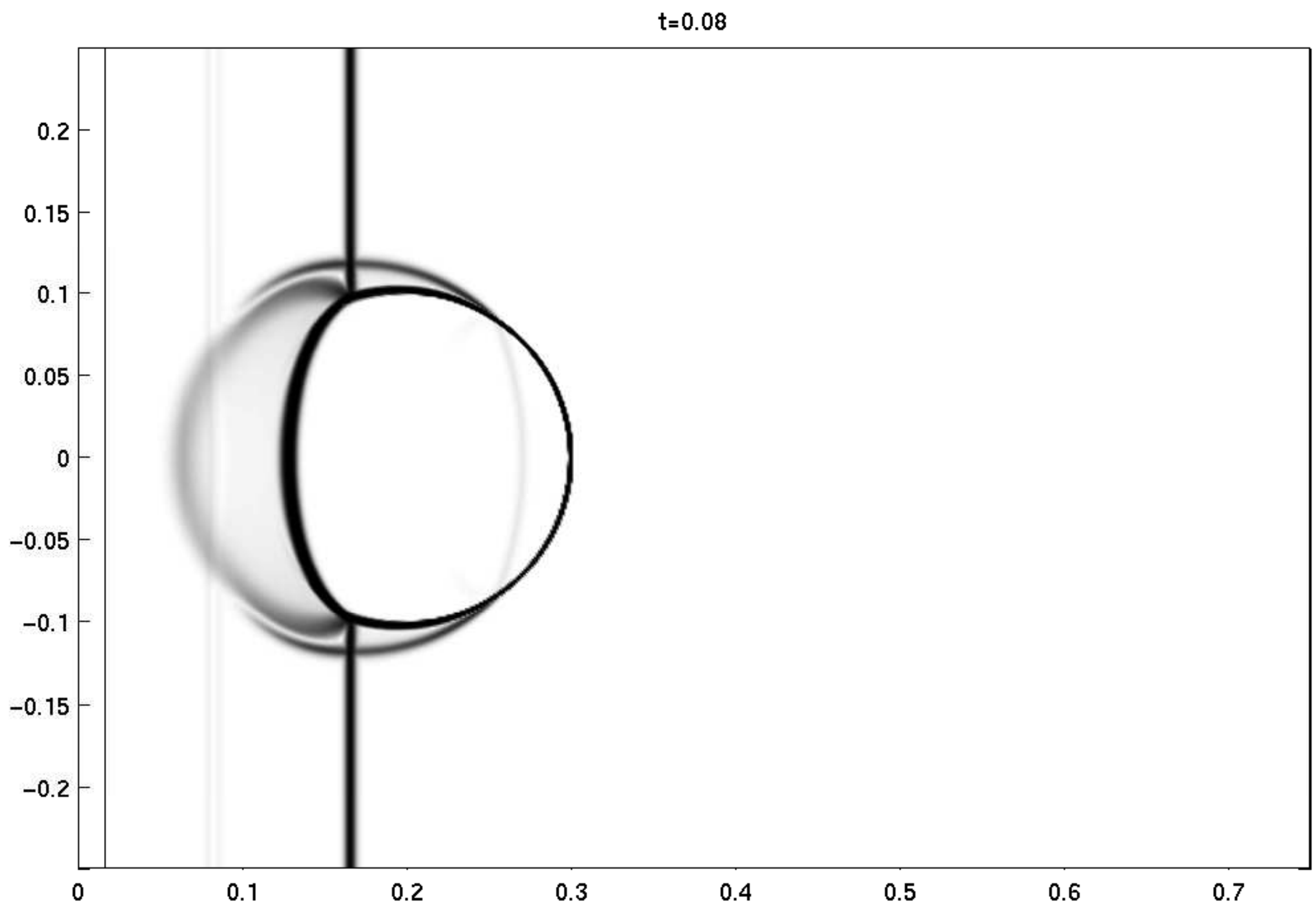

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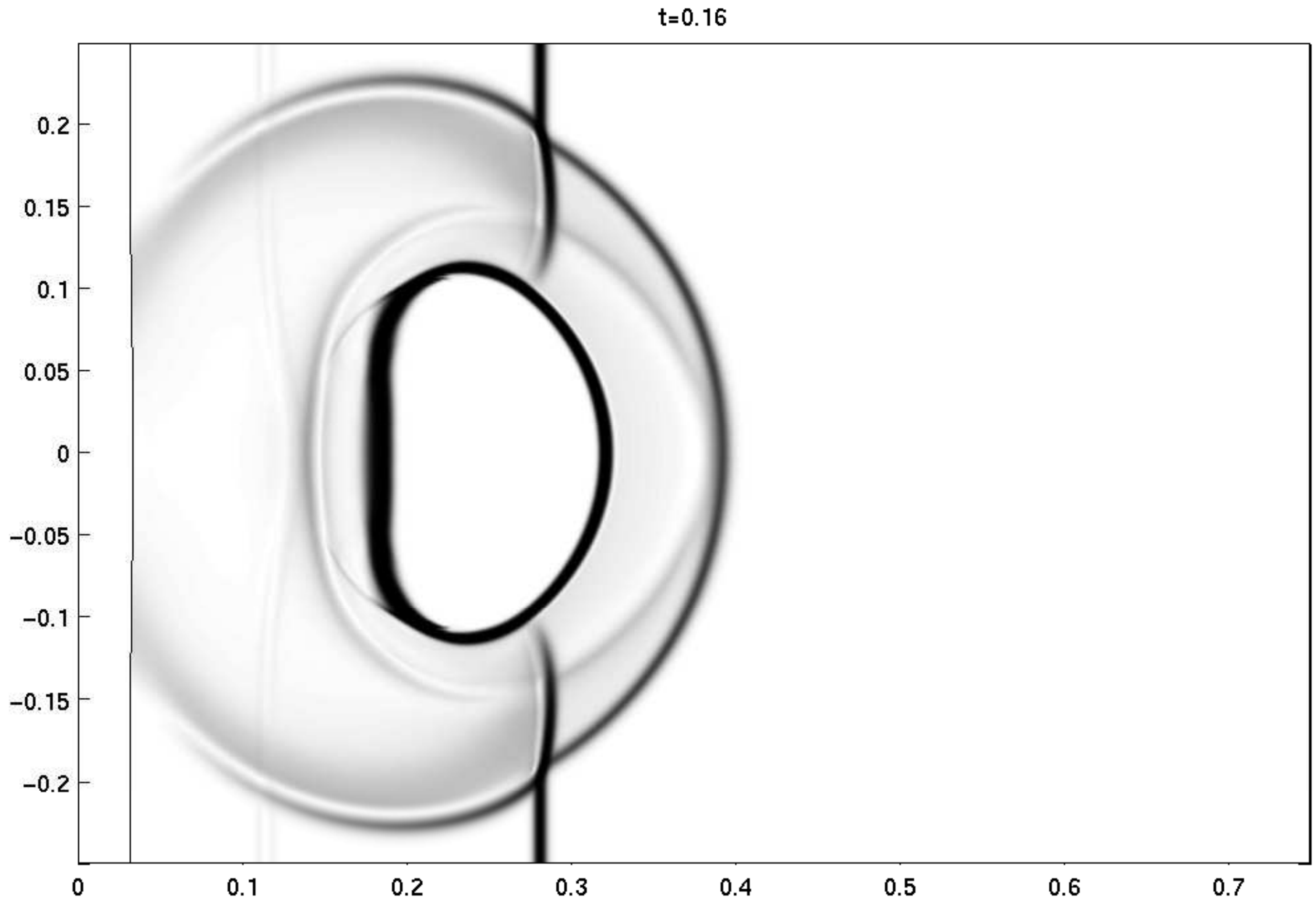

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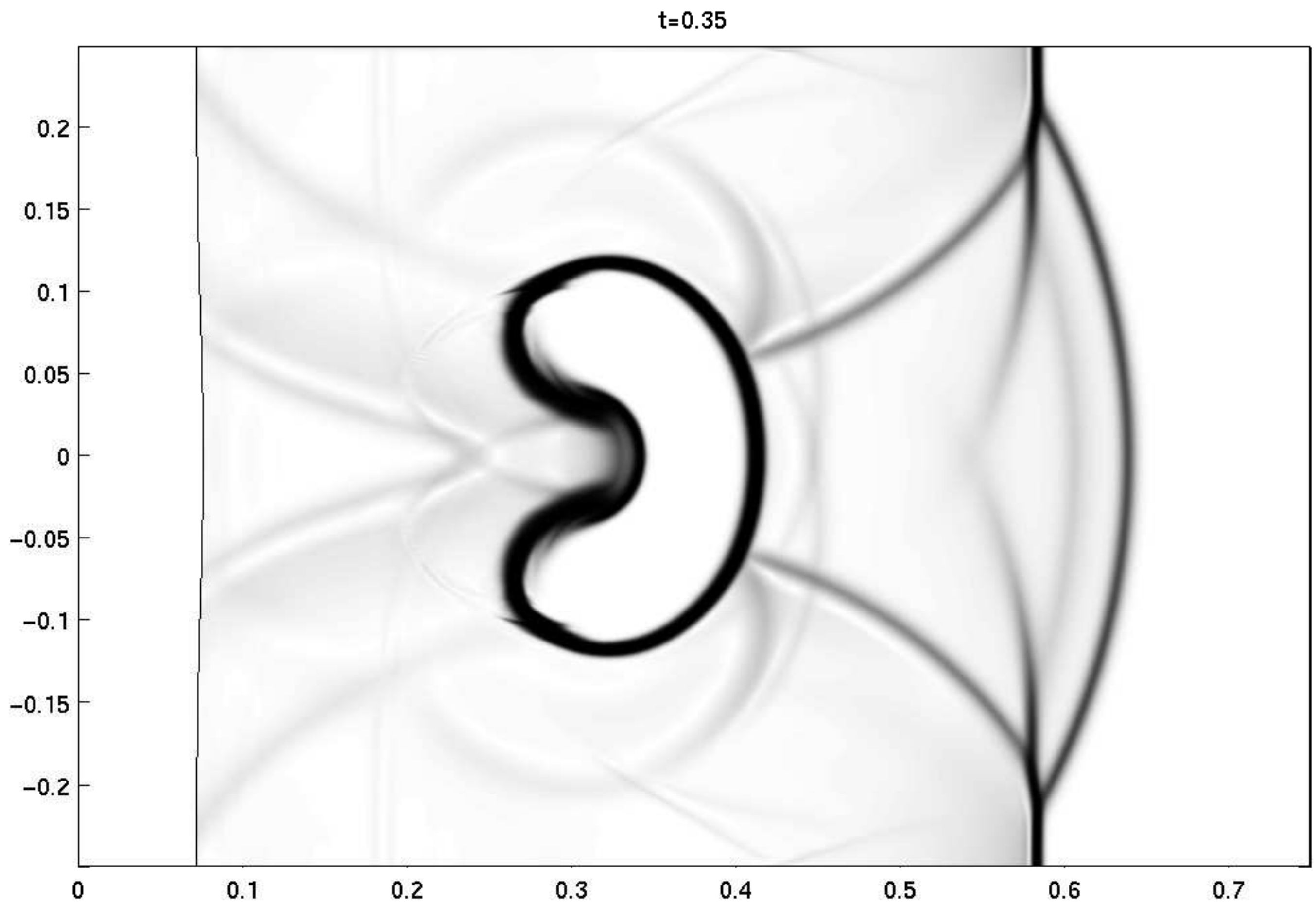
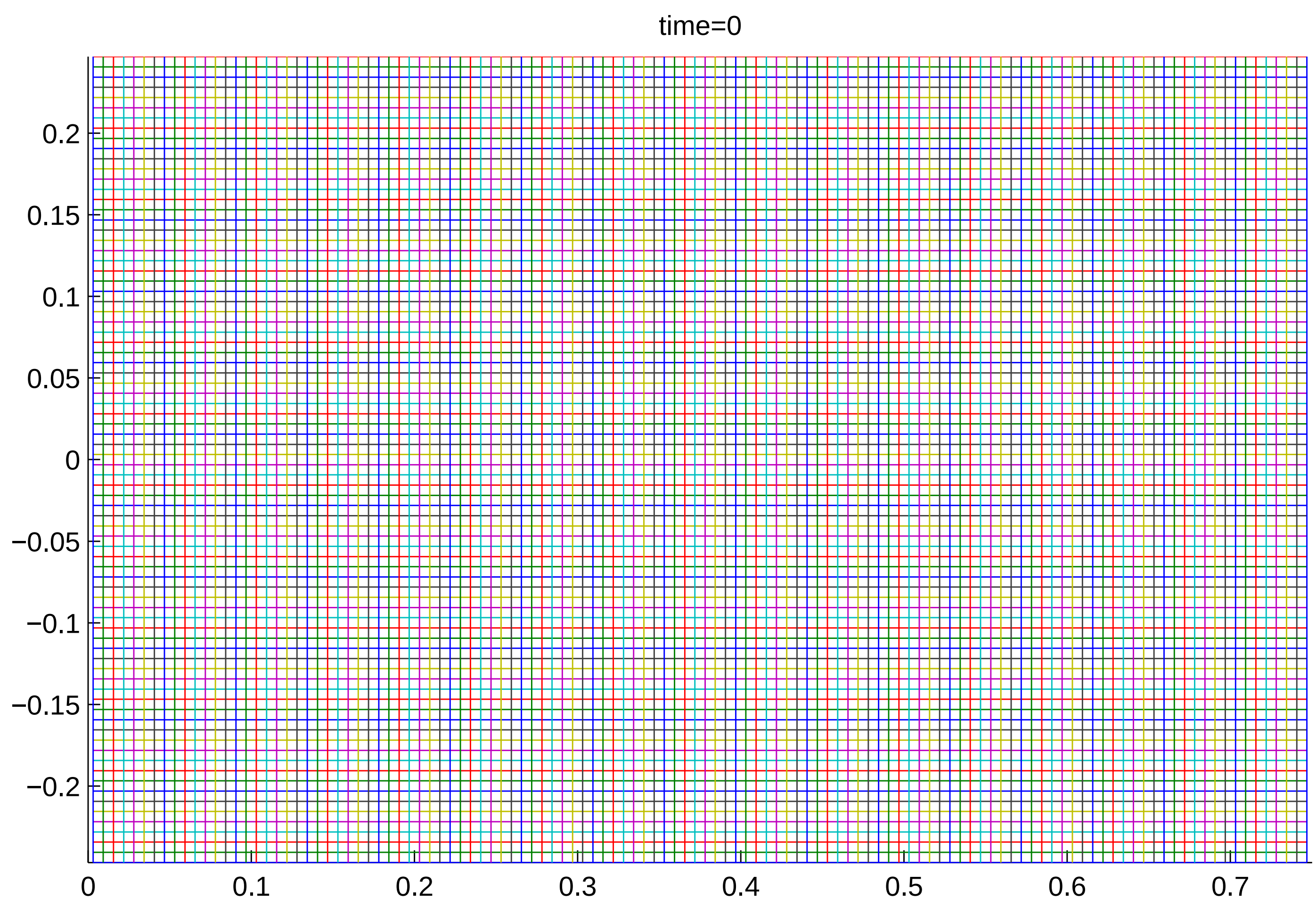


Shock-Bubble (Helium) (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.5$



Shock-Bubble (Helium) (Cont.)

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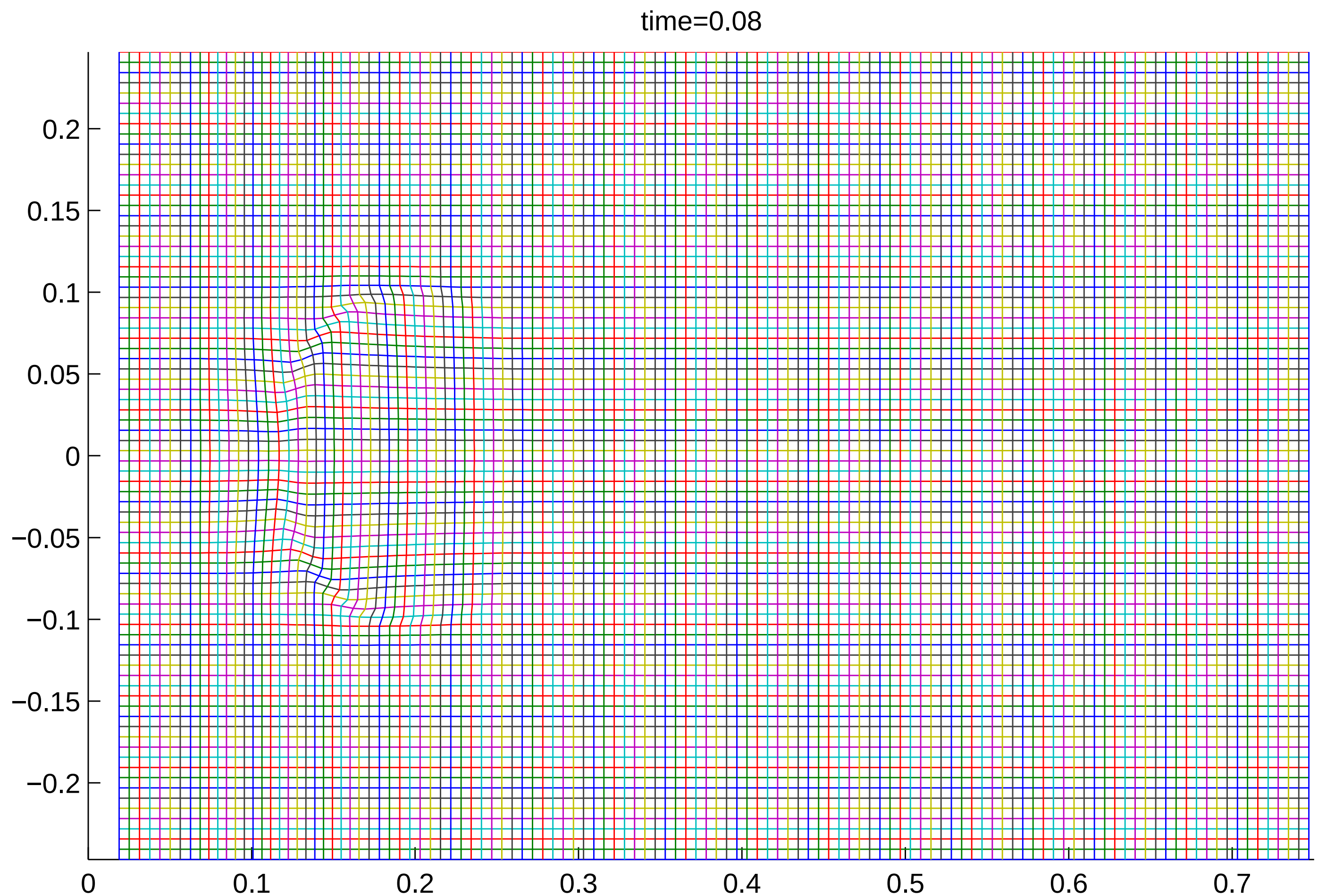
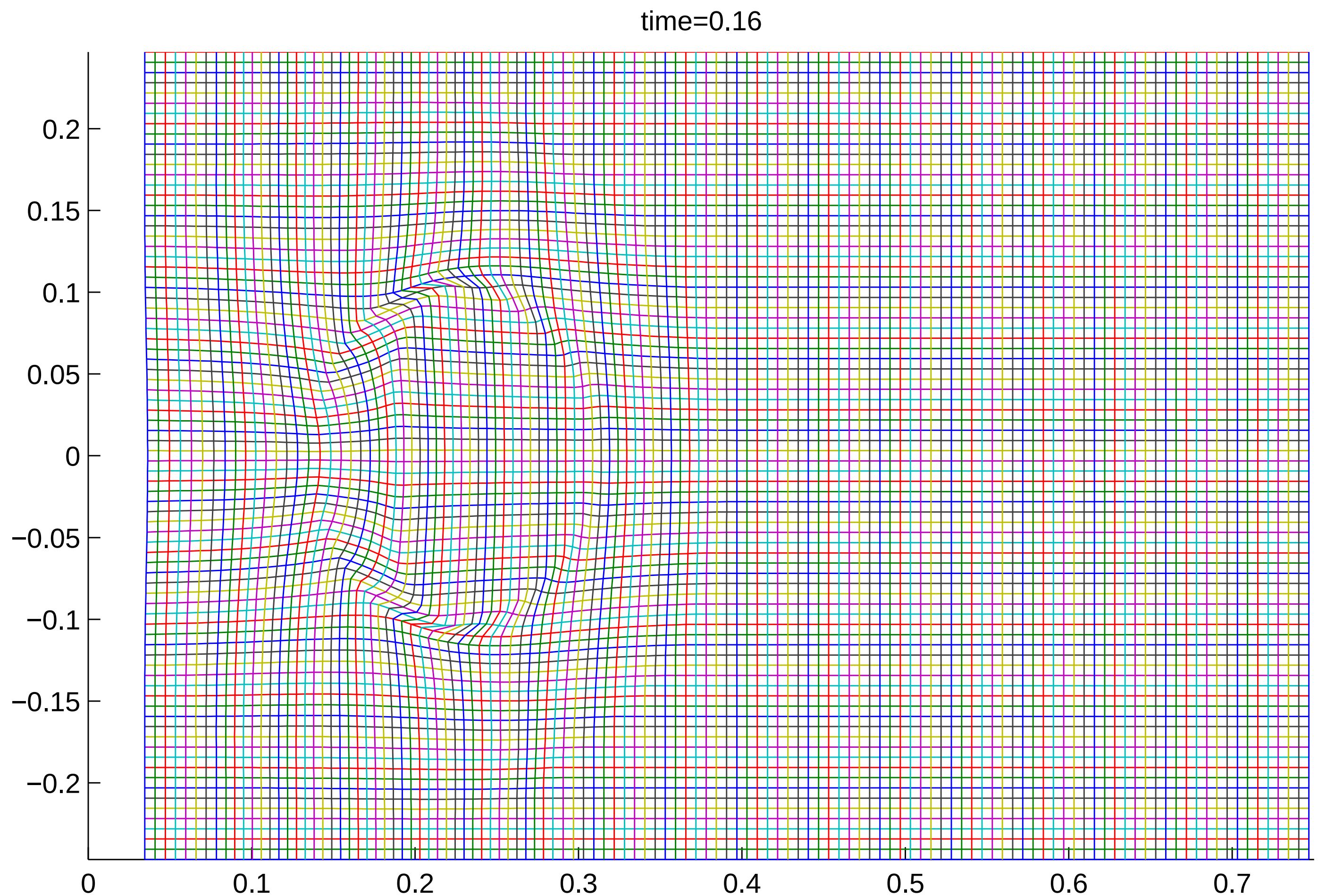


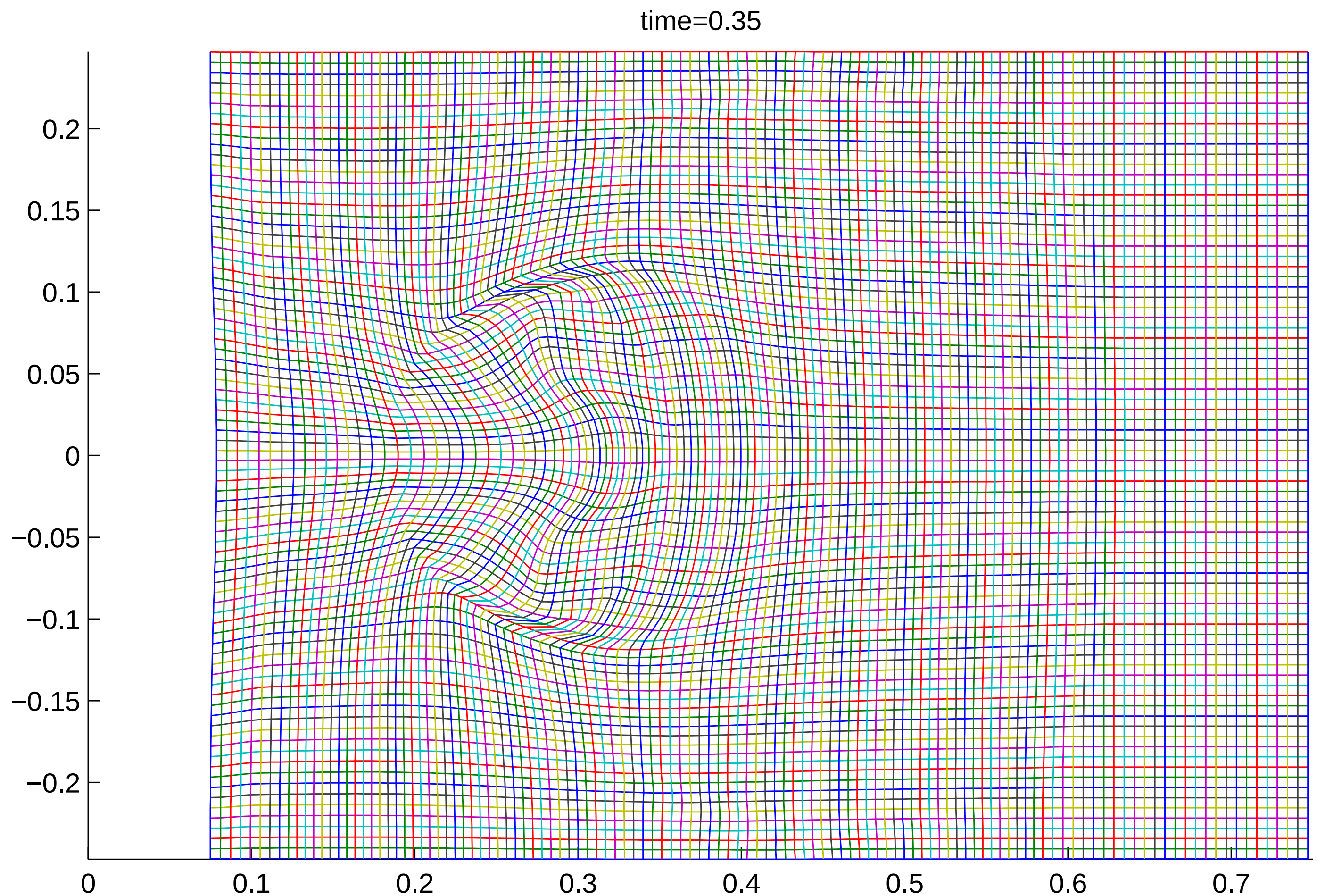
Shock-Bubble (Helium) (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.5$



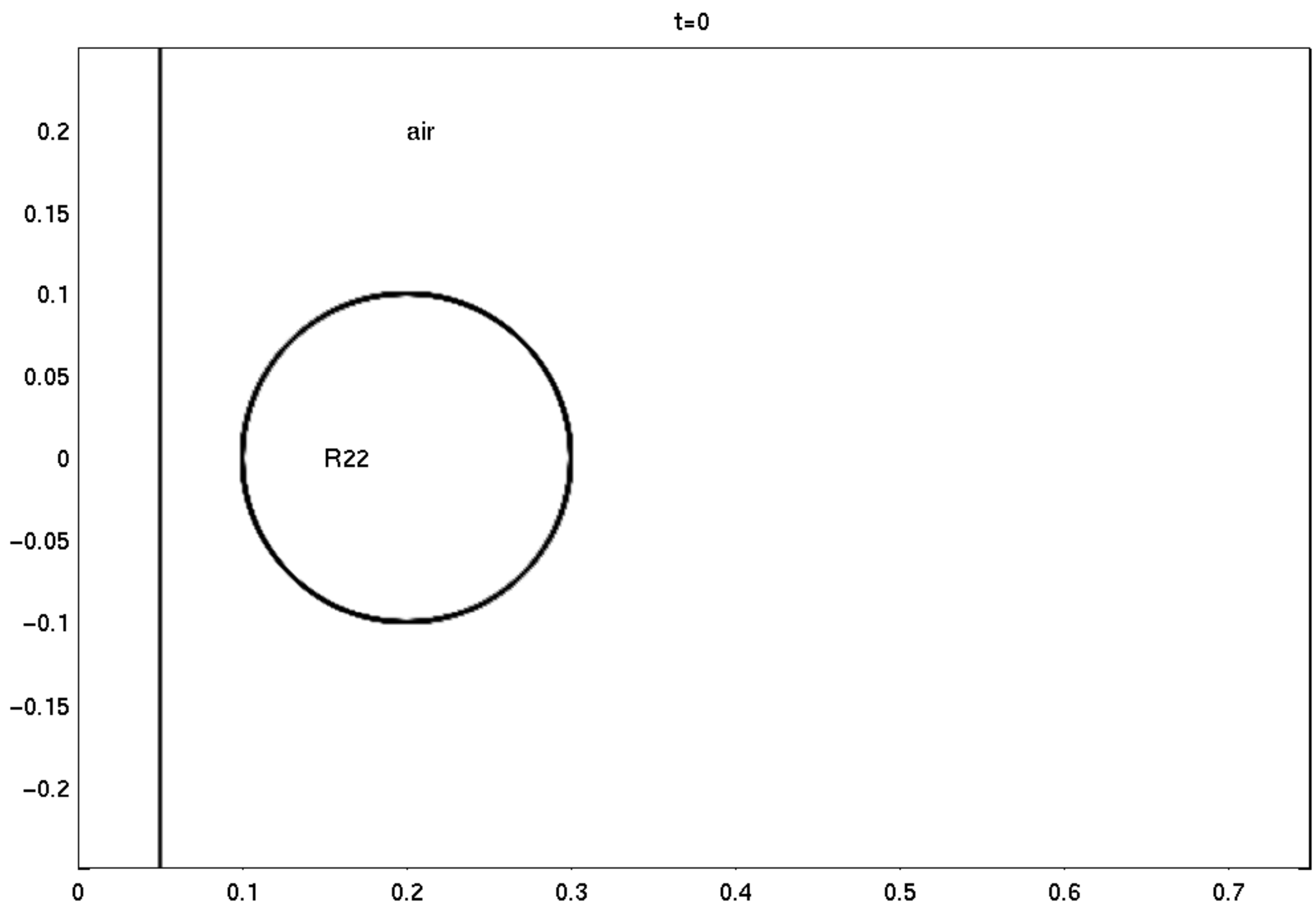
Shock-Bubble (Helium) (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.5$



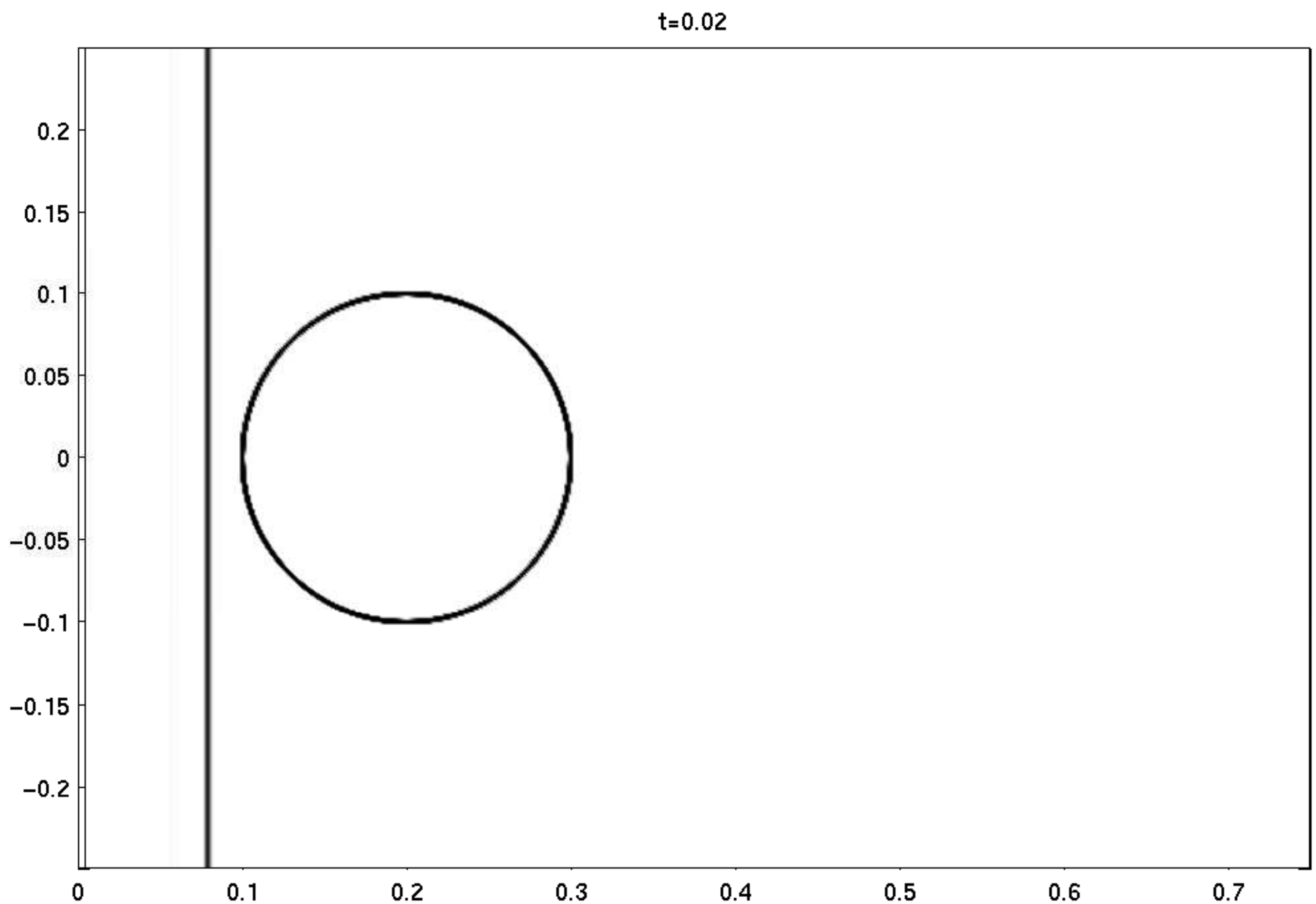
Shock-Bubble (Refrigerant)

- Numerical schlieren images: $h_0 = 0.5$, 600×400 grid



Shock-Bubble (Refrigerant)

- Numerical schlieren images: $h_0 = 0.5$, 600×400 grid



Shock-Bubble (Refrigerant)

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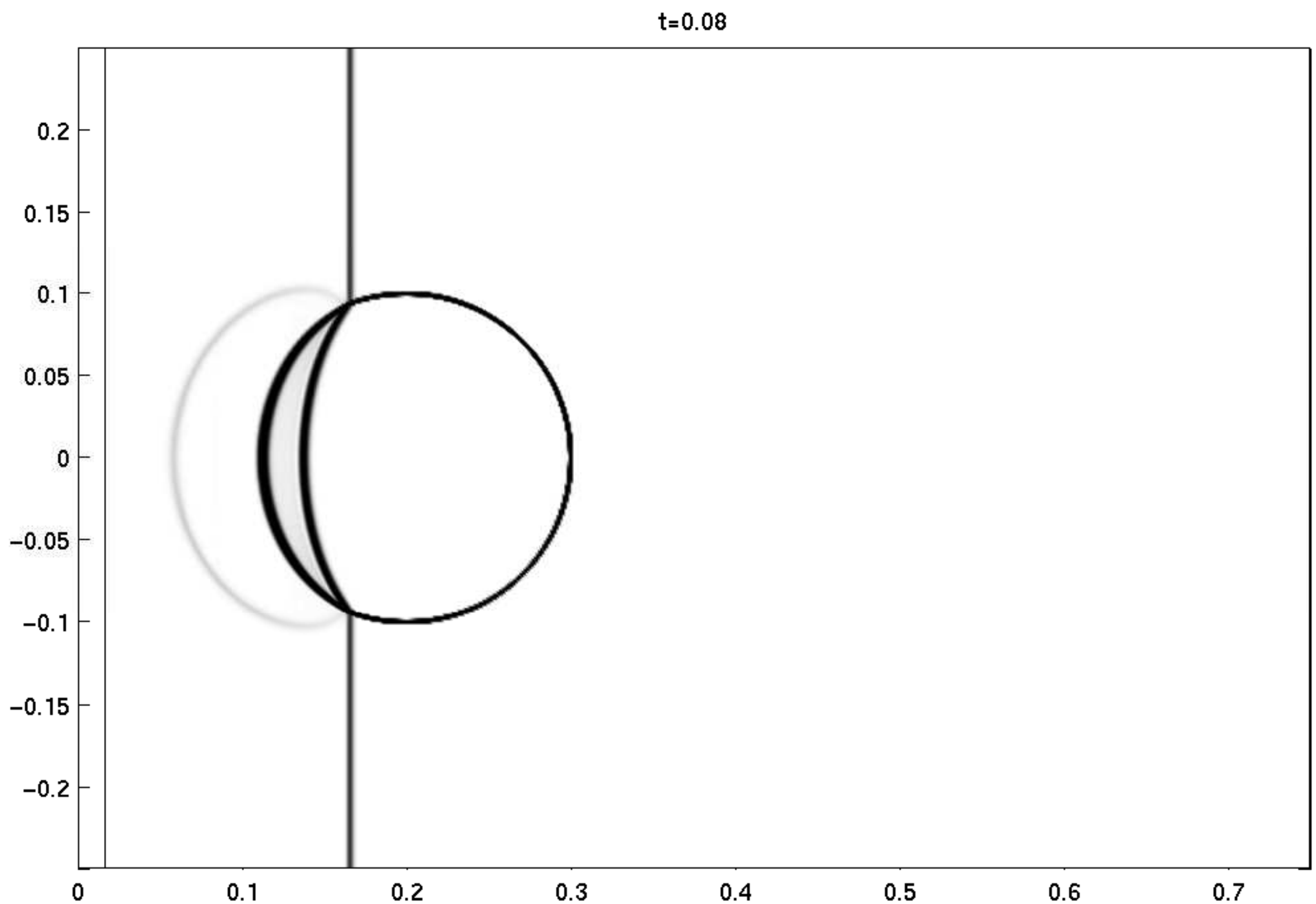

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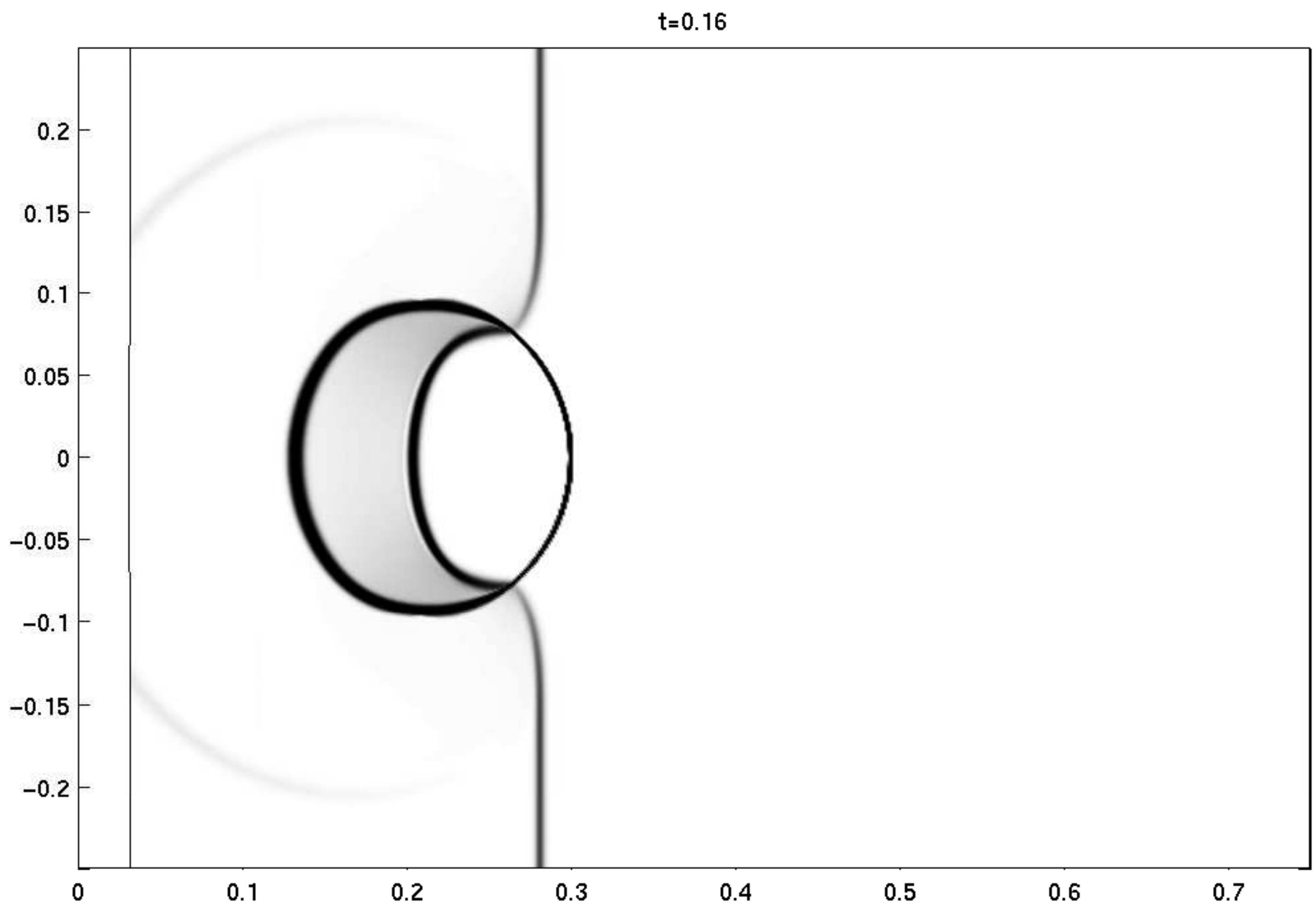
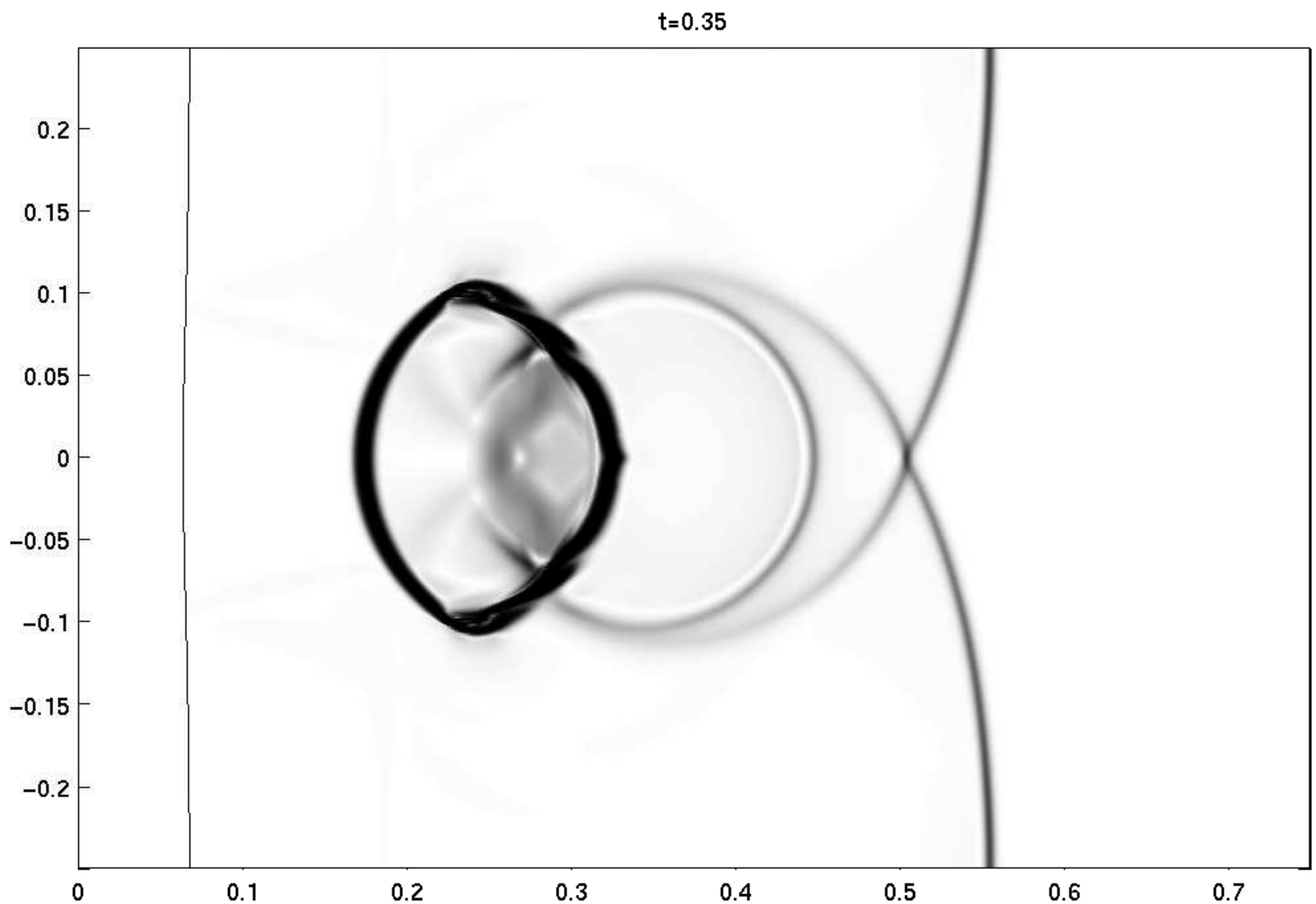
- Numerical schlieren images: $h_0 = 0.5$, 600×400 grid



Shock-Bubble (Refrigerant)

- Numerical schlieren images: $h_0 = 0.5$, 600×400 grid



Shock-Bubble (R22) (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.5$

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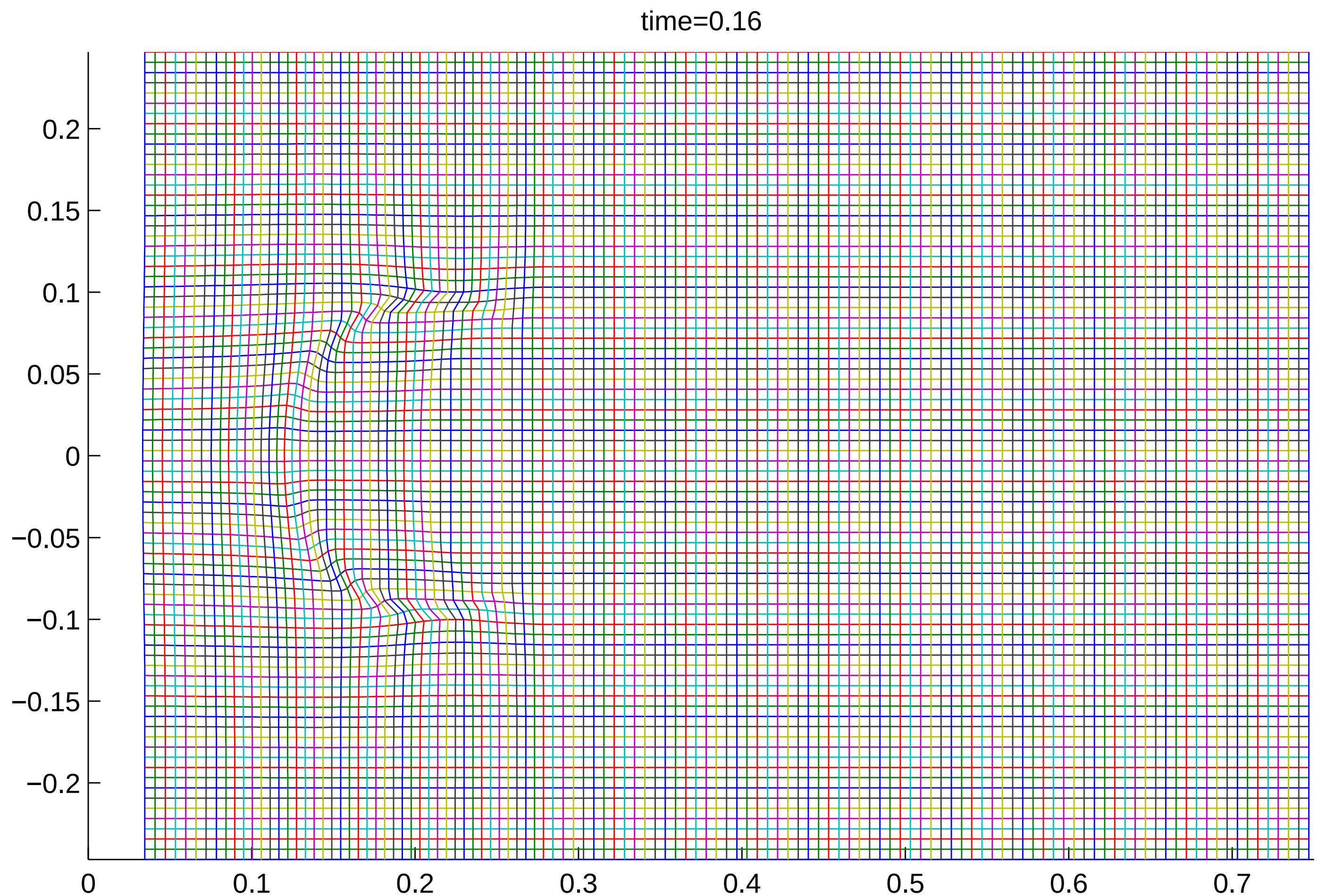
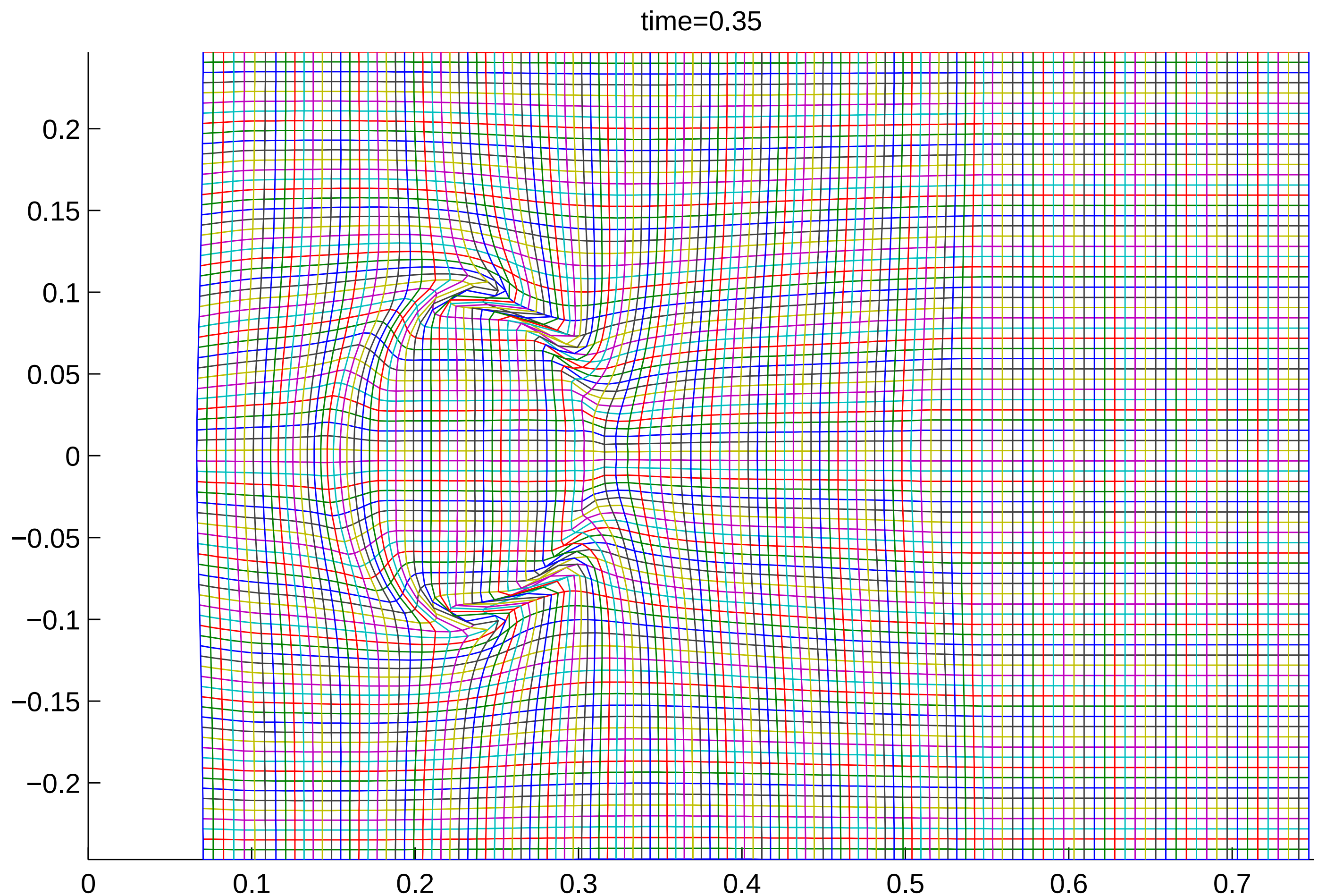


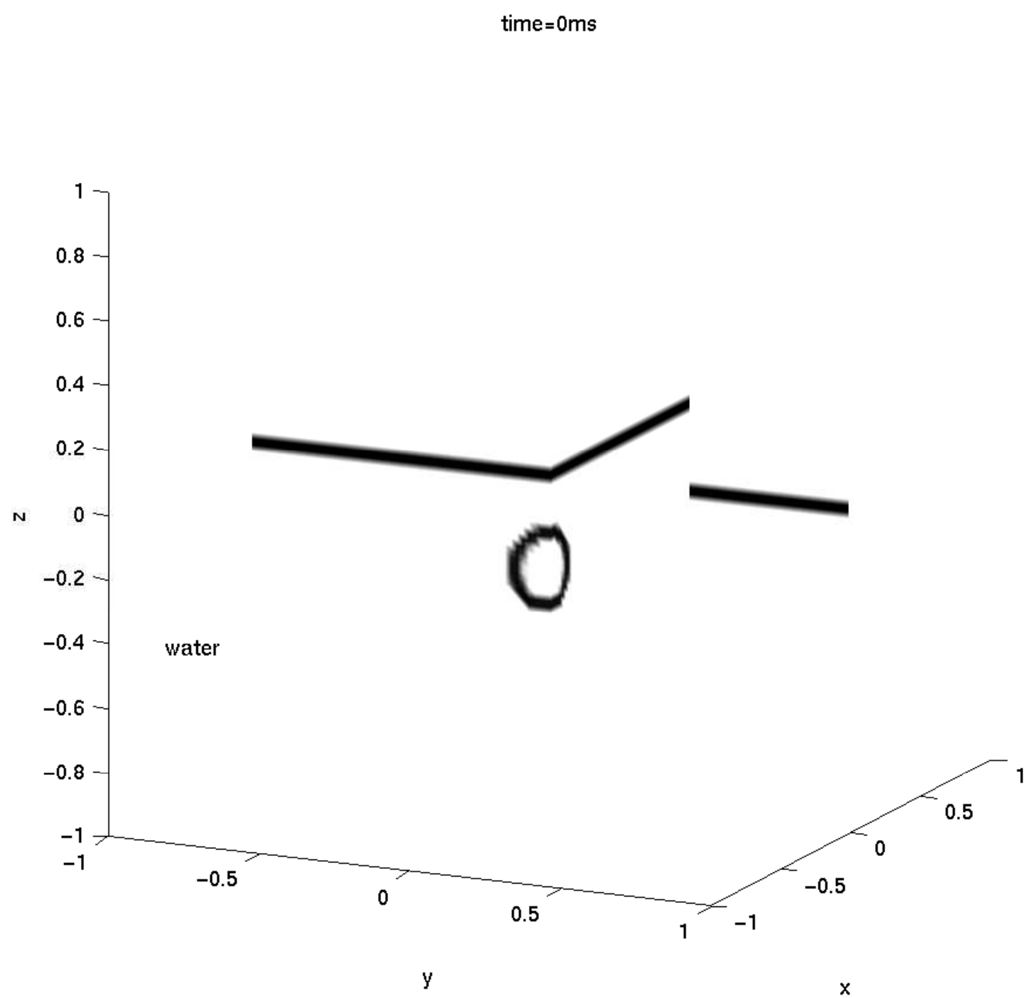
Shock-Bubble (R22) (Cont.)

- Grid system (coarsen by factor 5) with $h_0 = 0.5$



Underwater Explosions

- Numerical schlieren images $h_0 = 0.6$, 100^3 grid



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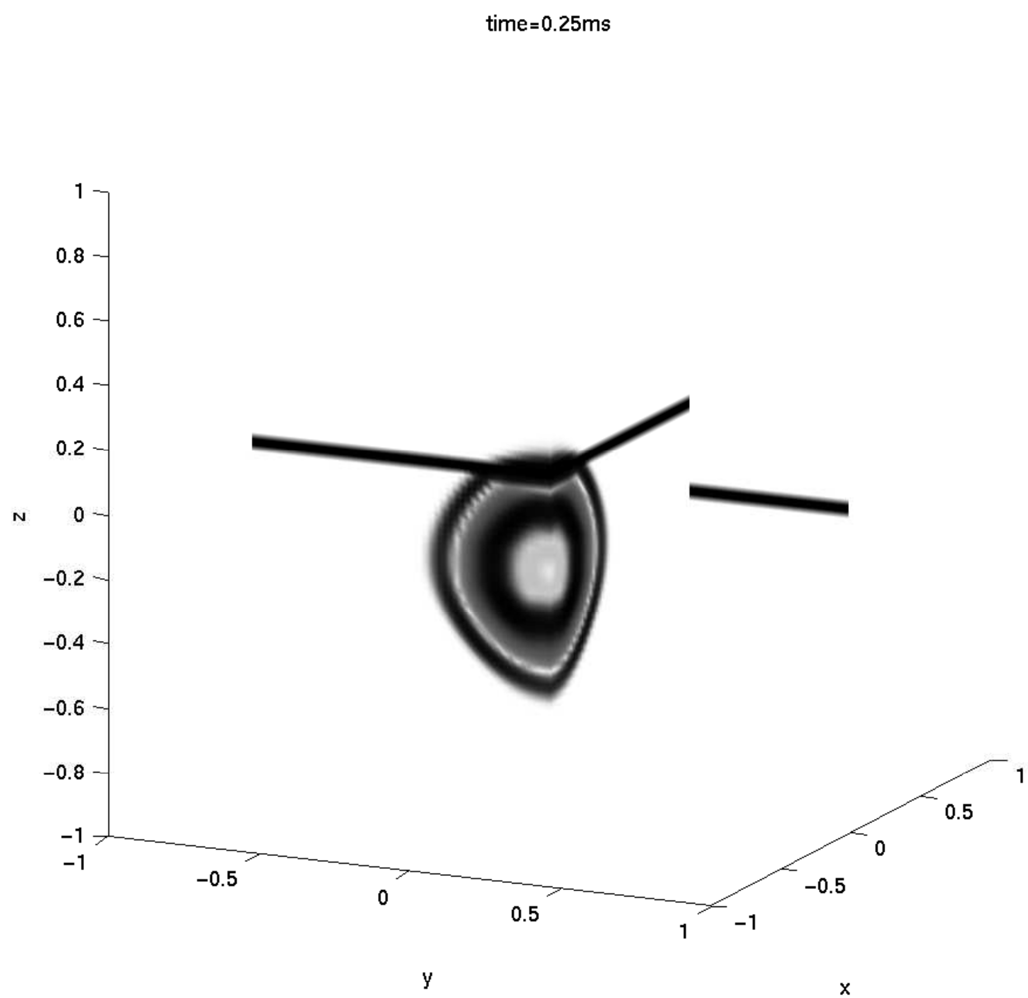

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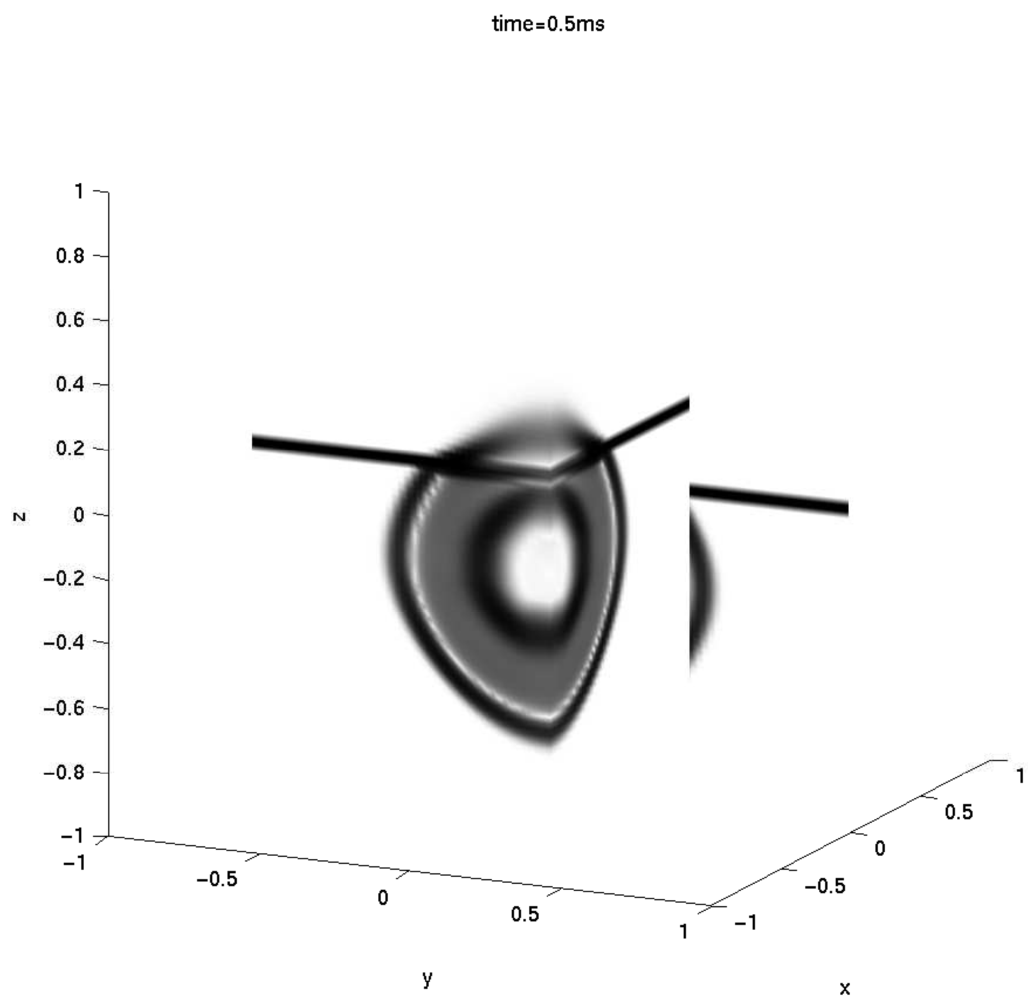

Underwater Explosions

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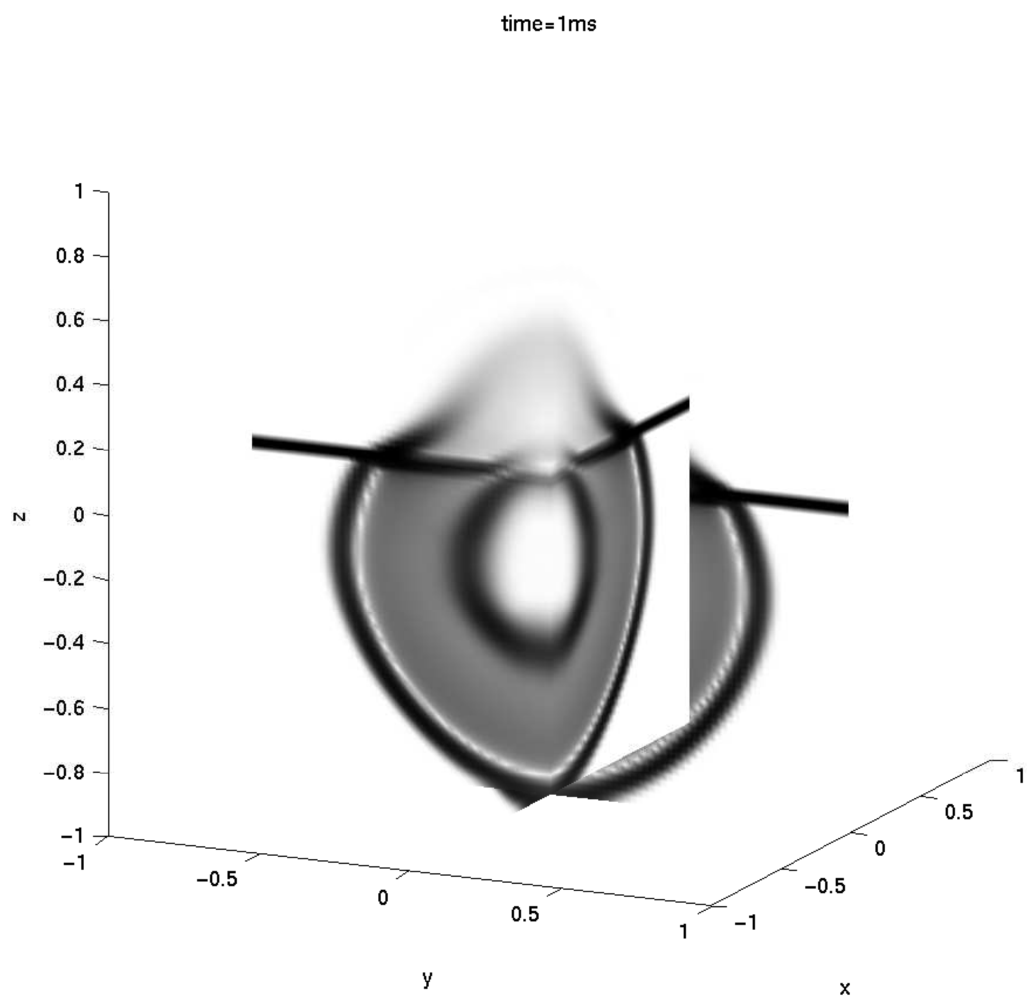

Underwater Explosions

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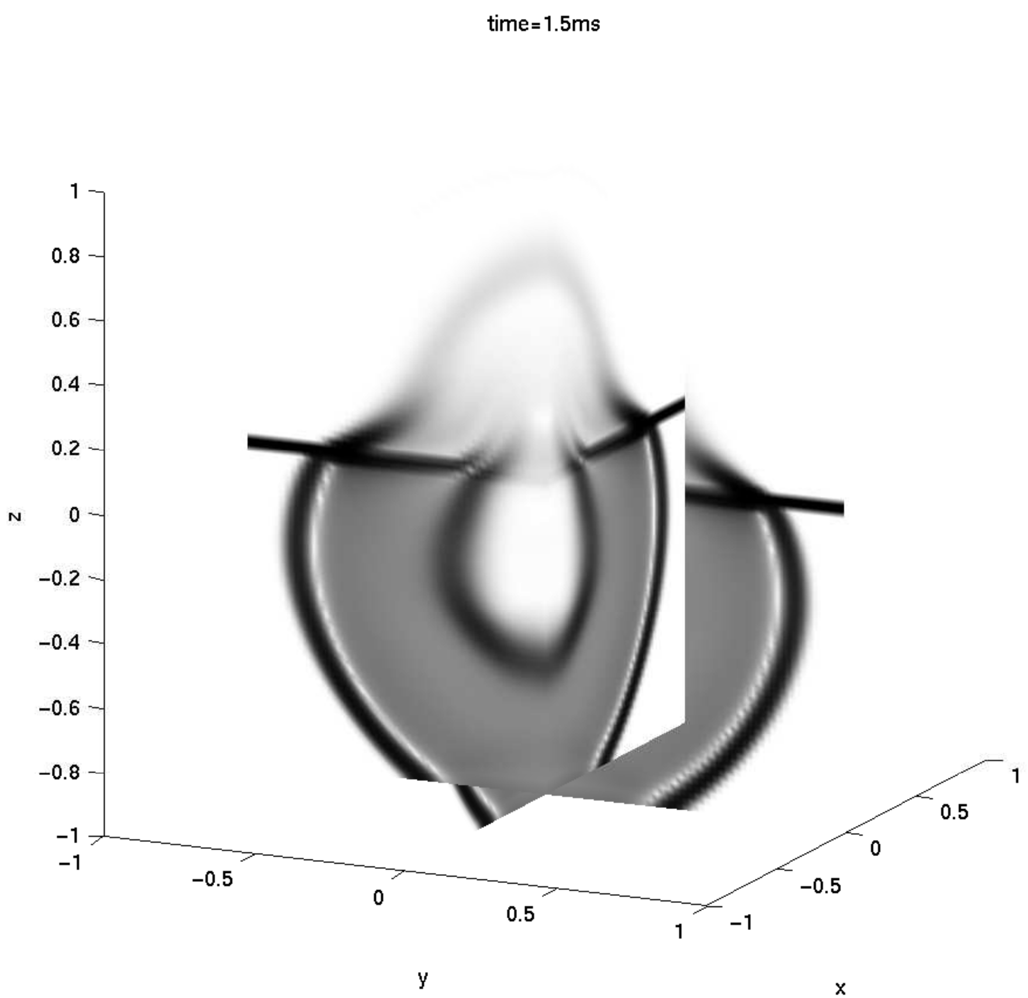
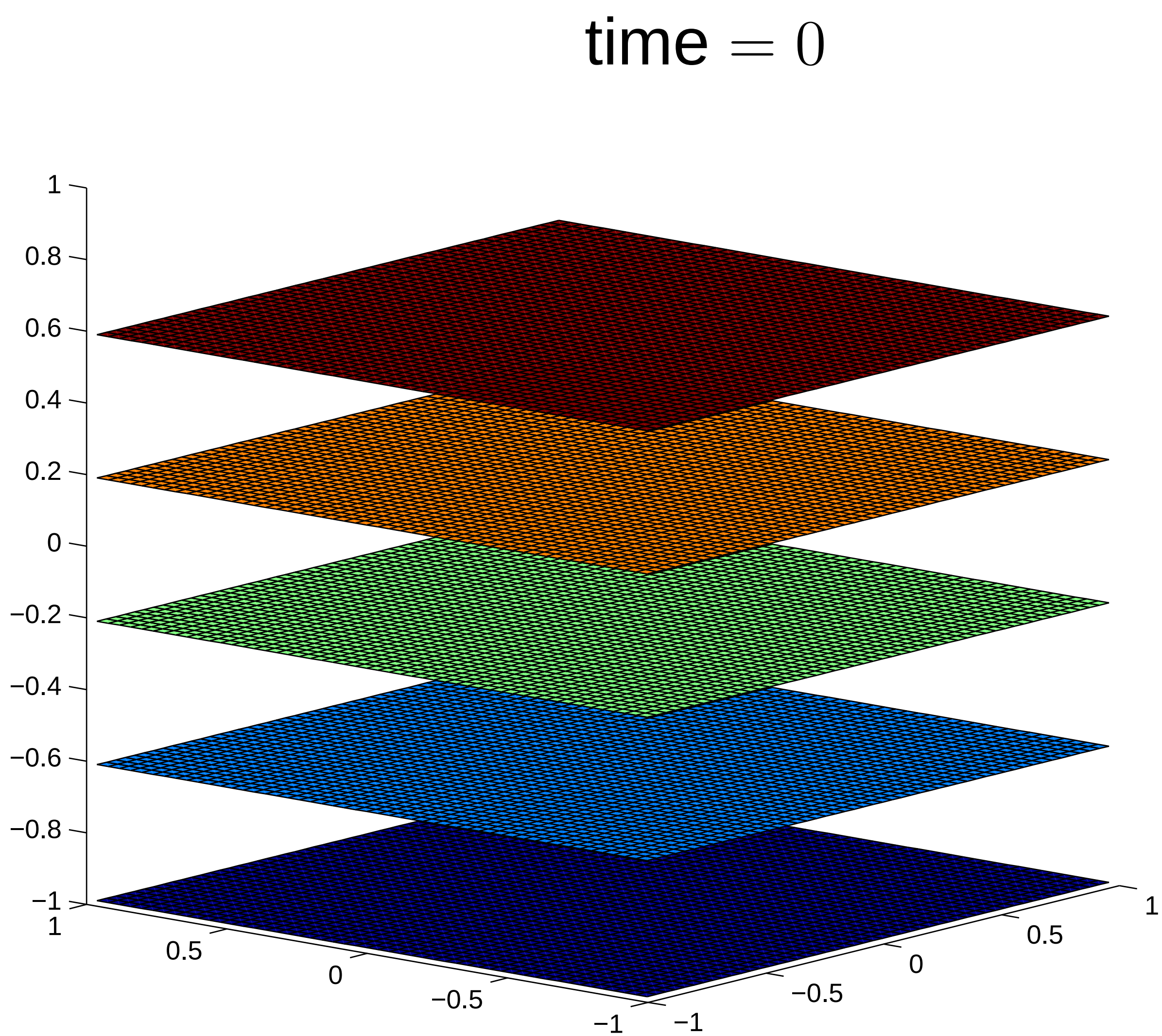


3D Underwater Explosions (Cont.)

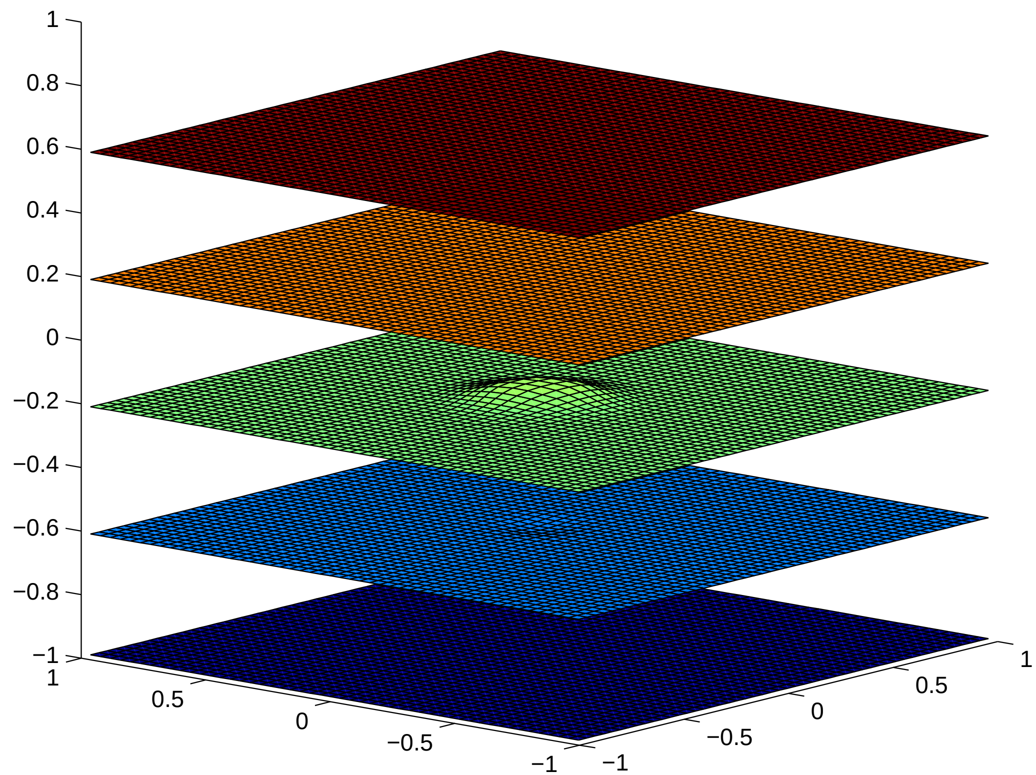
- Grid system (coarsen by factor 2) with $h_0 = 0.6$



3D Underwater Explosions (Cont.)

- Grid system (coarsen by factor 2) with $h_0 = 0.6$

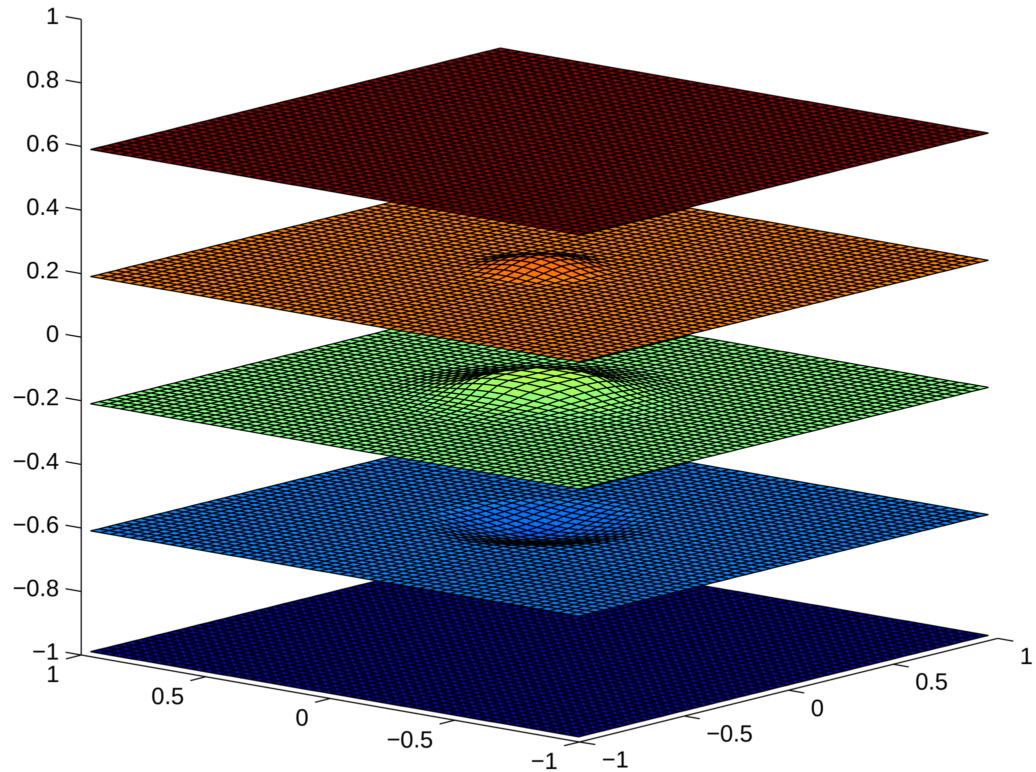
time $= 0.25$ms



3D Underwater Explosions (Cont.)

- Grid system (coarsen by factor 2) with $h_0 = 0.6$

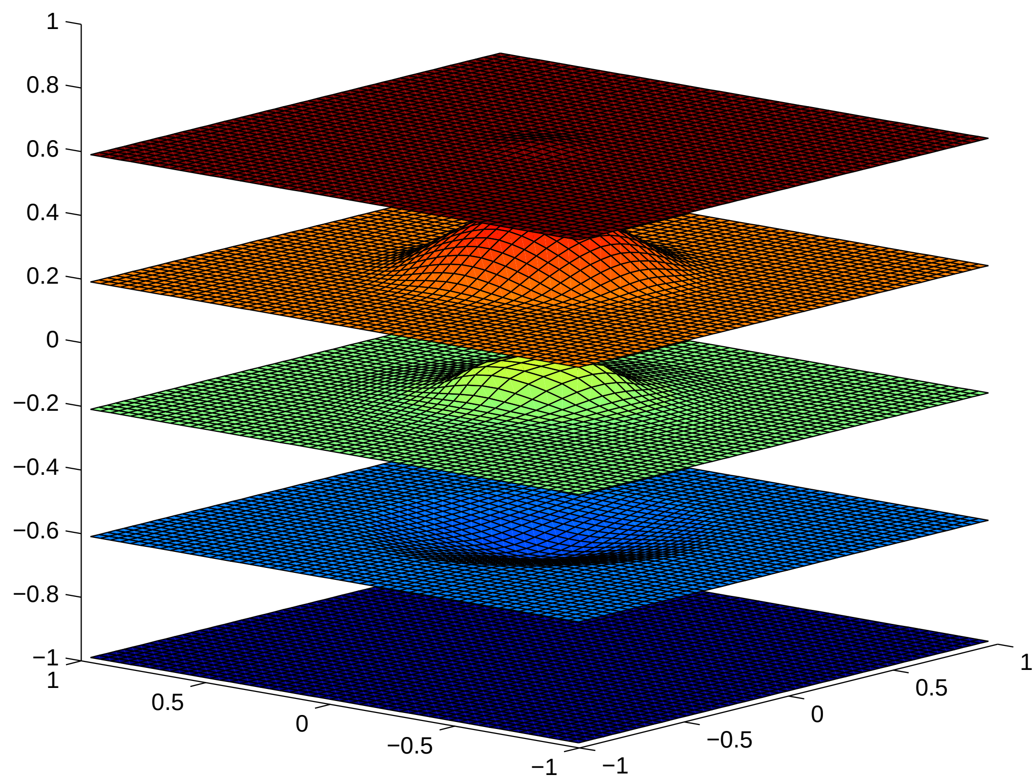
time $= 0.5$ms



3D Underwater Explosions (Cont.)

- Grid system (coarsen by factor 2) with $h_0 = 0.6$

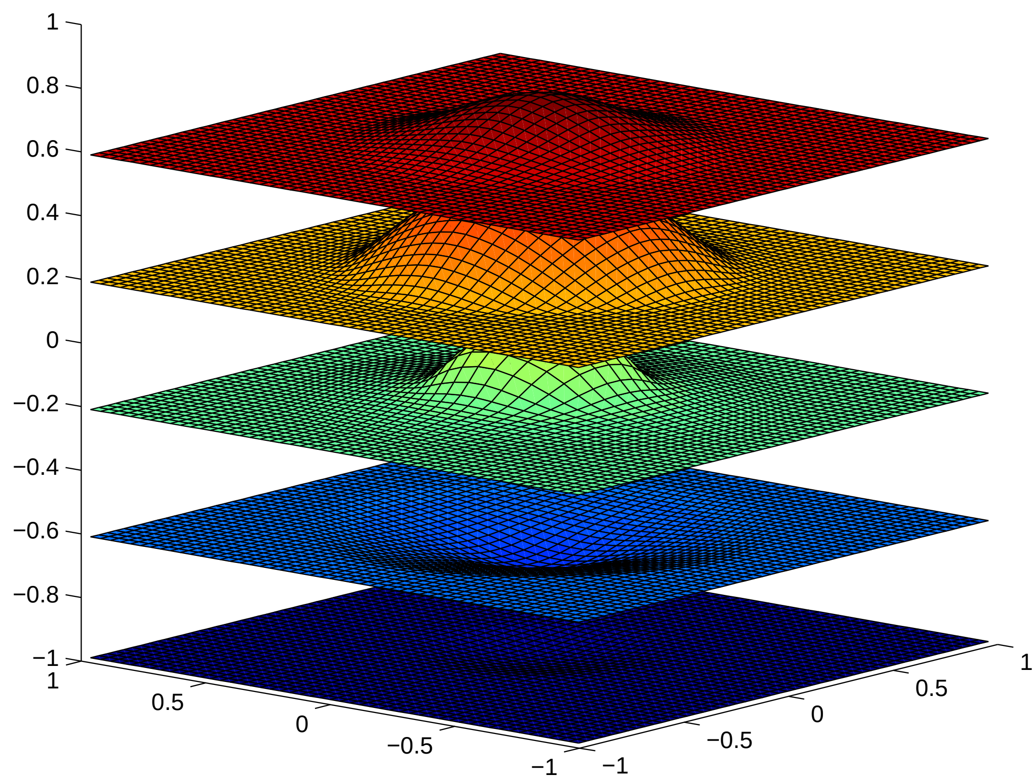
time $= 1.0$ms



3D Underwater Explosions (Cont.)

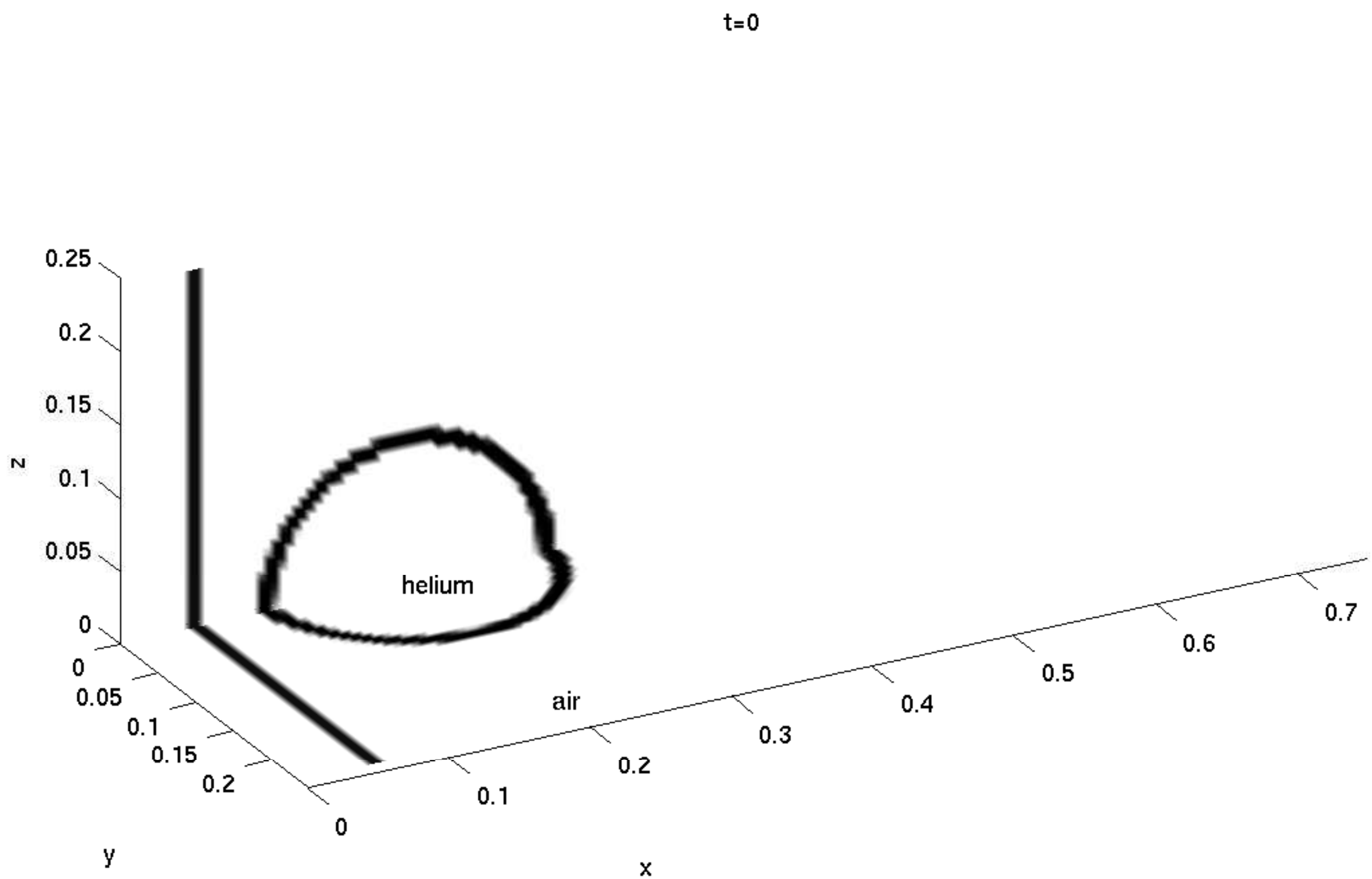
- Grid system (coarsen by factor 2) with $h_0 = 0.6$

time $= 1.5$ms



3D Shock-Bubble (Helium)

- Numerical schlieren images: $h_0 = 0.6$, $150 \times 50 \times 50$ grid



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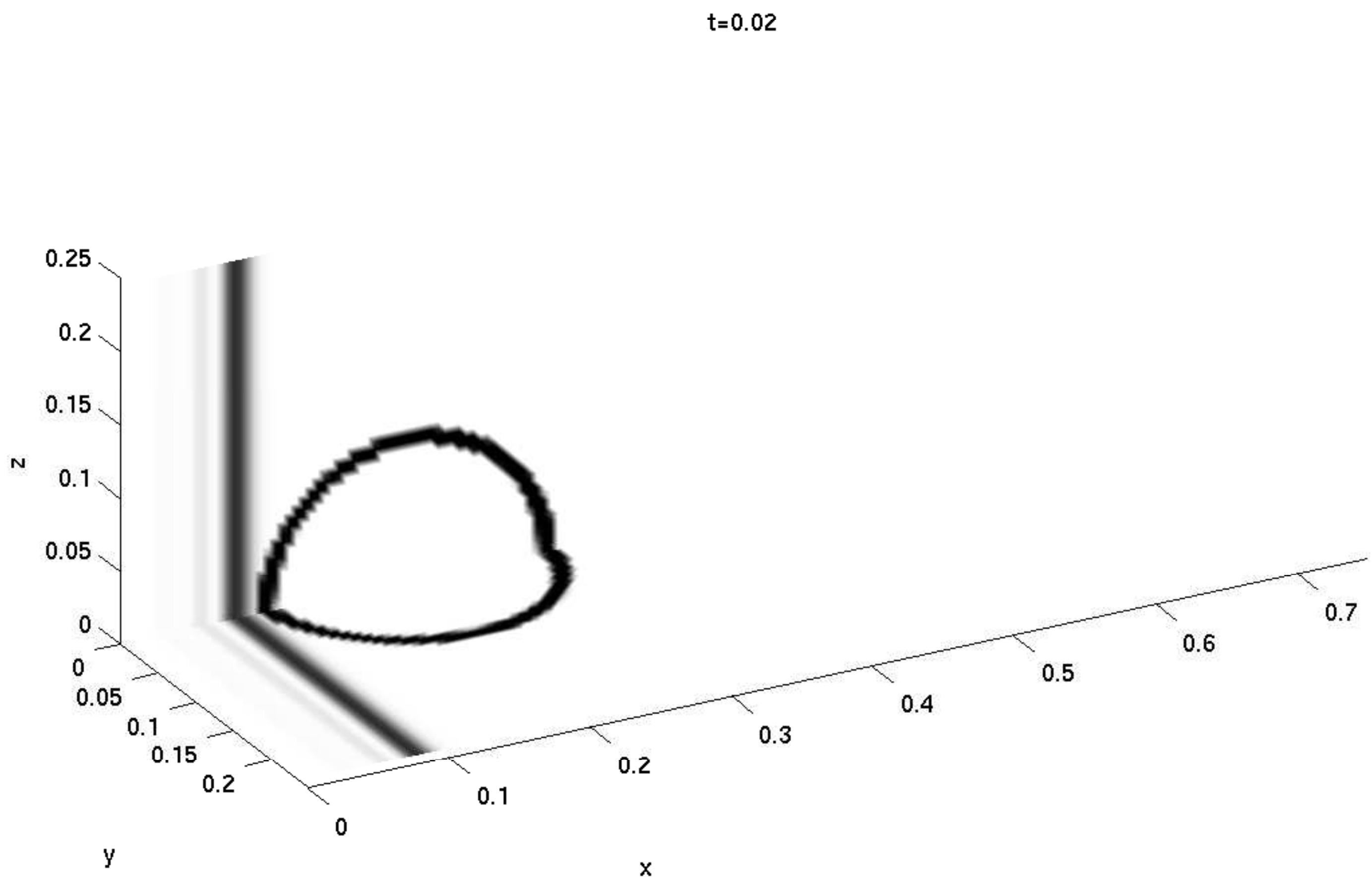

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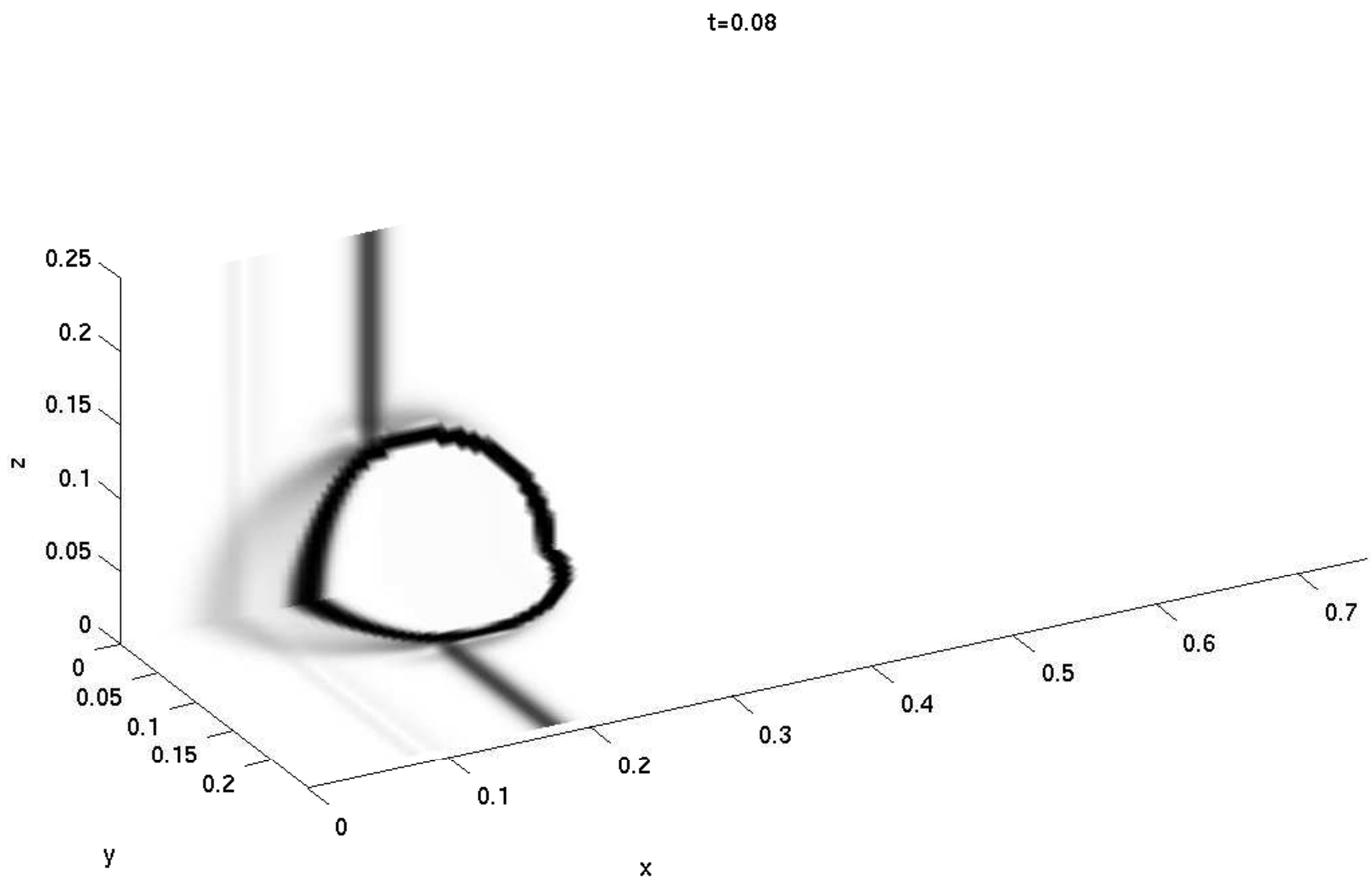

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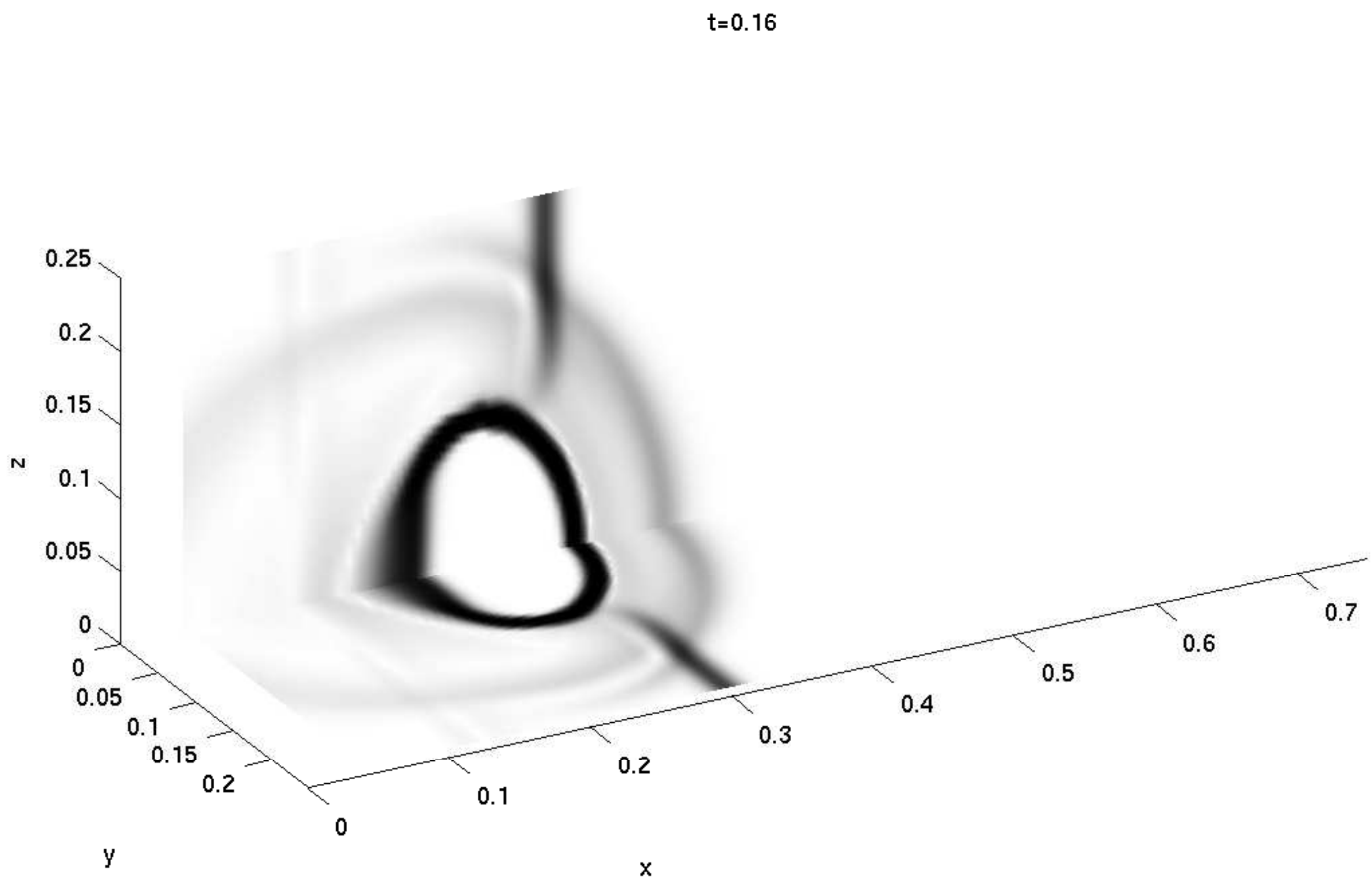

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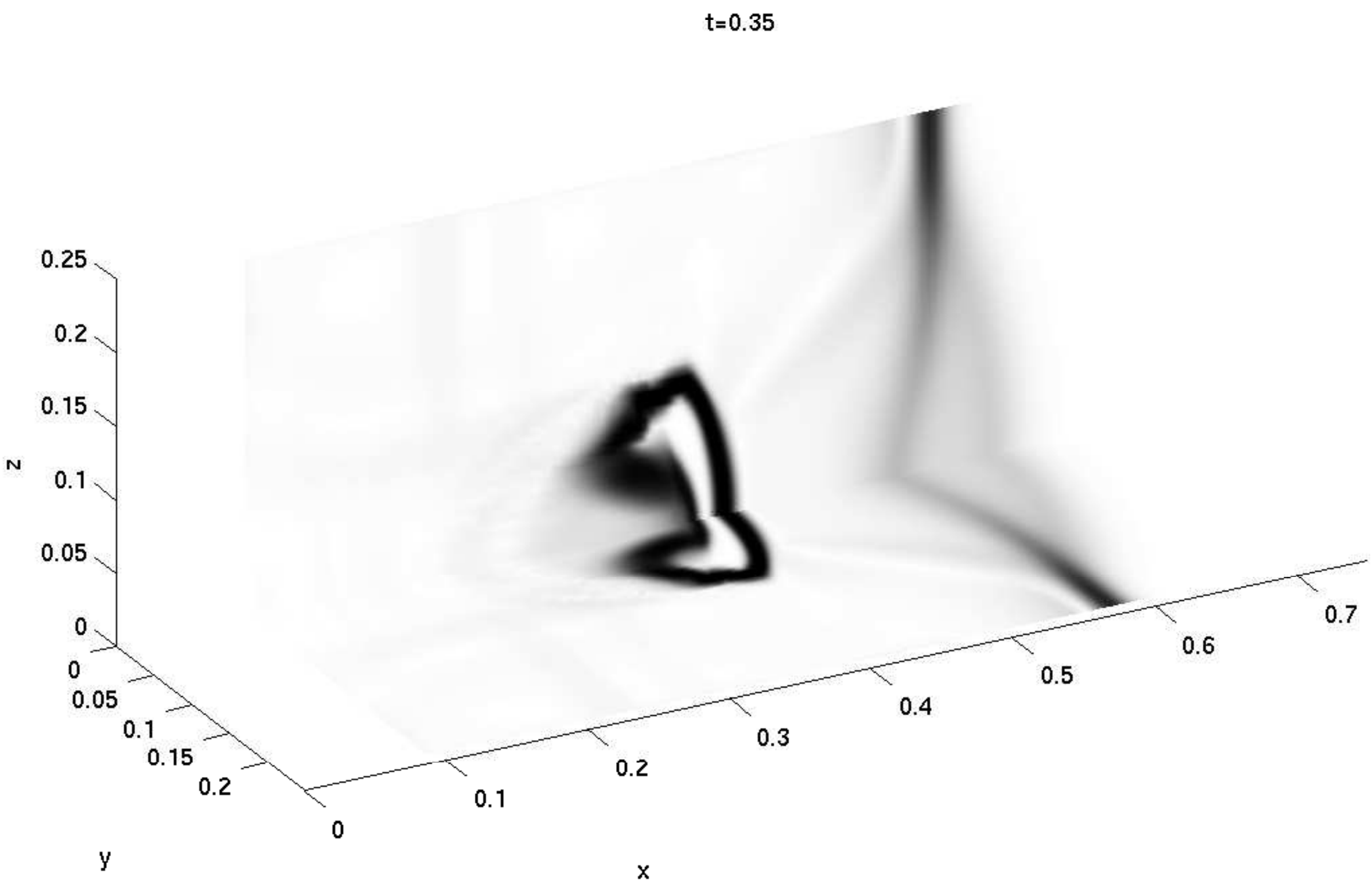
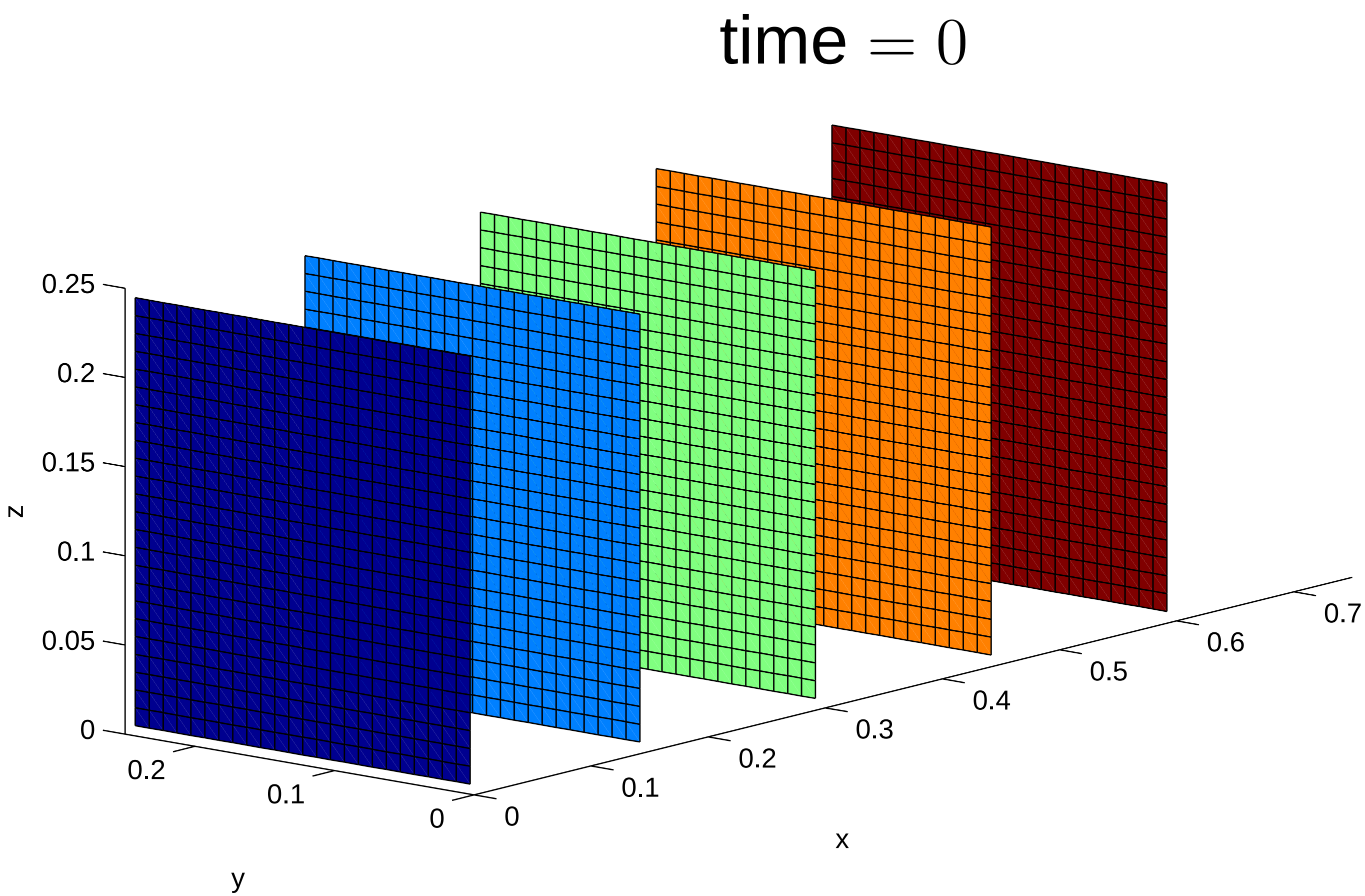


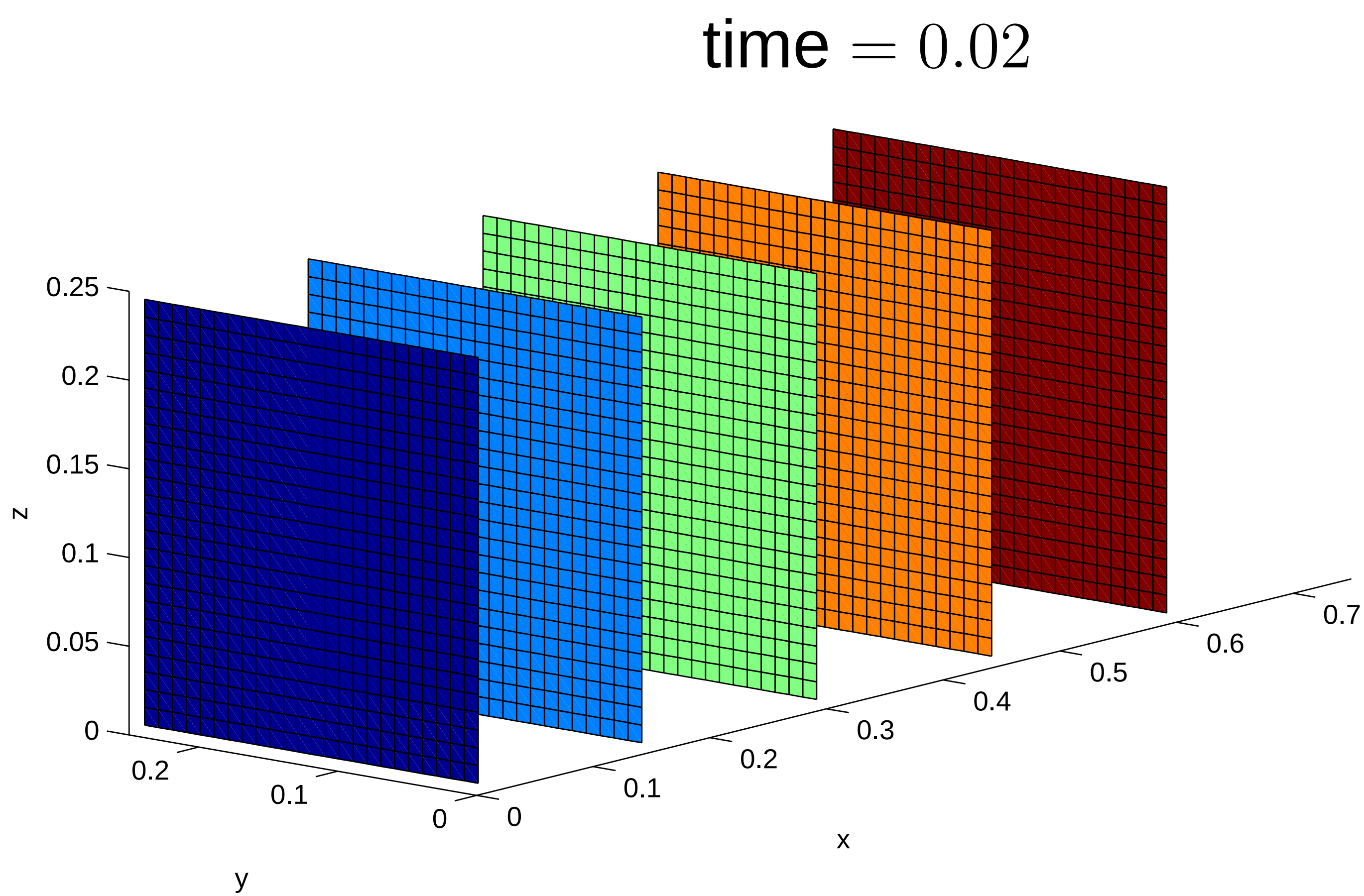
Shock-Bubble (Helium) (Cont.)

- Grid system (coarsen by factor 2) with $h_0 = 0.6$



Shock-Bubble (Helium) (Cont.)

- Grid system (coarsen by factor 2) with $h_0 = 0.6$



Shock-Bubble (Helium) (Cont.)

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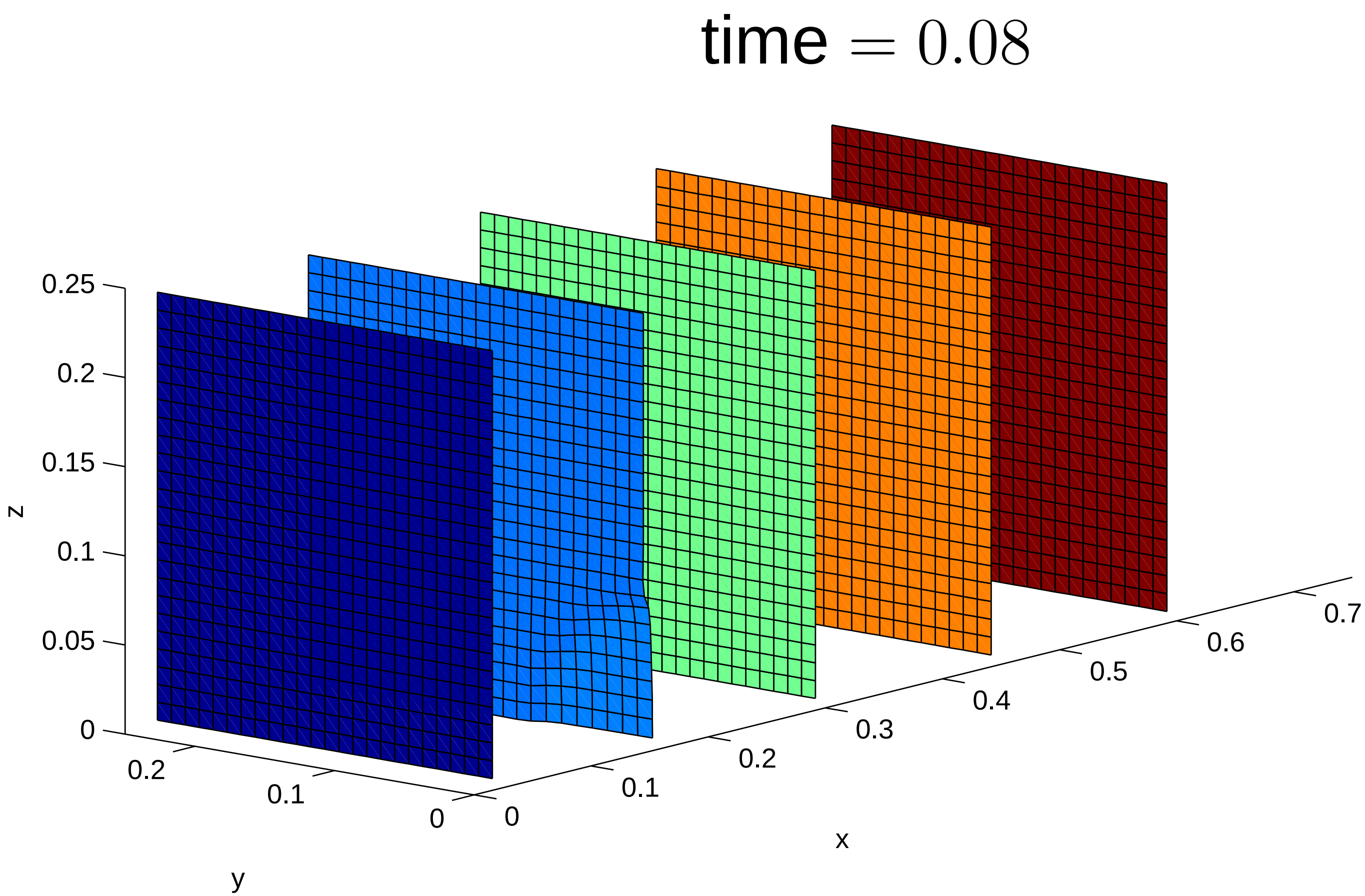
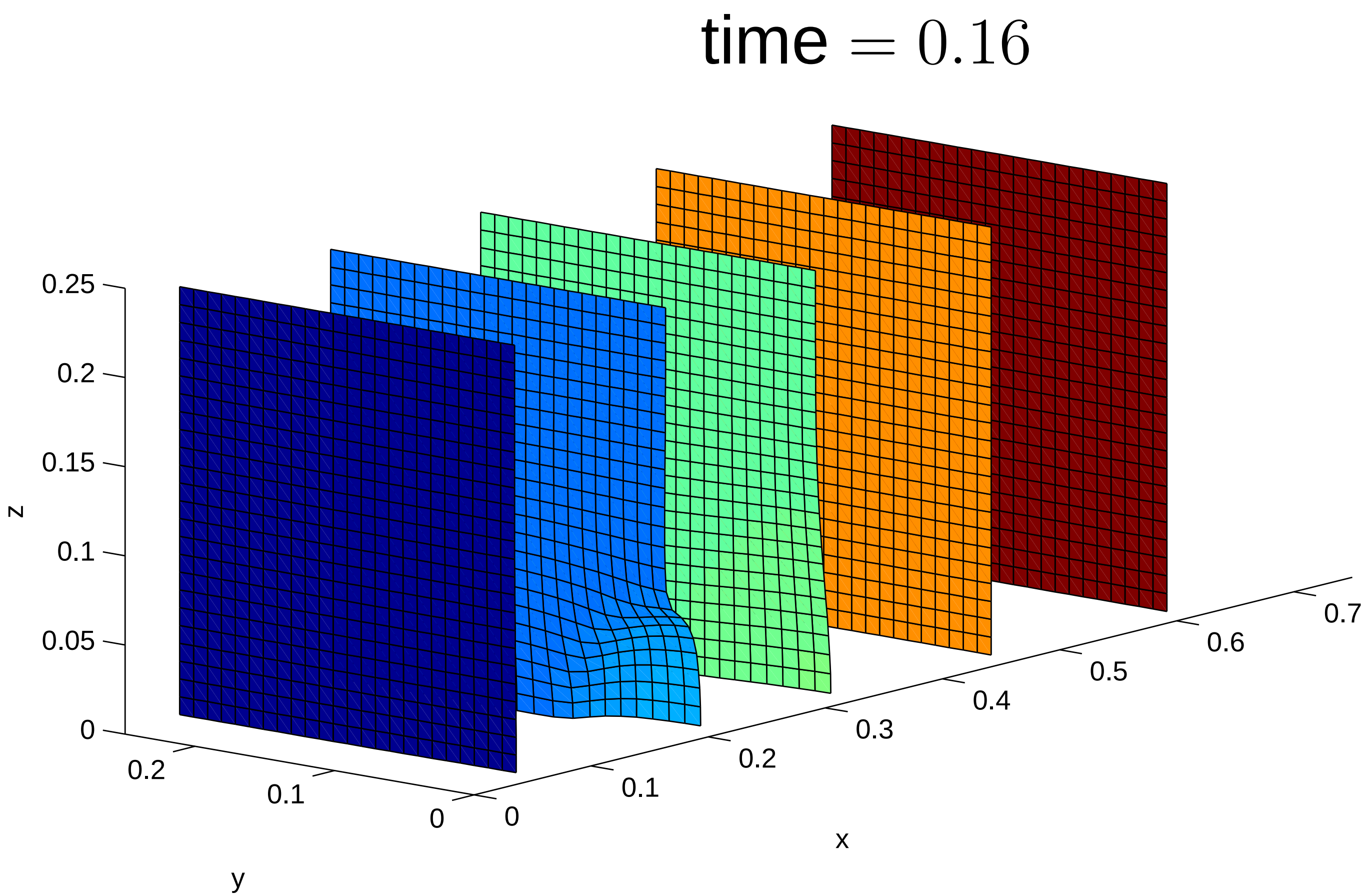


Shock-Bubble (Helium) (Cont.)

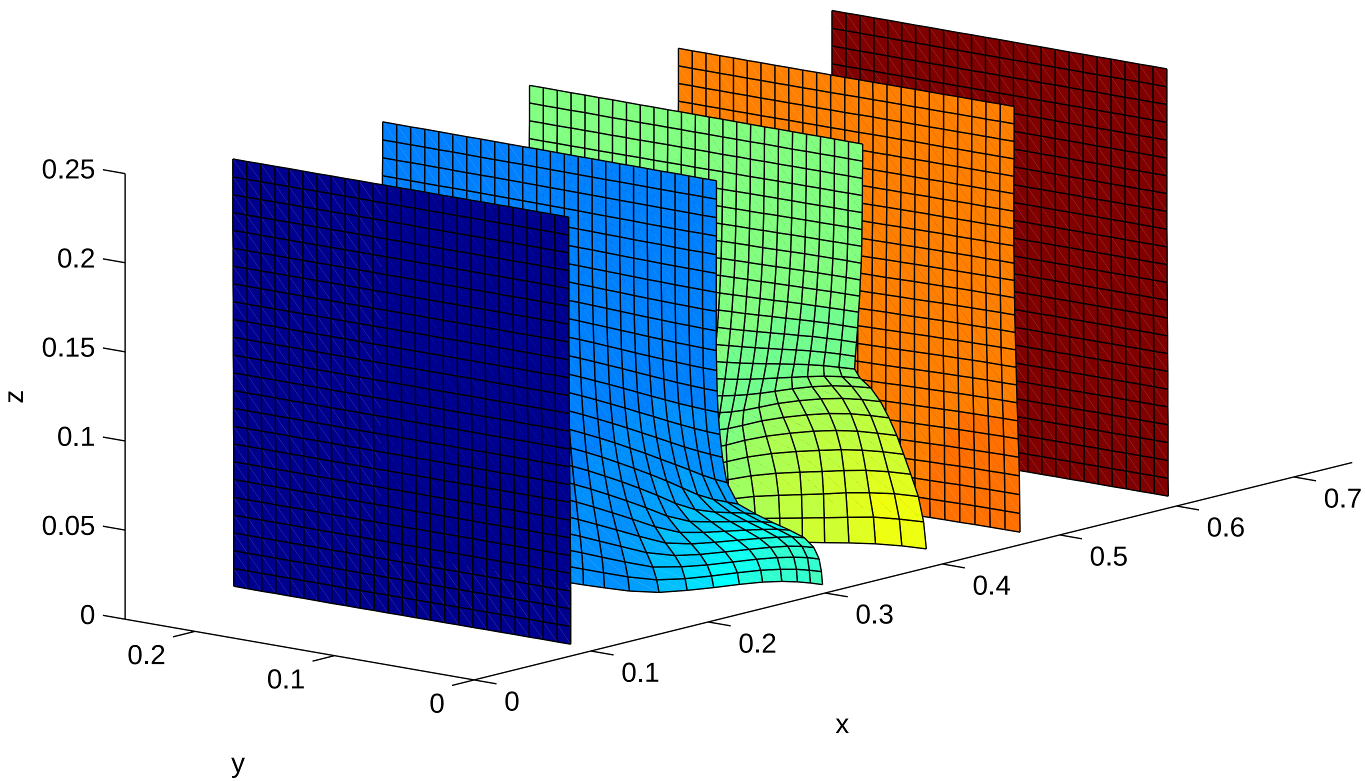
- Grid system (coarsen by factor 2) with $h_0 = 0.6$



Shock-Bubble (Helium) (Cont.)

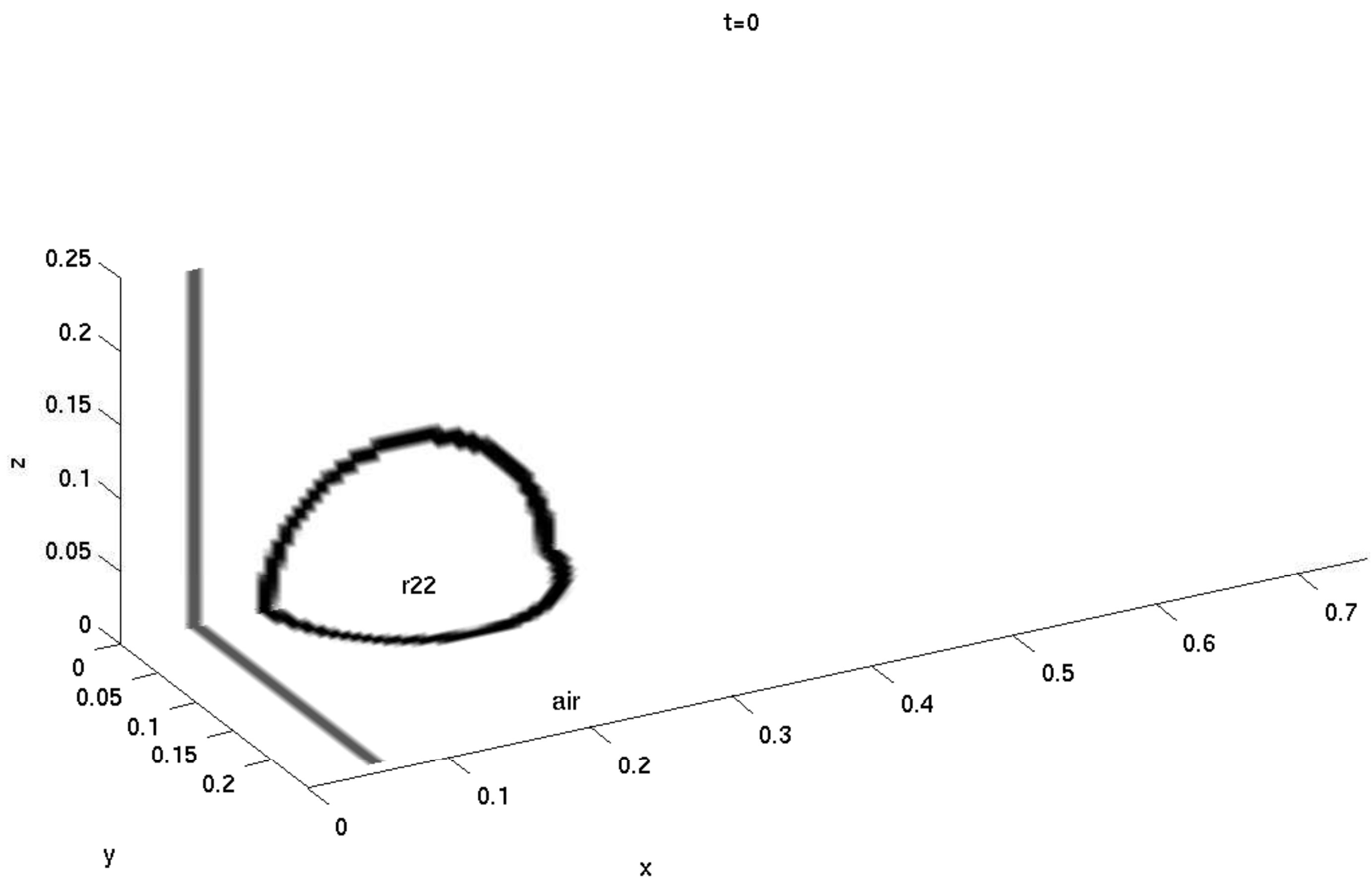
- Grid system (coarsen by factor 2) with $h_0 = 0.6$

time $= 0.35$



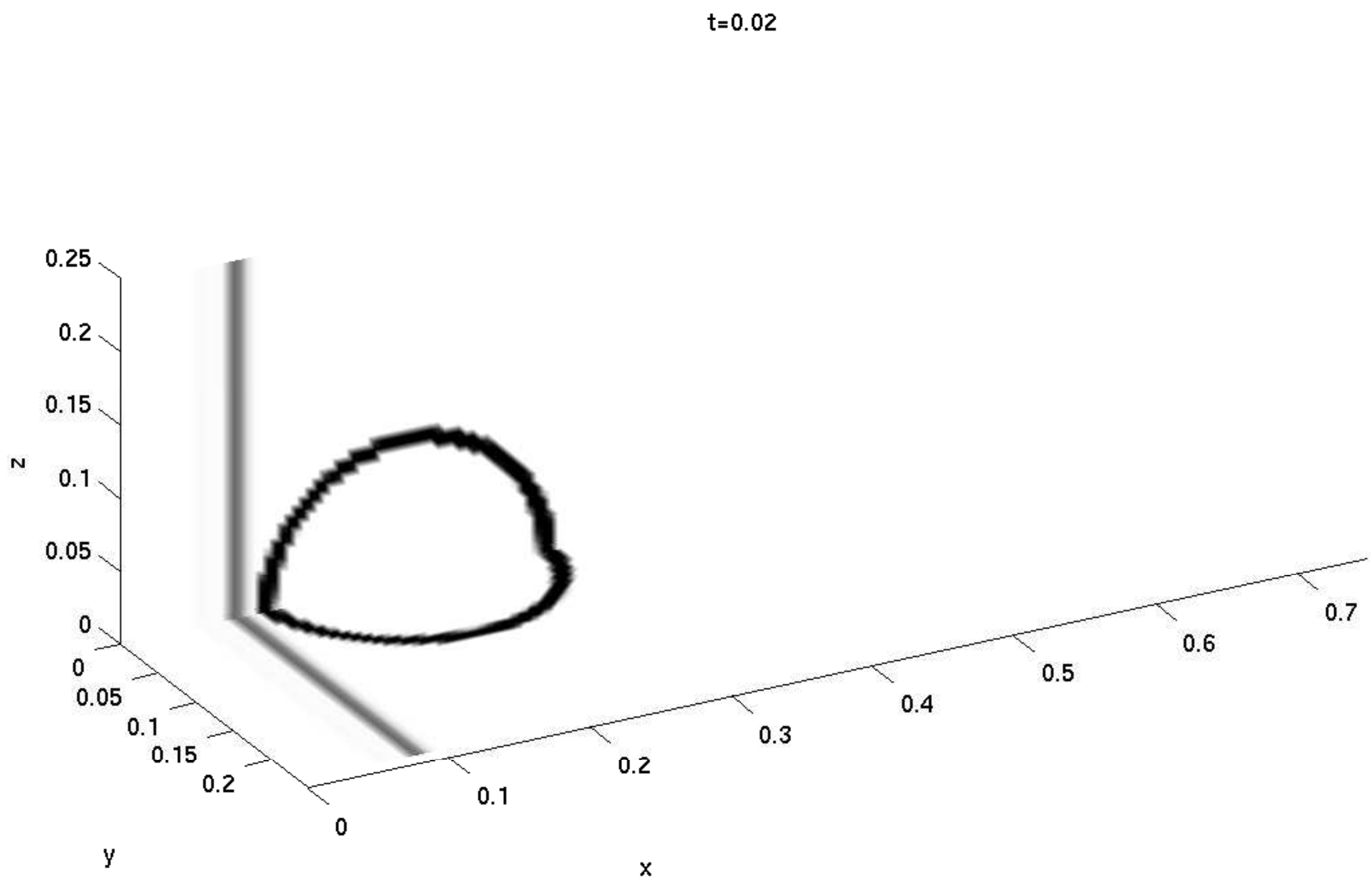
3D Shock-Bubble (Refrigerant)

- Numerical schlieren images: $h_0 = 0.6$, $150 \times 50 \times 50$ grid



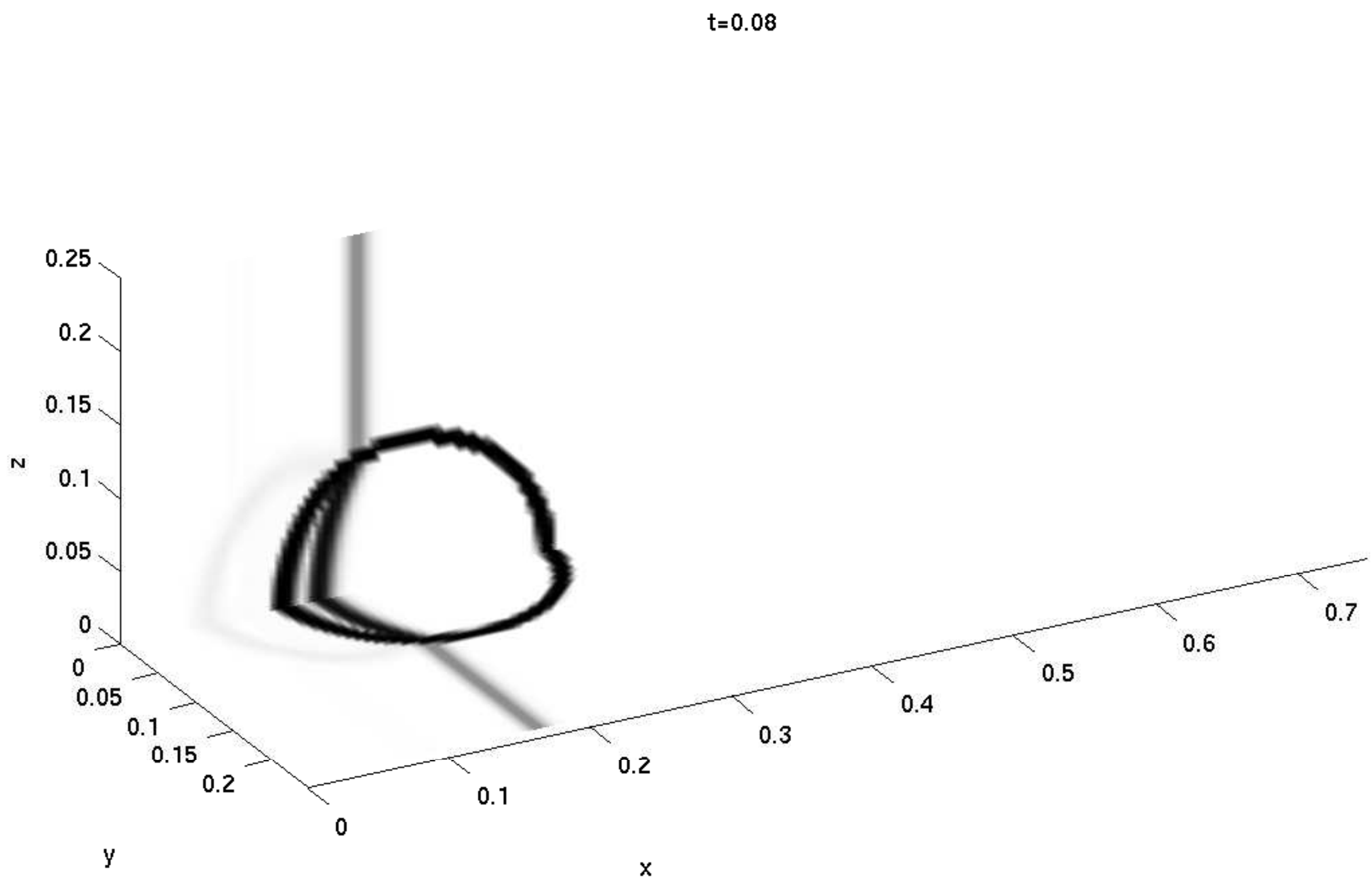
3D Shock-Bubble (Refrigerant)

- Numerical schlieren images: $h_0 = 0.6$, $150 \times 50 \times 50$ grid



3D Shock-Bubble (Refrigerant)

- Numerical schlieren images: $h_0 = 0.6$, $150 \times 50 \times 50$ grid



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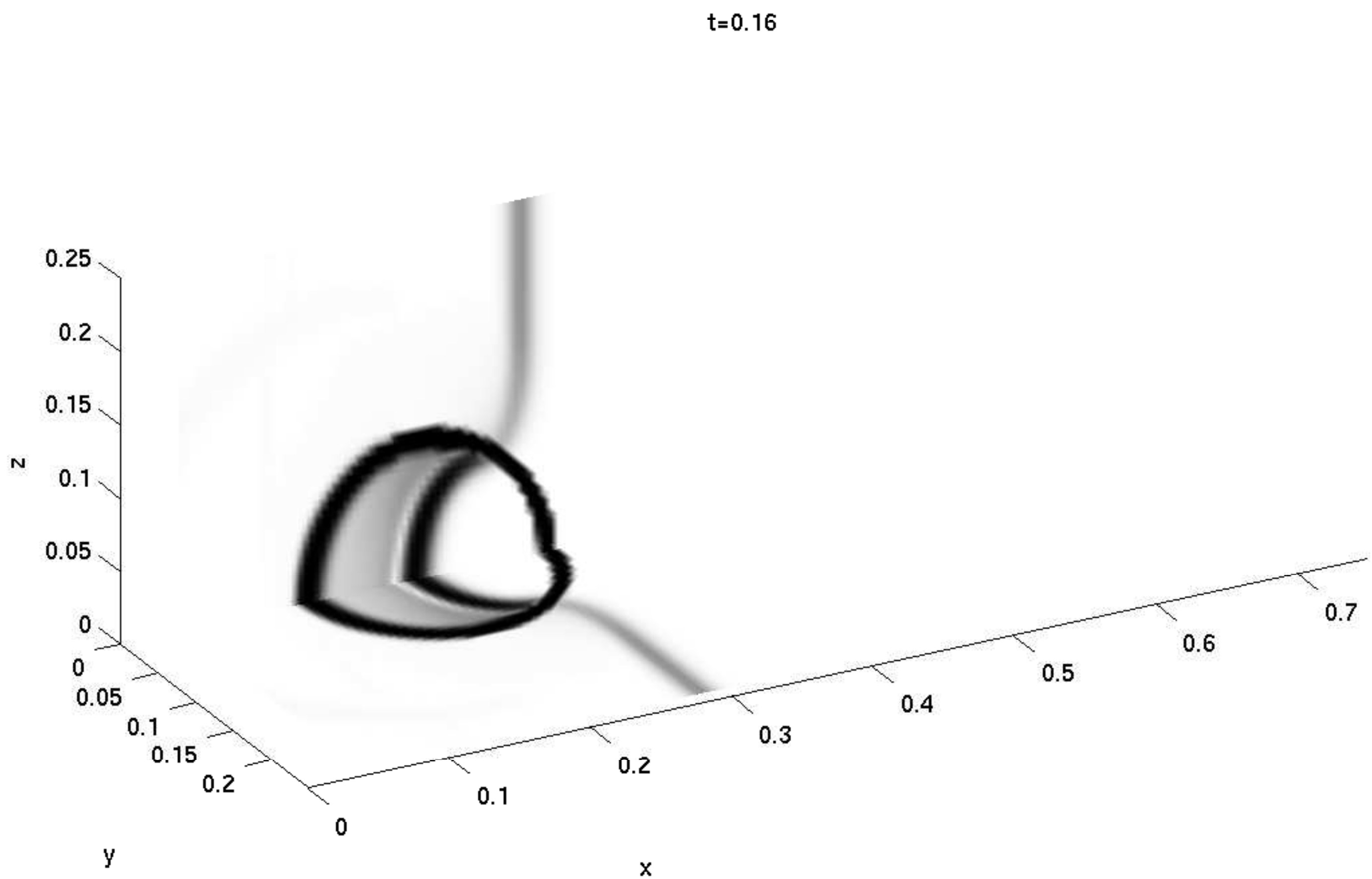

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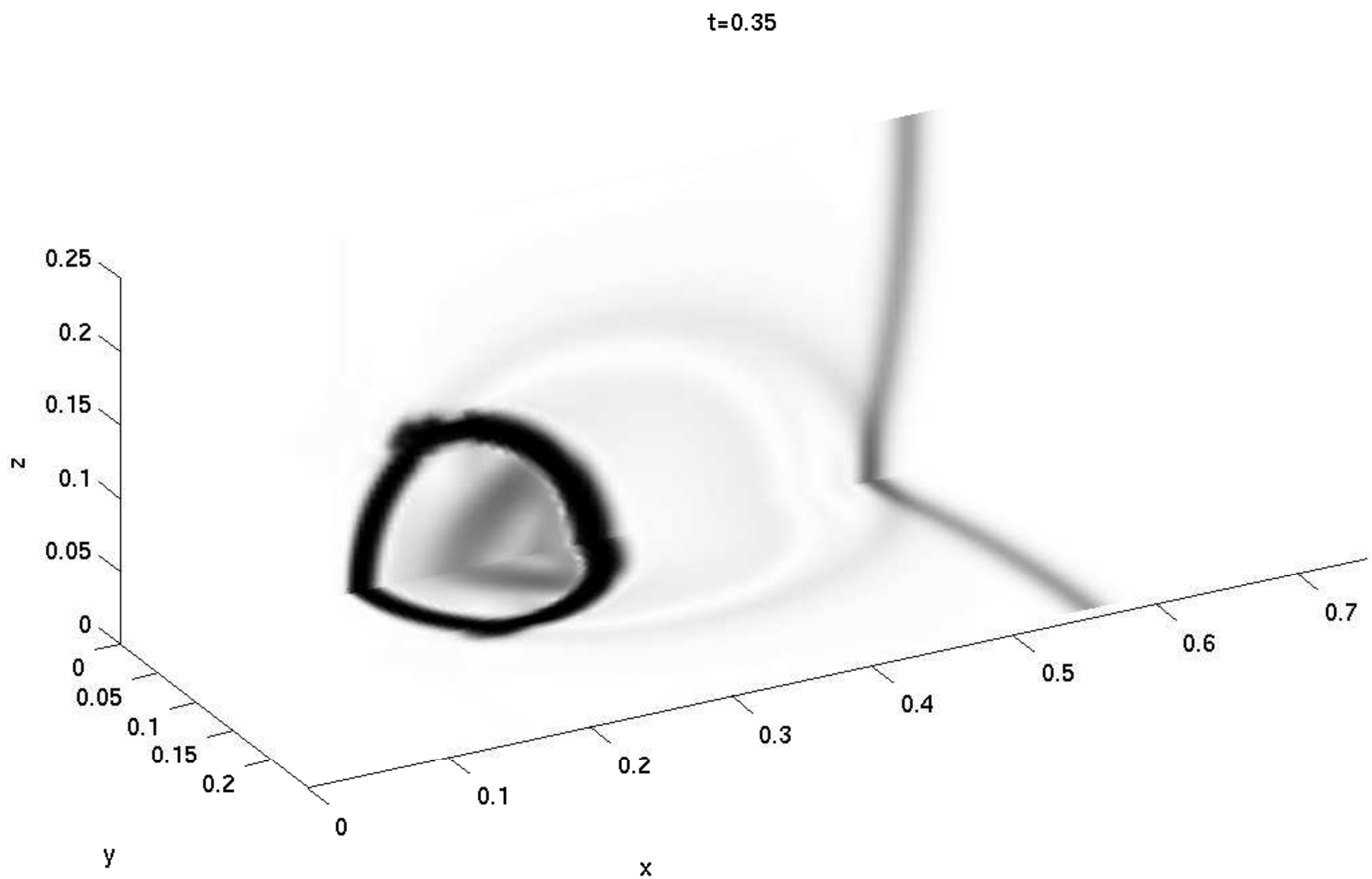
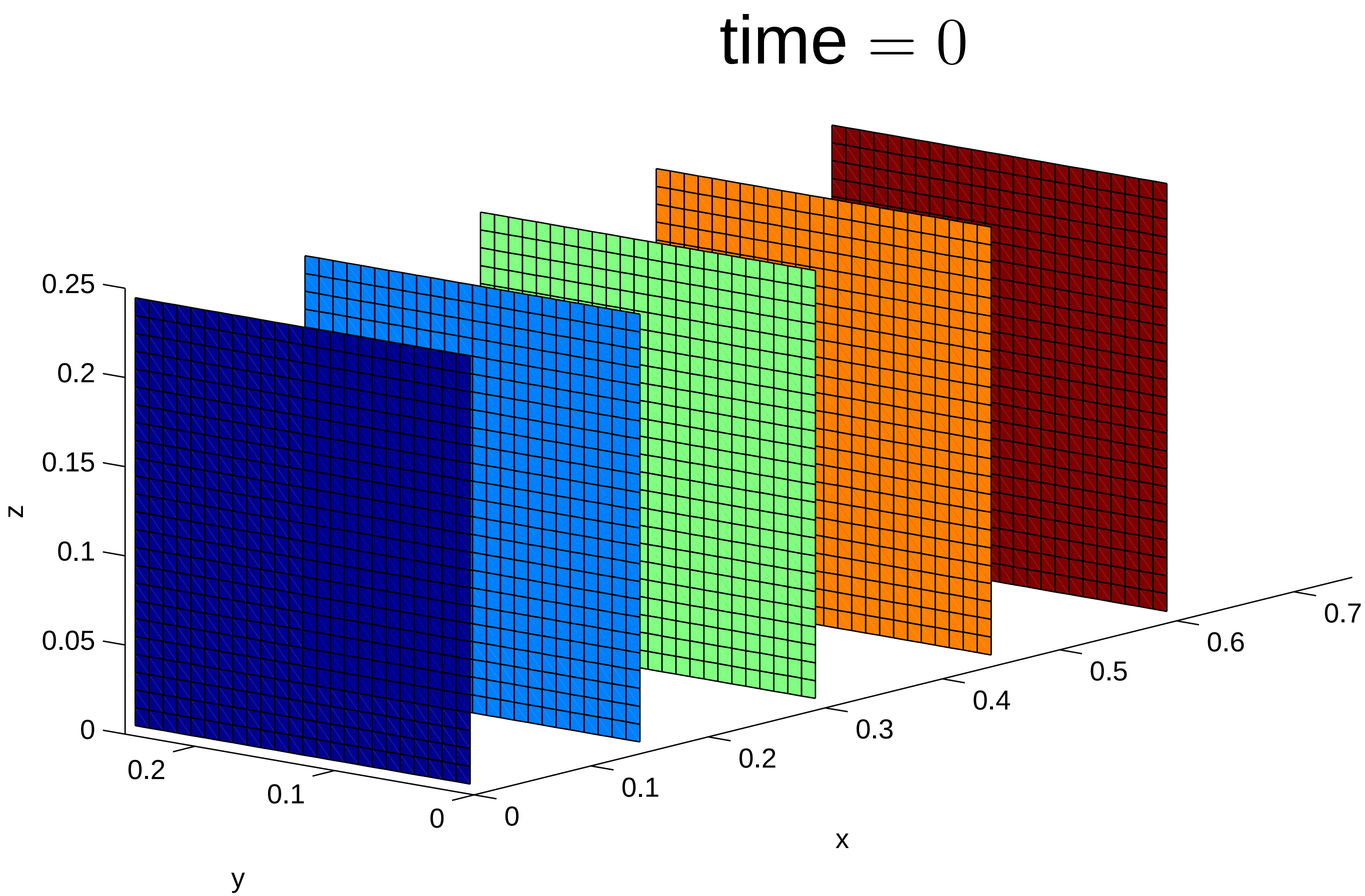


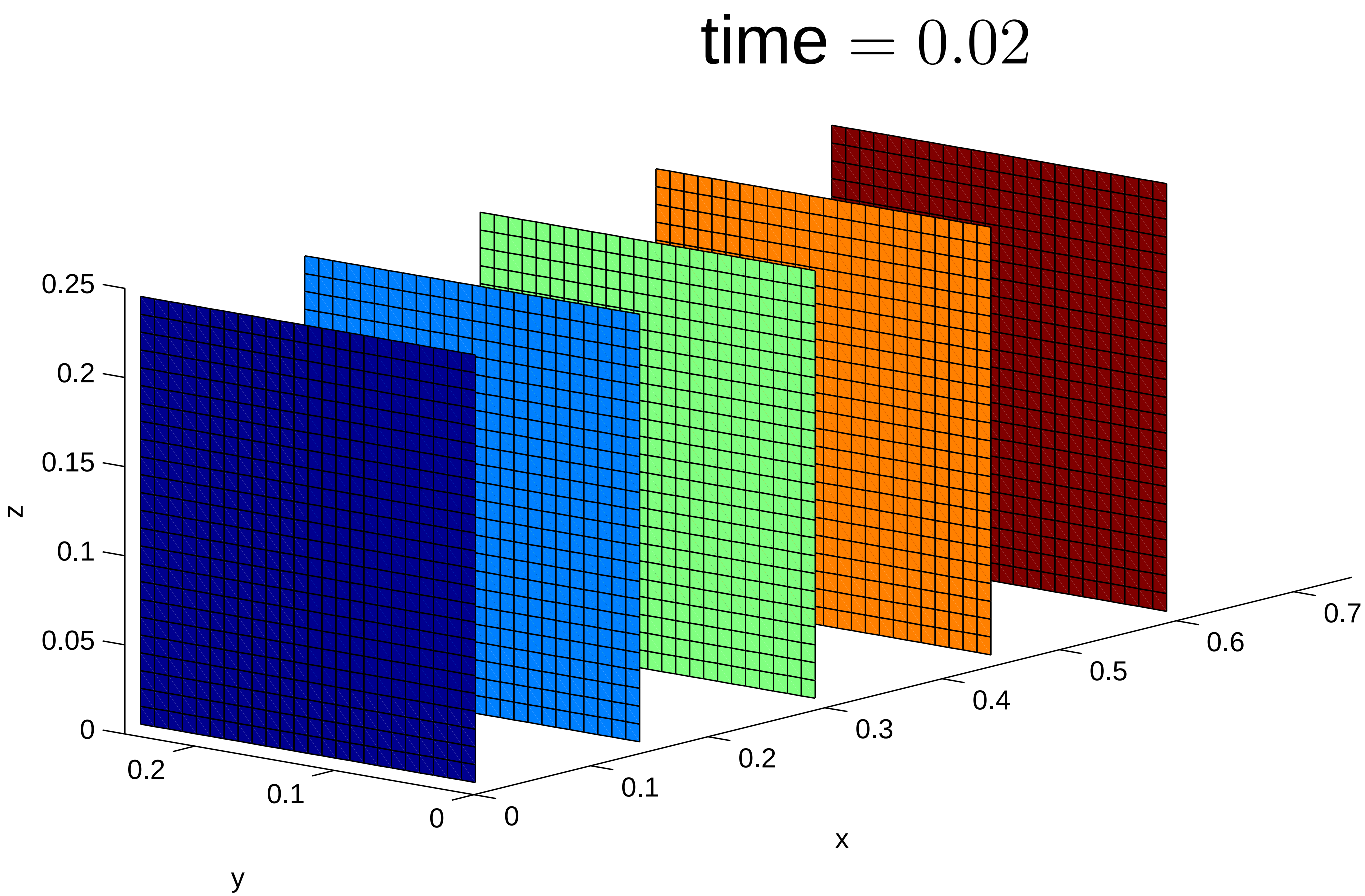
Shock-Bubble (R22) (Cont.)

- Grid system (coarsen by factor 2) with $h_0 = 0.6$



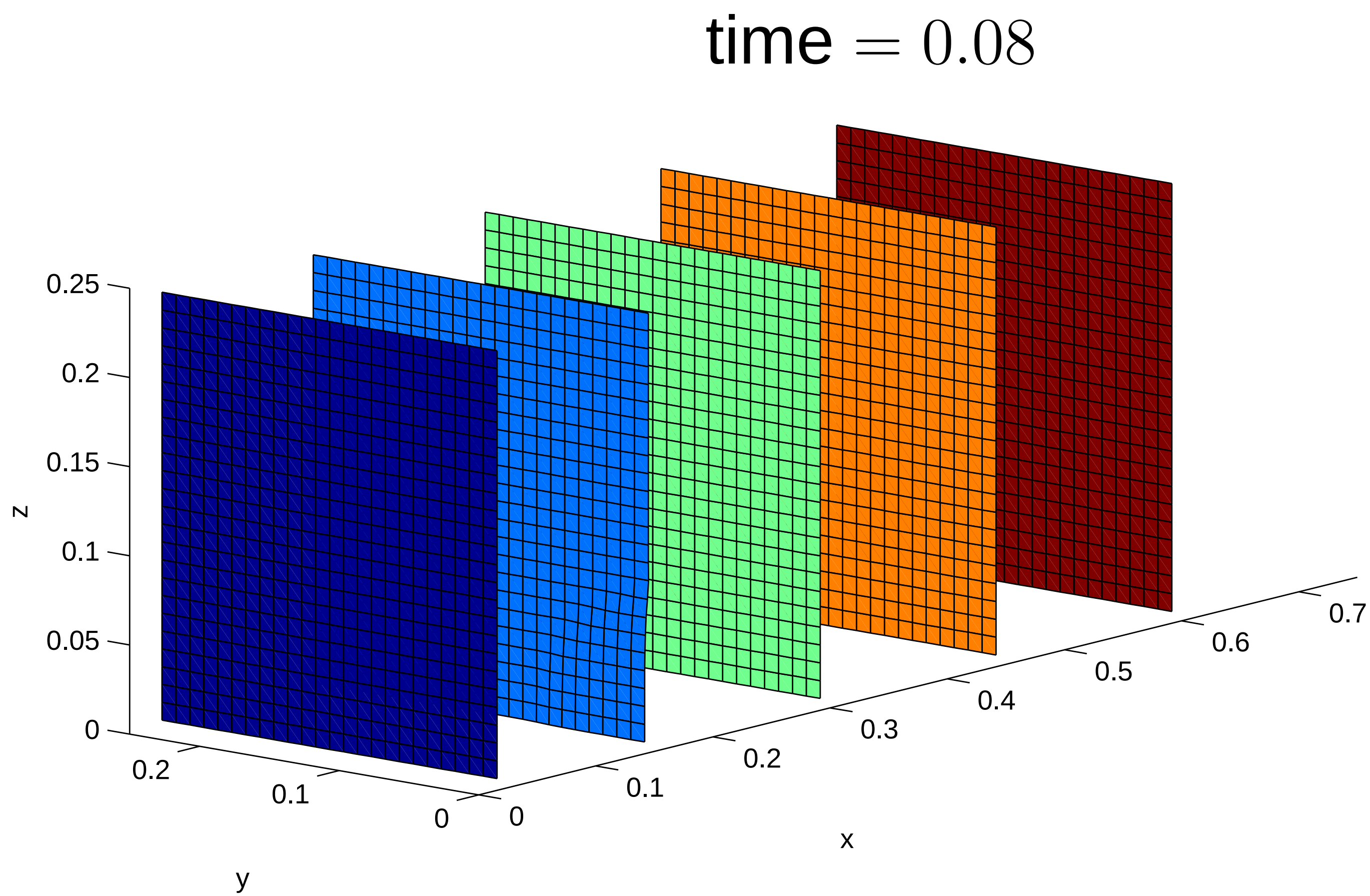
Shock-Bubble (R22) (Cont.)

- Grid system (coarsen by factor 2) with $h_0 = 0.6$



Shock-Bubble (R22) (Cont.)

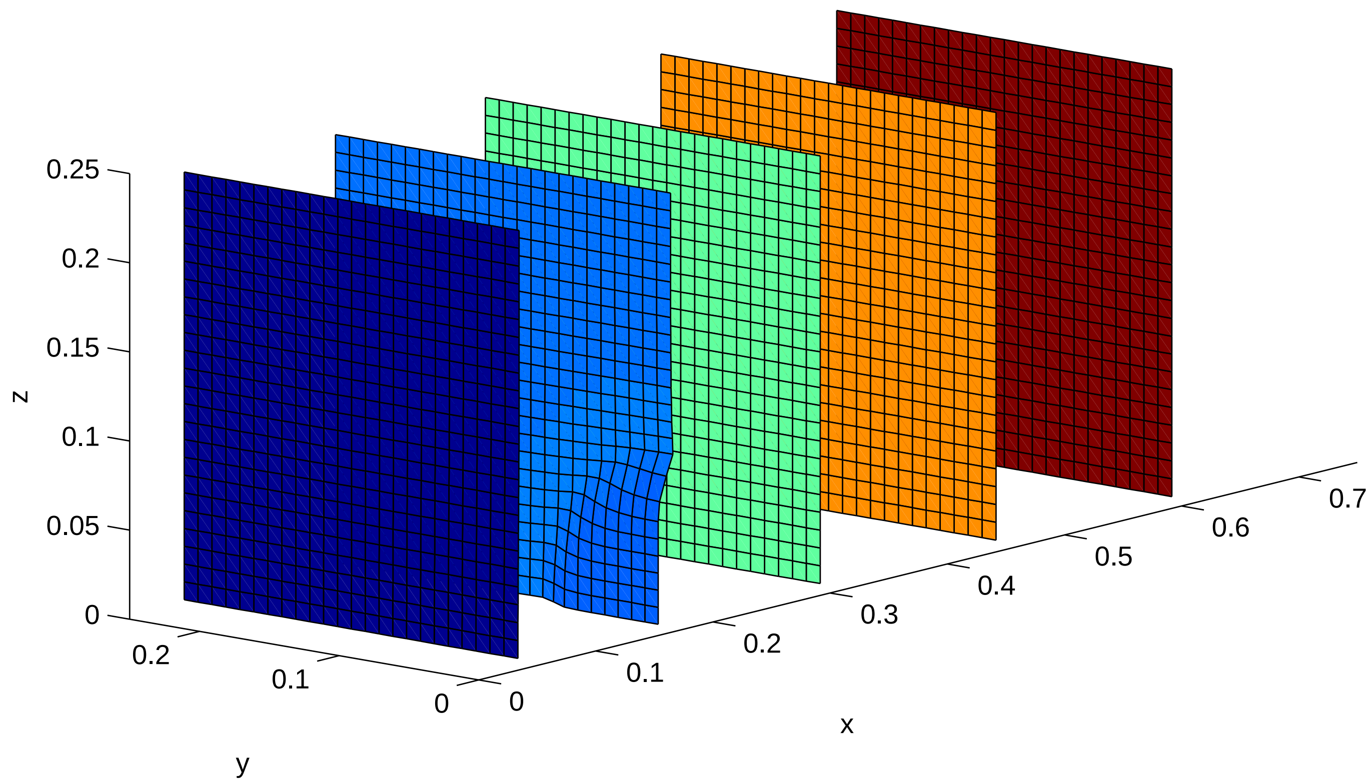
- Grid system (coarsen by factor 2) with $h_0 = 0.6$



Shock-Bubble (R22) (Cont.)

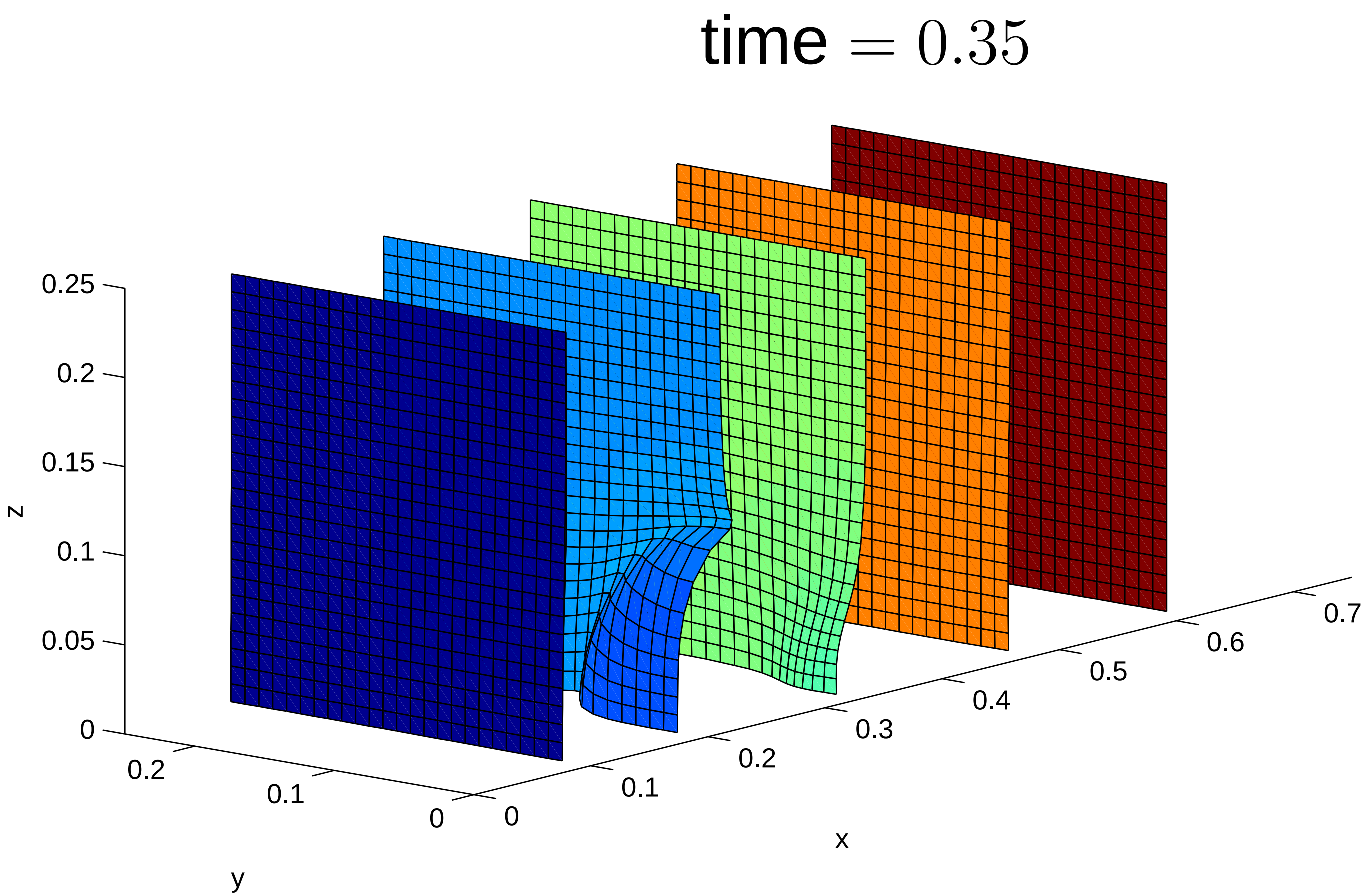
- Grid system (coarsen by factor 2) with $h_0 = 0.6$

time $= 0.16$



Shock-Bubble (R22) (Cont.)

- Grid system (coarsen by factor 2) with $h_0 = 0.6$



Conclusion

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  - Weakly compressible flow
  - Viscous flow extension
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Thank You