# A unified moving grid method for hyperbolic systems of partial differential equations

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# Talk objective

Describe a unified-coordinate moving grid approach for numerical approximation of first-order hyperbolic system

$$\frac{\partial}{\partial t} q\left(\vec{x},\ t\right) + \sum_{j=1}^{N} A_j \frac{\partial q}{\partial x_j} = 0 \qquad \text{or} \qquad \frac{\partial}{\partial t} q\left(\vec{x},\ t\right) + \sum_{j=1}^{N} \frac{\partial}{\partial x_j} f_j\left(q,\ \vec{x}\right) = 0$$

with discontinuous initial data in general $N \geq 1$ geometry

- $\vec{x} = (x_1, x_2, \ldots, x_N)$: spatial vector, $t$: time
- $q \in \mathbb{R}^m$: vector of $m$ state quantities
- $A_j \in \mathbb{R}^{m \times m}$: $m \times m$ matrix, $f_j \in \mathbb{R}^m$: flux vector

Model is assumed to be hyperbolic, where $\sum_{j=1}^{N} \alpha_j A_j$ or $\sum_{j=1}^{N} \alpha_j \left(\partial f_j / \partial q\right)$ is diagonalizable with real e-values, $\alpha_j \in \mathbb{R}$

# Talk outline

- Preliminary
  - Sample models in Cartesian coordinates
  - Cartesian cut-cell method & results
- Mathematical model in unified coordinates
  - Basic physical equations
  - Moving grid condition & geometric conservation law
- Finite volume approximation
  - Riemann problem & approximate solution
  - Godunov-type method
- Numerical examples
- Future work

# Preliminary: model equations

- Acoustics in heterogeneous media

$$\frac{\partial}{\partial t}\begin{pmatrix} p \\ u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} 0 & K & 0 \\ 1/\rho & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \frac{\partial}{\partial x_1}\begin{pmatrix} p \\ u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} 0 & 0 & K \\ 0 & 0 & 0 \\ 1/\rho & 0 & 0 \end{pmatrix} \frac{\partial}{\partial x_2}\begin{pmatrix} p \\ u_1 \\ u_2 \end{pmatrix} = 0$$

- Shallow water equations with bottom topography

$$\frac{\partial}{\partial t}\begin{pmatrix} h \\ hu_i \end{pmatrix} + \sum_{j=1}^{N} \frac{\partial}{\partial x_j}\begin{pmatrix} hu_j \\ hu_i u_j + \frac{1}{2} g h^2 \delta_{ij} \end{pmatrix} = \begin{pmatrix} 0 \\ -gh \frac{\partial B}{\partial x_i} \end{pmatrix}, \quad i = 1, \ldots, N$$

$p$: pressure, $\rho$: density, $K$: bulk modulus, $u_i$: $x_i$-velocity
$h$: water height, $\delta_{ij}$: Kronecker delta, $B$: bottom topo.
$g$: gravitational constant

# Model equations (Cont.)

- Compressible Euler equations

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u_i\\ E\end{pmatrix}+\sum_{j=1}^{N}\frac{\partial}{\partial x_j}\begin{pmatrix}\rho u_j\\ \rho u_i u_j+p\delta_{ij}\\ E u_j+p u_j\end{pmatrix}=0,\quad i=1,\ldots,N$$

$E=\rho e+\rho\sum_{j=1}^{N}u_j^2/2$: total energy, $e(\rho,p)$: internal energy

Note constitutive law for $p$ is required to complete the model, for example,

- Polytropic gas: $p=(\gamma-1)\rho e$
- Stiffened gas: $p=(\gamma-1)\rho e-\gamma\mathcal{B}$
- van der Waals gas: $p=\frac{\gamma-1}{1-b\rho}\left(\rho e+a\rho^2\right)-a\rho^2$

# Model equations (Cont.)

- Compressible reduced $2$-phase flow model
  - Proposed by Murrone & Guillard (JCP 2005)
  - Derive from Baer & Nunziato's model by assuming $1$-pressure & $1$-velocity across interfaces

$$\frac{\partial}{\partial t}\begin{pmatrix}\alpha_1\rho_1\\ \alpha_2\rho_2\\ \rho u_i\\ E\end{pmatrix}+\sum_{j=1}^{N}\frac{\partial}{\partial x_j}\begin{pmatrix}\alpha_1\rho_1 u_j\\ \alpha_2\rho_2 u_j\\ \rho u_i u_j+p\delta_{ij}\\ E u_j+p u_j\end{pmatrix}=0, \quad i=1,\ldots,N$$

$$\frac{\partial \alpha_1}{\partial t}+\sum_{j=1}^{N}u_j\frac{\partial \alpha_1}{\partial x_j}=\alpha_1\alpha_2\left(\frac{\rho_1 c_1^2-\rho_2 c_2^2}{\sum_{k=1}^{2}\alpha_k\rho_k c_k^2}\right)\sum_{j=1}^{N}\frac{\partial u_j}{\partial x_j}$$

$\alpha_k$: volume fraction for phase $k$, $\alpha_1+\alpha_2=1$, $c_k$: sound speed, $\rho=\alpha_1\rho_1+\alpha_2\rho_2$: mixture (total) density

# Reduced $2$-phase 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
  - For some complex EOS, from $(\alpha_2, \rho_1, \rho_2, \rho e)$ in model equations we recover $p$ by solving

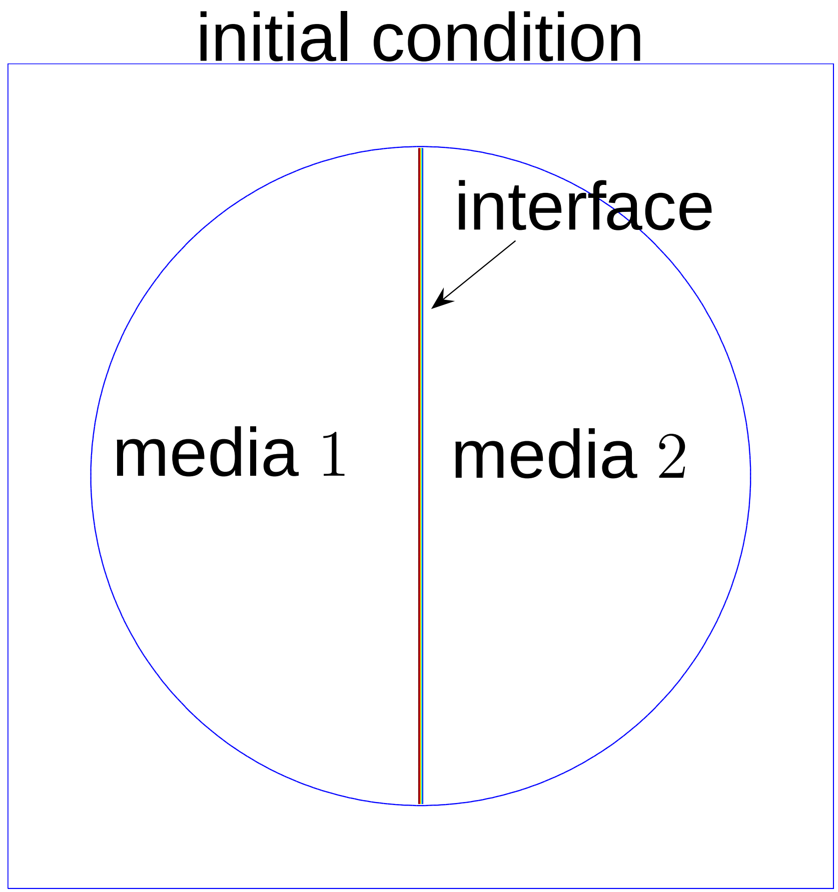
$$p_1(\rho_1, \rho_1 e_1) = p_2(\rho_2, \rho_2 e_2) \quad \& \quad \sum_{k=1}^{2} \alpha_k \rho_k e_k = \rho e$$

- Shyue (JCP 1998) & Allaire *et al.* (JCP 2002) proposed

$$\frac{\partial \alpha_1}{\partial t} + \sum_{j=1}^{N} u_j \frac{\partial \alpha_1}{\partial x_j} = 0$$

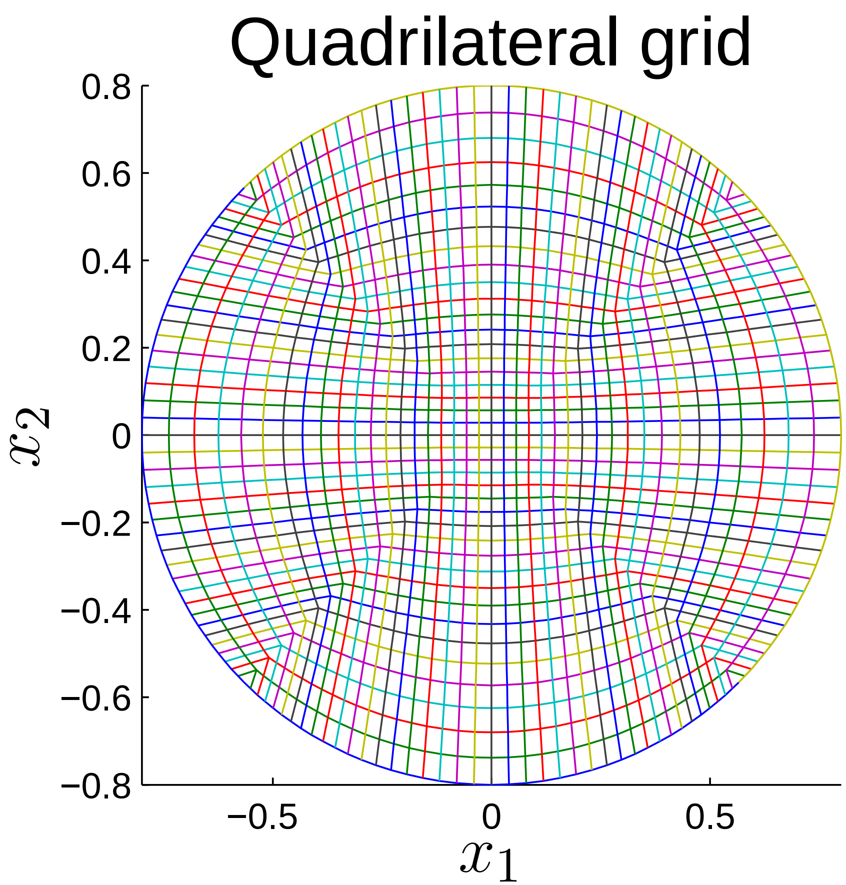
# Preliminary: model problem

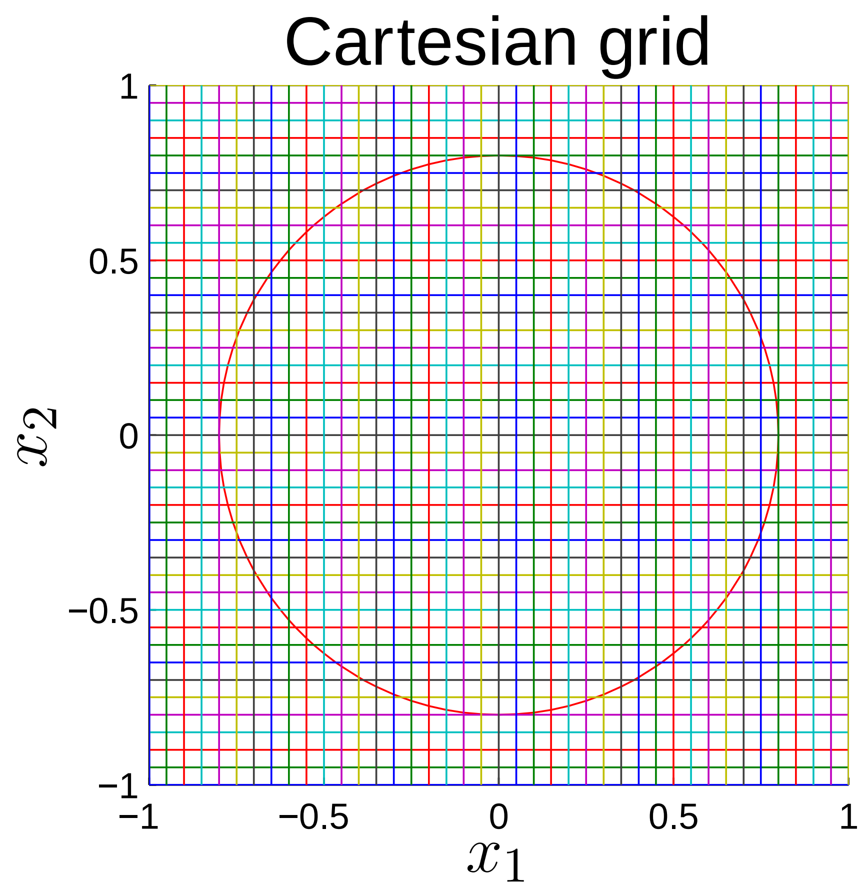
- Moving cylindrical vessel with $\vec{u}_b = (1, 0)$



# Model problem: grid system

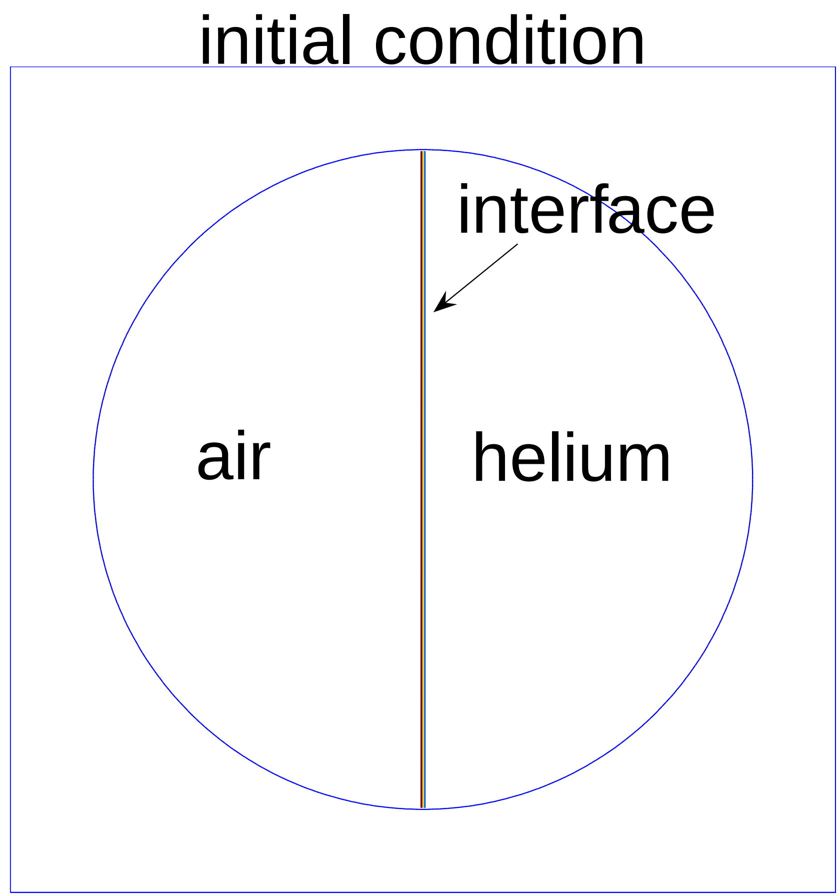
- Typical discrete grid systems for cylindrical vessel



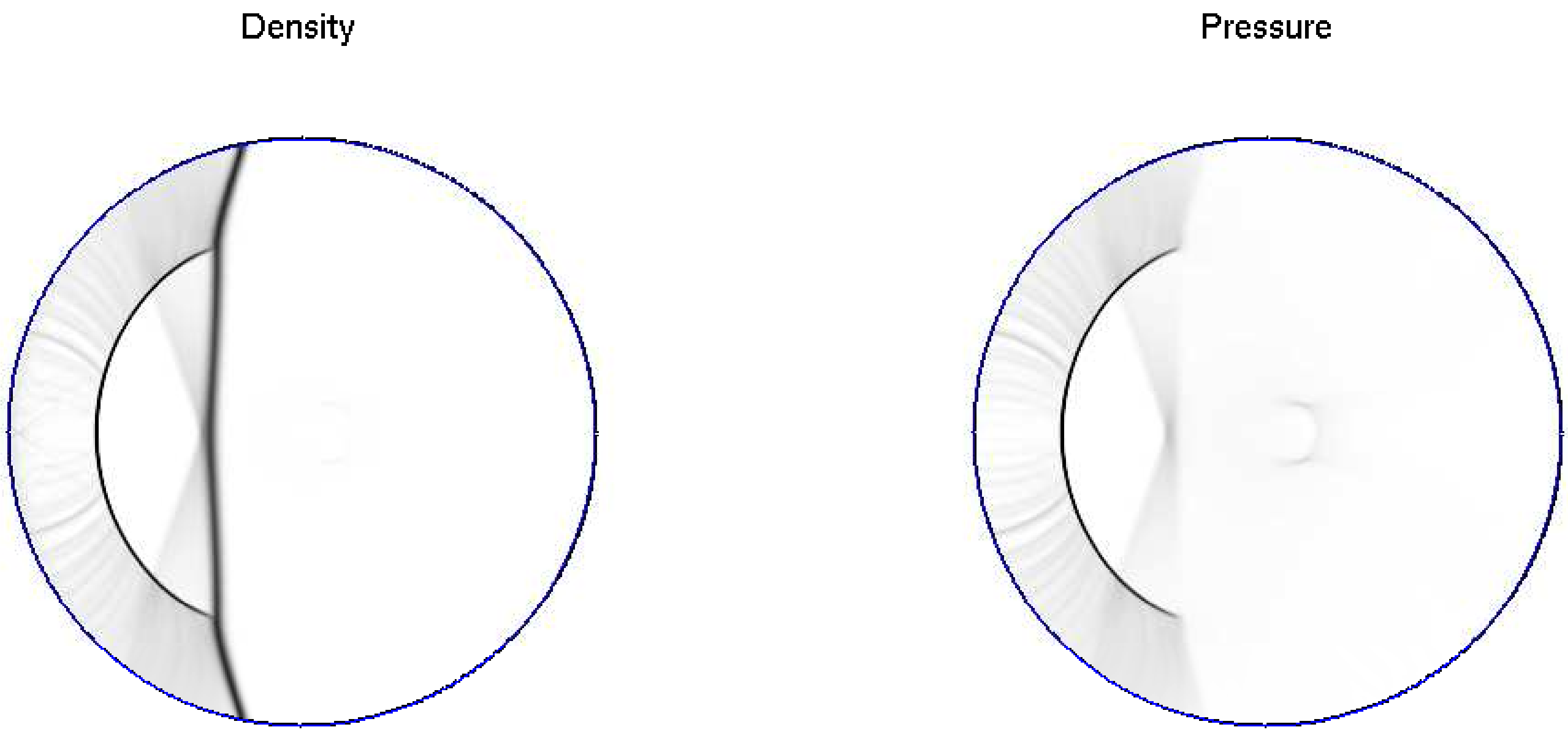
# Model problem: Cartesian results

- Compressible flow case with air-helium interface



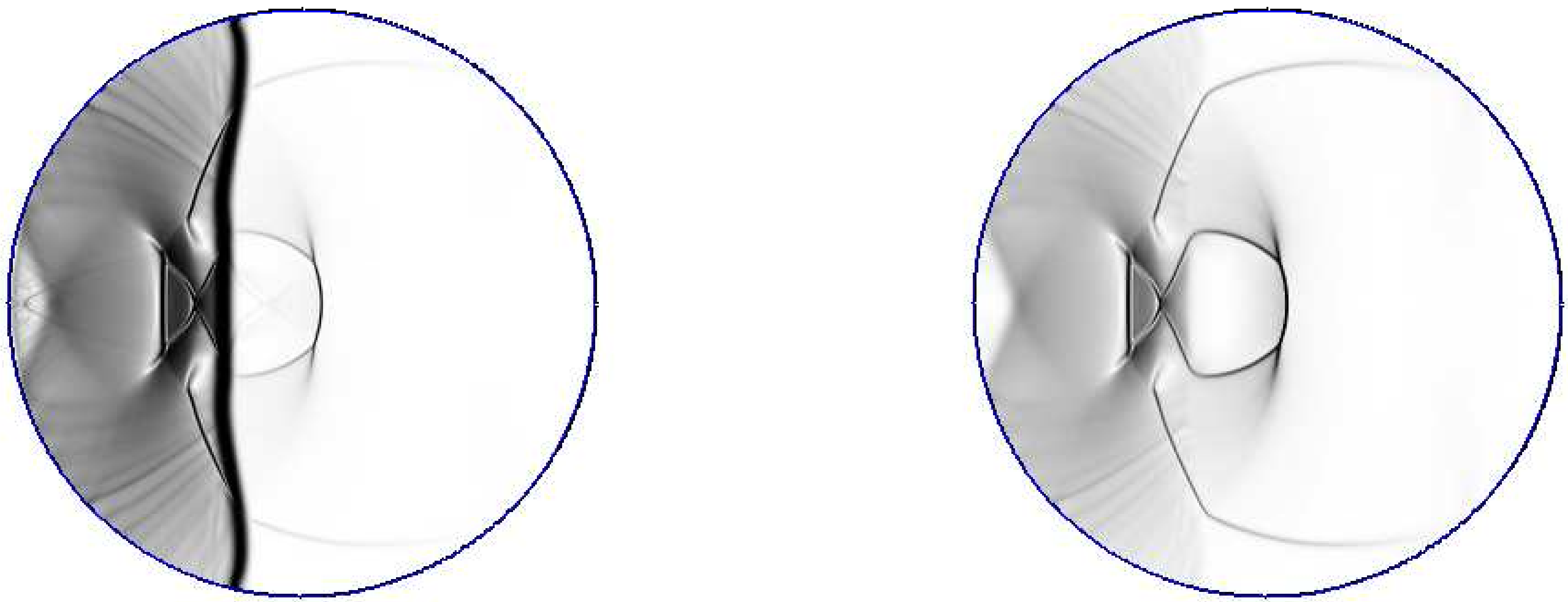
# Model problem: Cartesian results

- Compressible flow case with air-helium interface
  - Solution at time $t = 0.25$



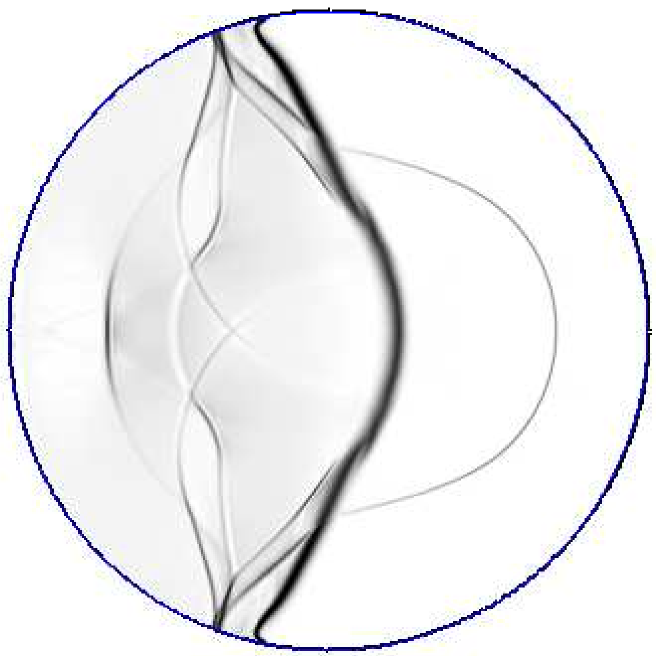
# Model problem: Cartesian results

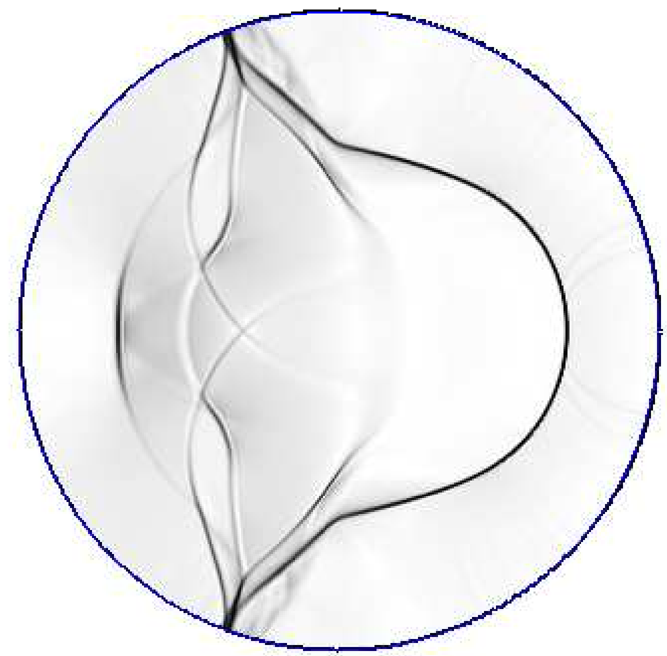
- Compressible flow case with air-helium interface
  - Solution at time $t = 0.5$



# Model problem: Cartesian results

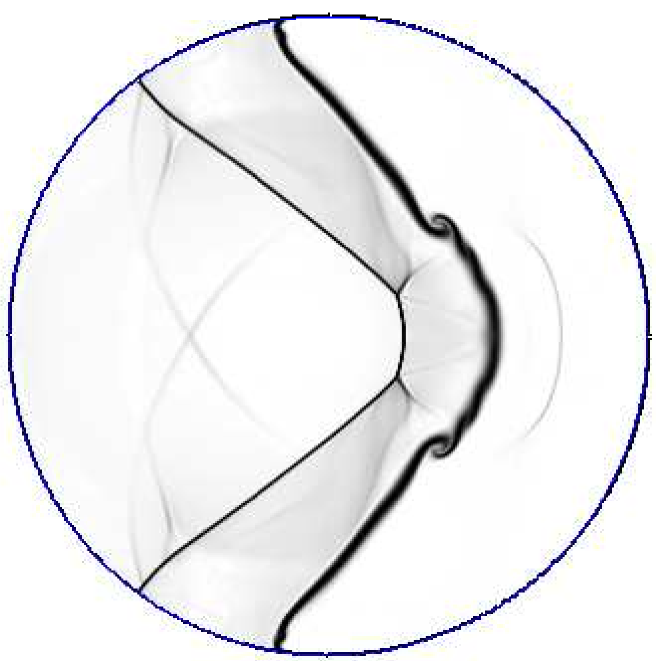
- Compressible flow case with air-helium interface
  - Solution at time $t = 0.75$

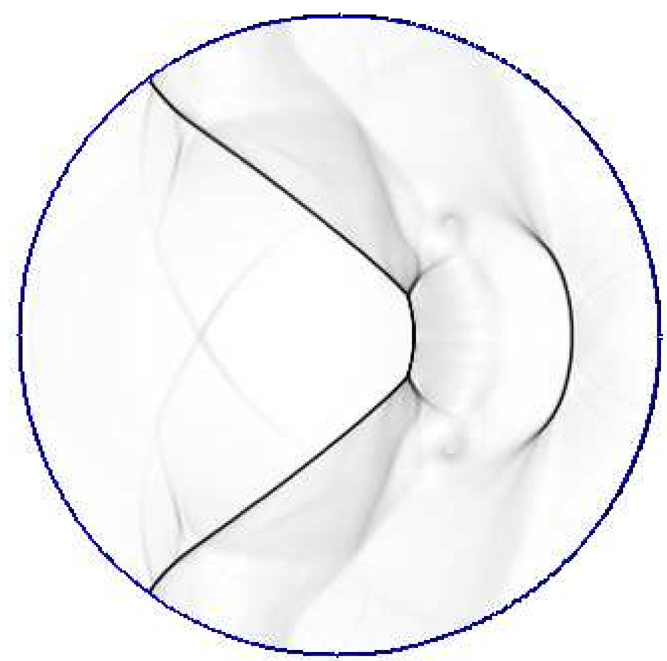




# Model problem: Cartesian results

- Compressible flow case with air-helium interface
  - Solution at time $t = 1$



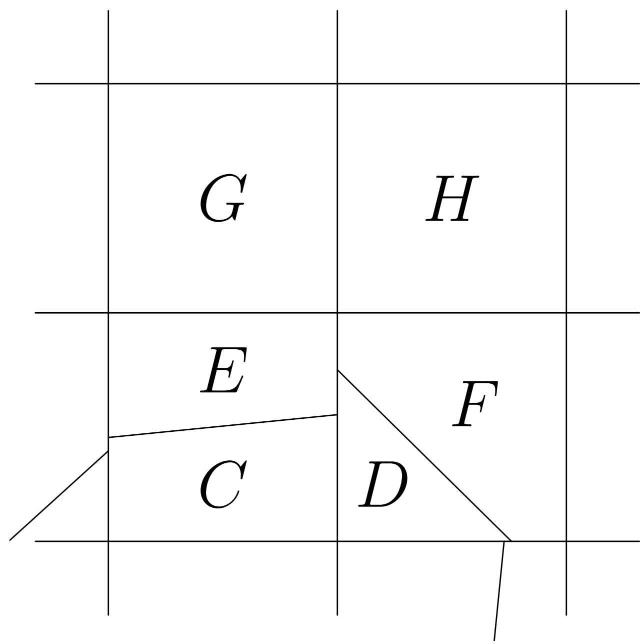


# Cartesian cut-cell method

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

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

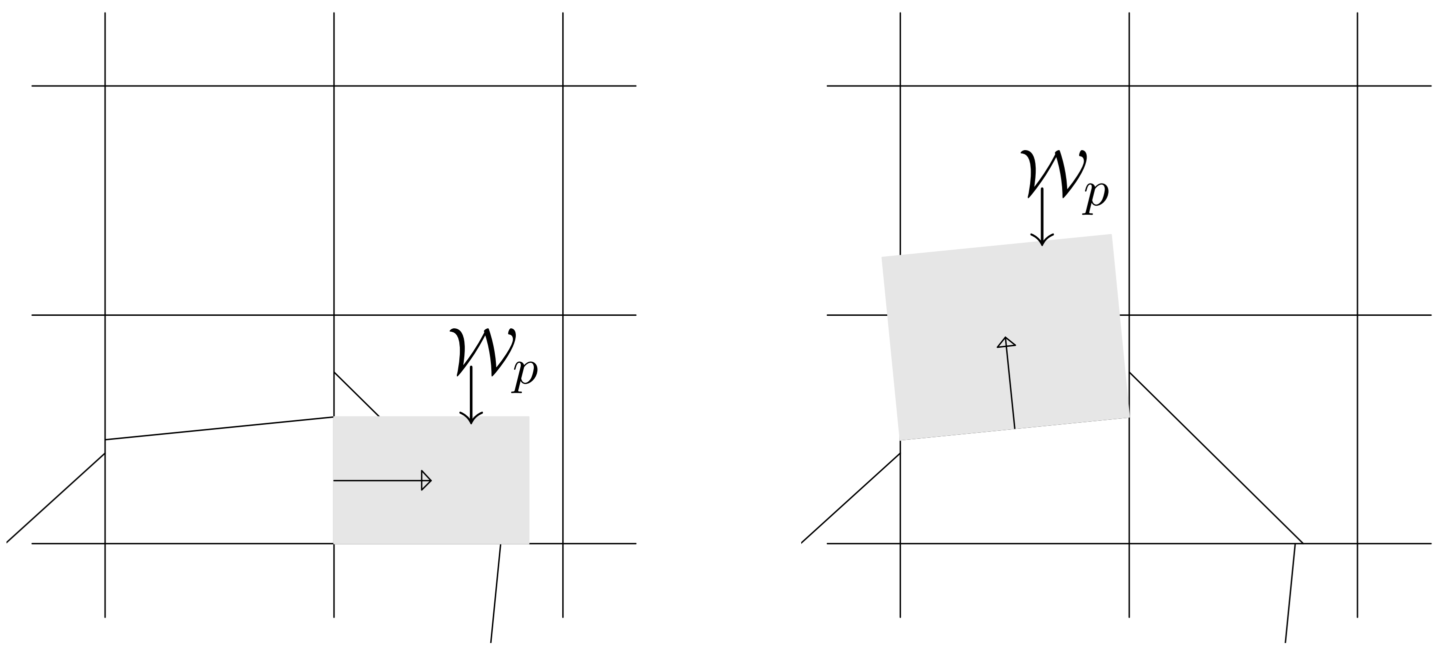
$\mathcal{M}(S)$: measure (area in $2$D or volume in $3$D) of cell $S$



# Cartesian cut-cell method (Cont.)

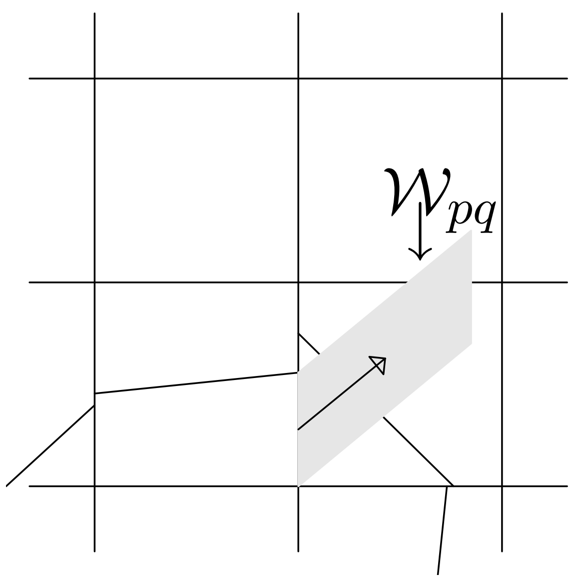
- First order version: Piecewise constant wave update
  - Godunov-type method: Solve Riemann problem at each cell interface in normal direction & use resulting waves to update cell averages

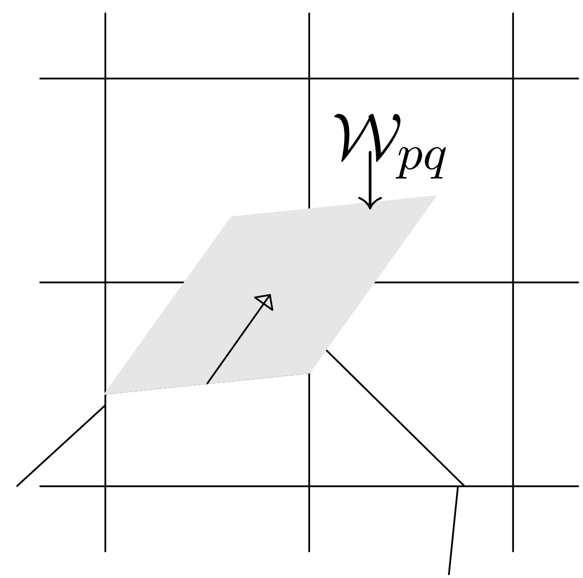
$$Q_S^{n+1} := Q_S^{n+1} - \frac{\mathcal{M}\left(\mathcal{W}_p \cap S\right)}{\mathcal{M}(S)} R_p, \qquad R_p \text{ being jump from RP}$$



# Cartesian cut-cell 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

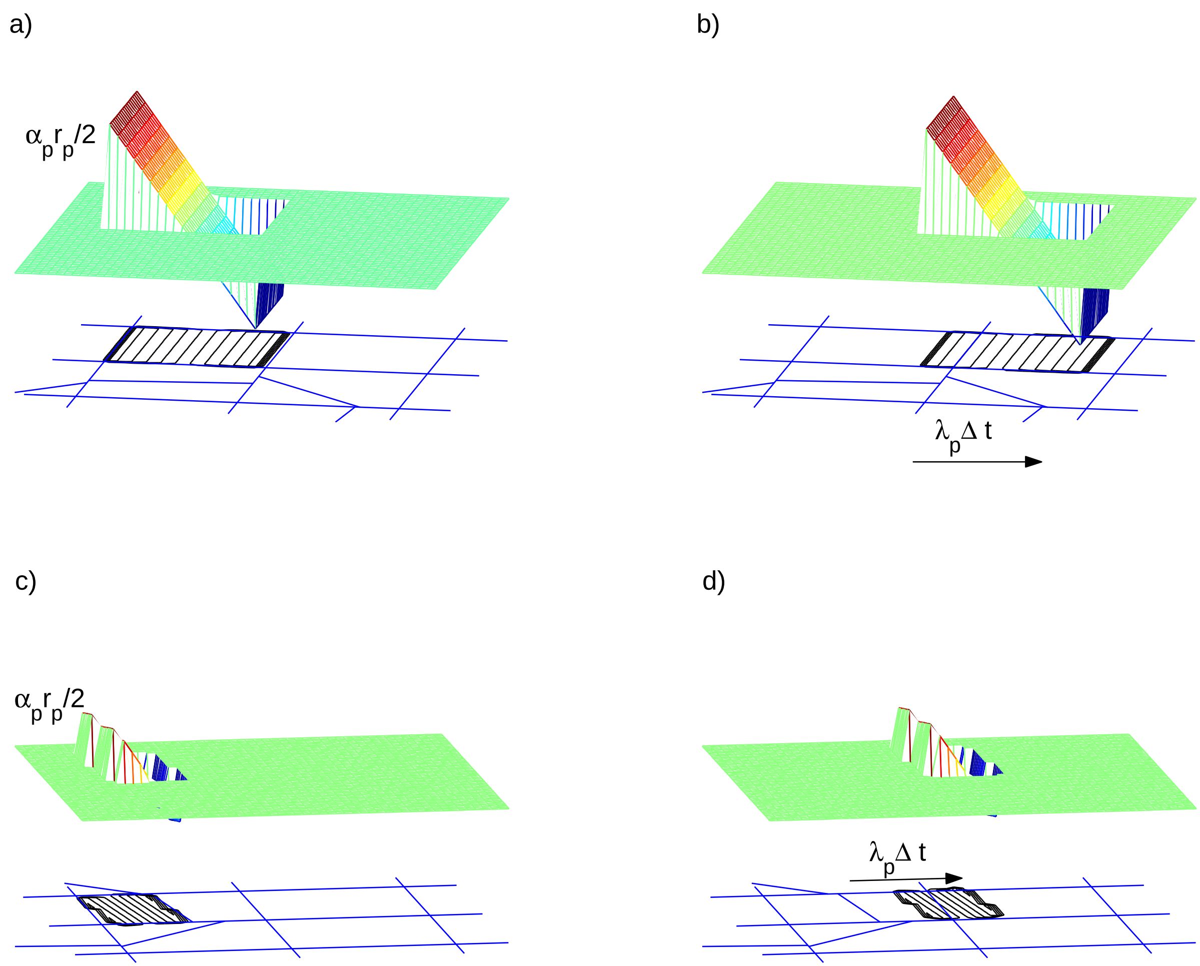


# Cartesian cut-cell method (Cont.)

- High resolution version: Piecewise linear wave update

wave before propagation after propagation



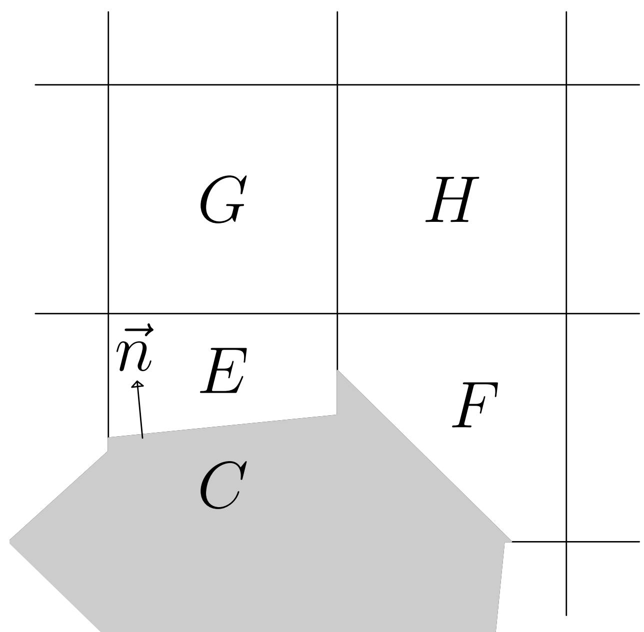
# Embedded boundary conditions

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:

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

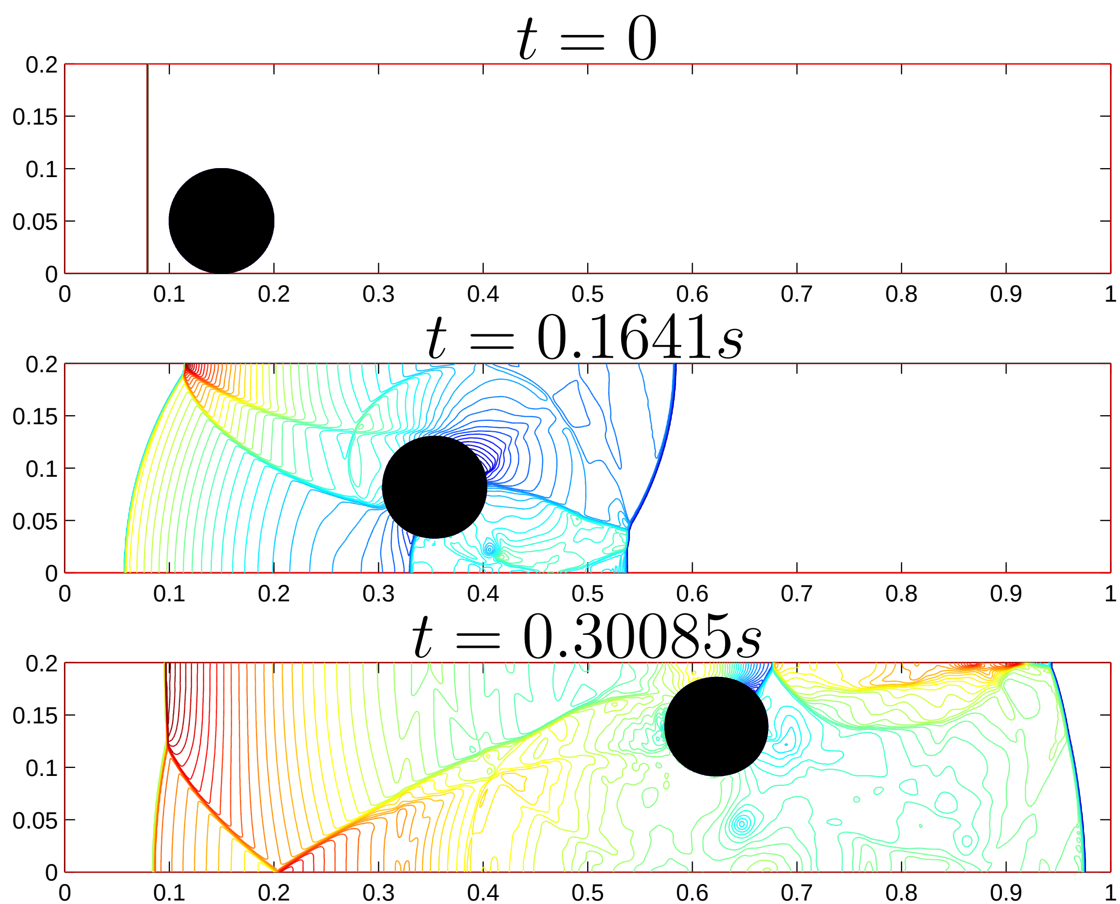
$$\vec{u}_C := \vec{u}_E - 2(\vec{u}_E \cdot \vec{n})\vec{n} + 2(\vec{u}_b \cdot \vec{n})$$

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



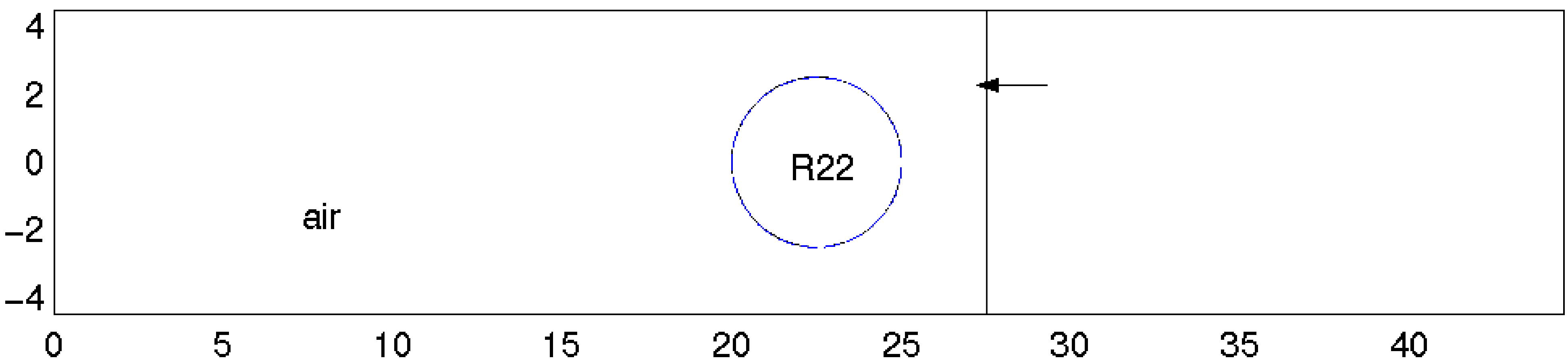
# Cylinder lift-off problem

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



# Shock-Bubble Interaction Problem

- Cartesian grid results



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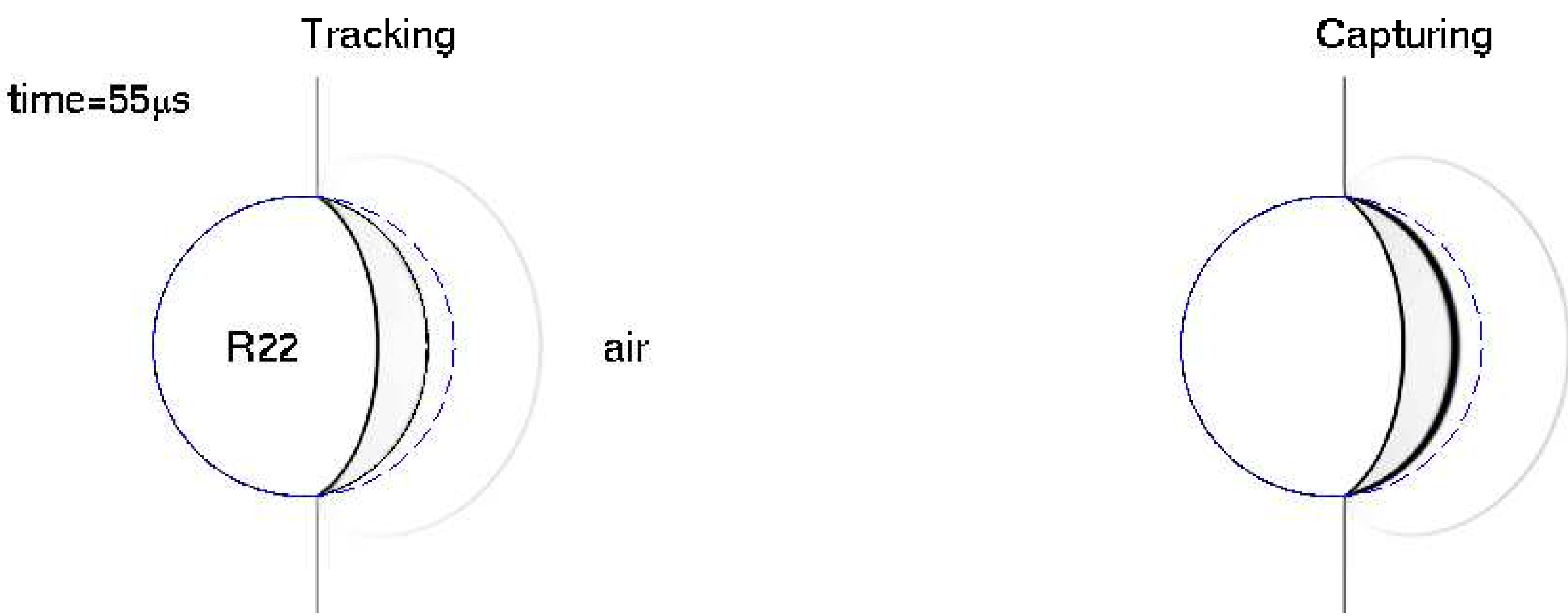

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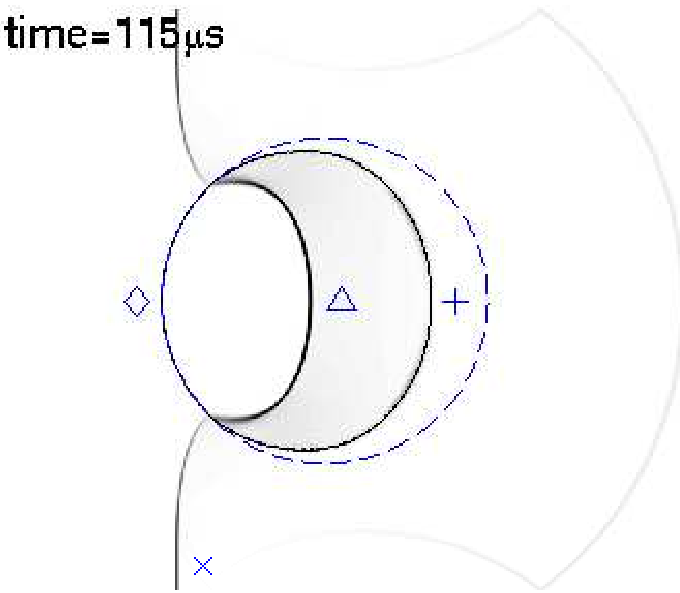


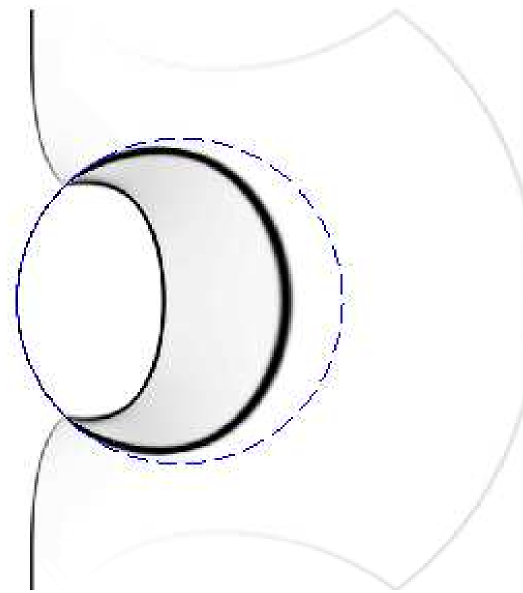

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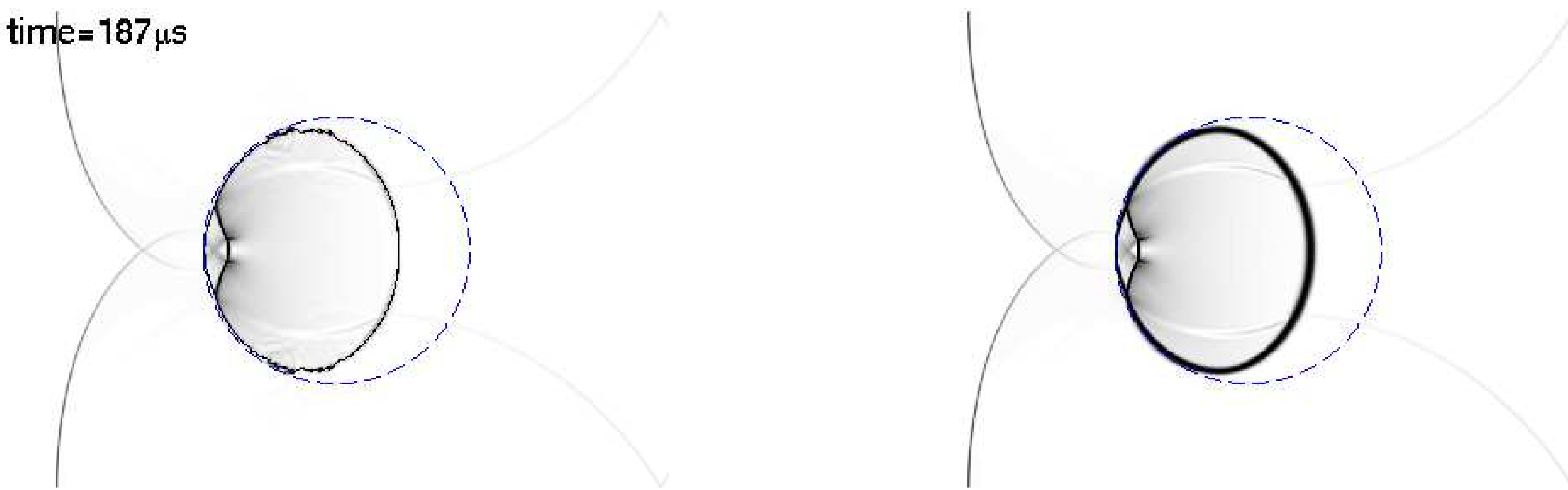

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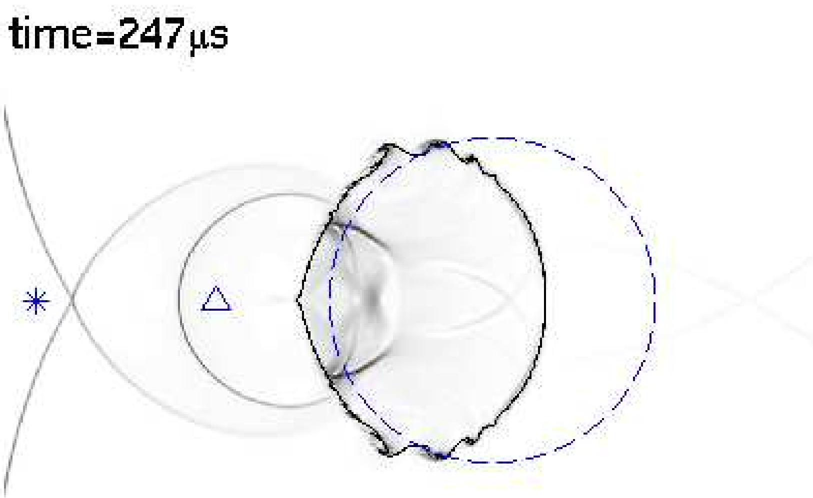


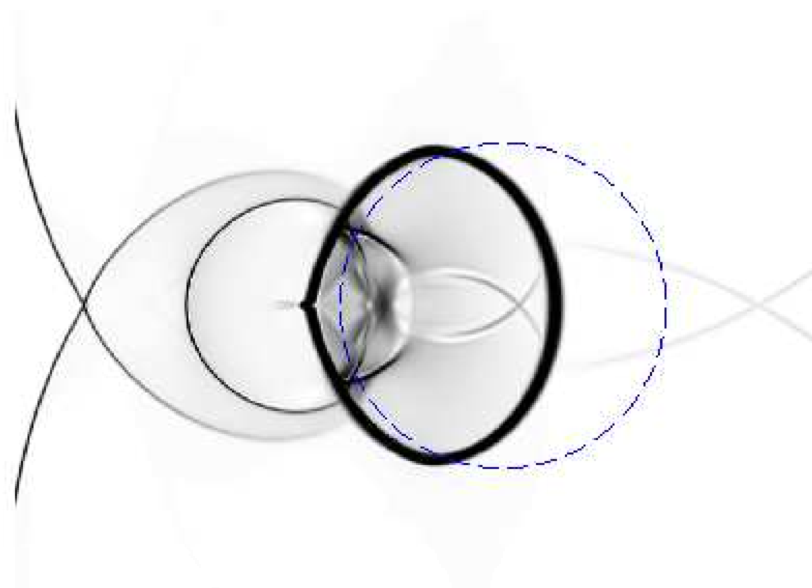

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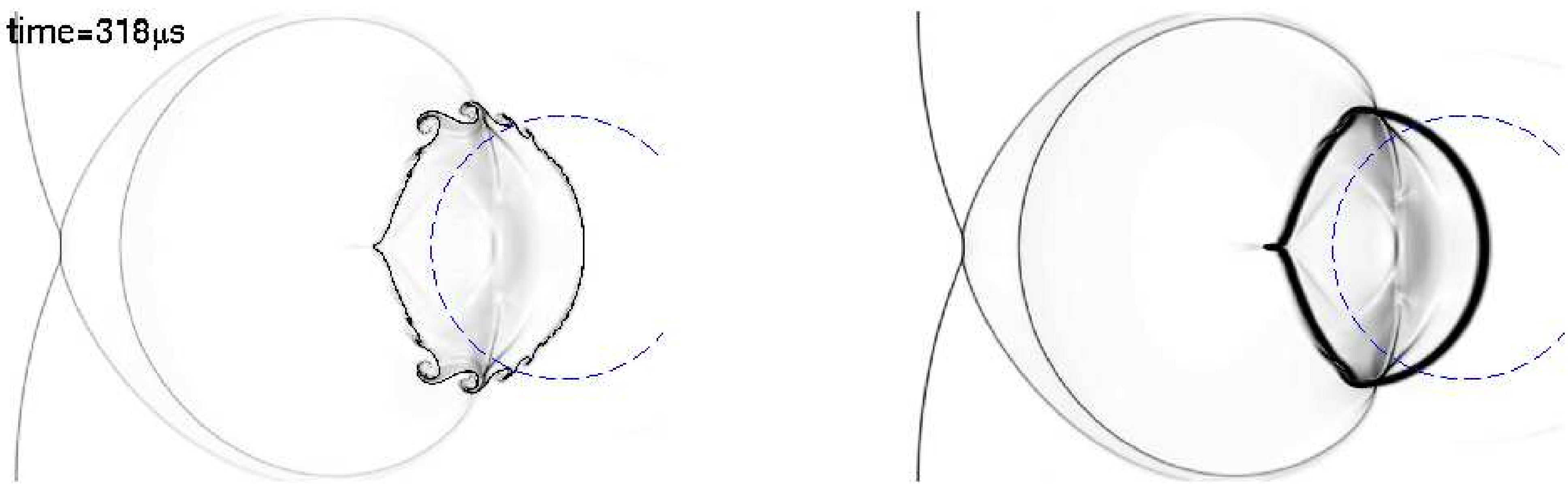

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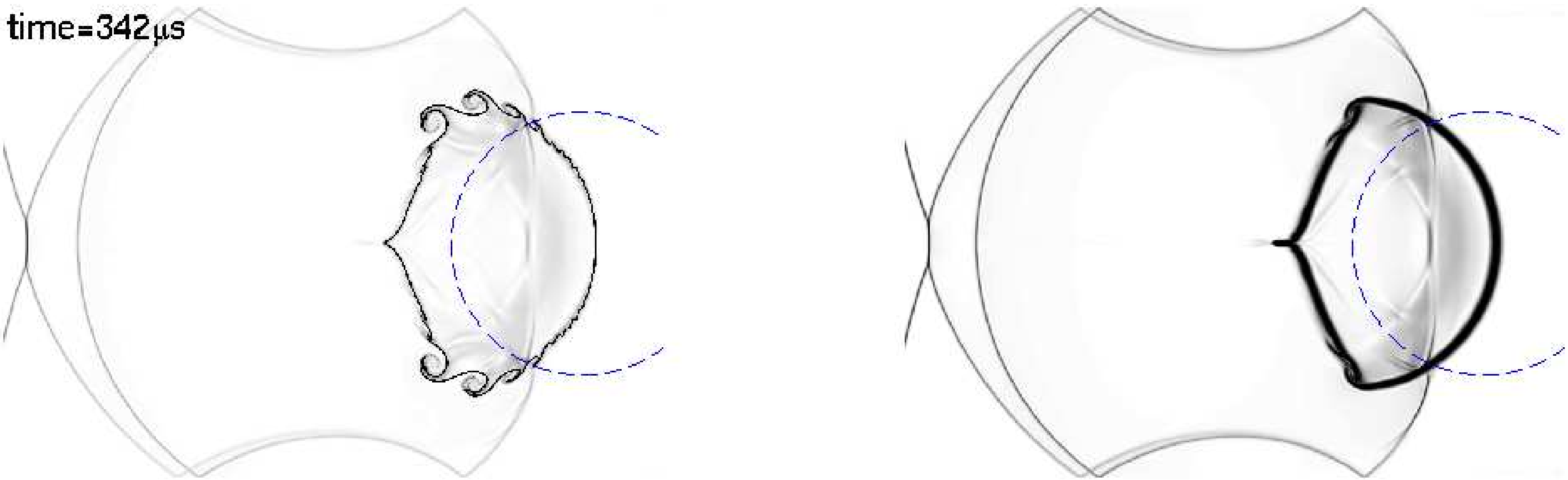

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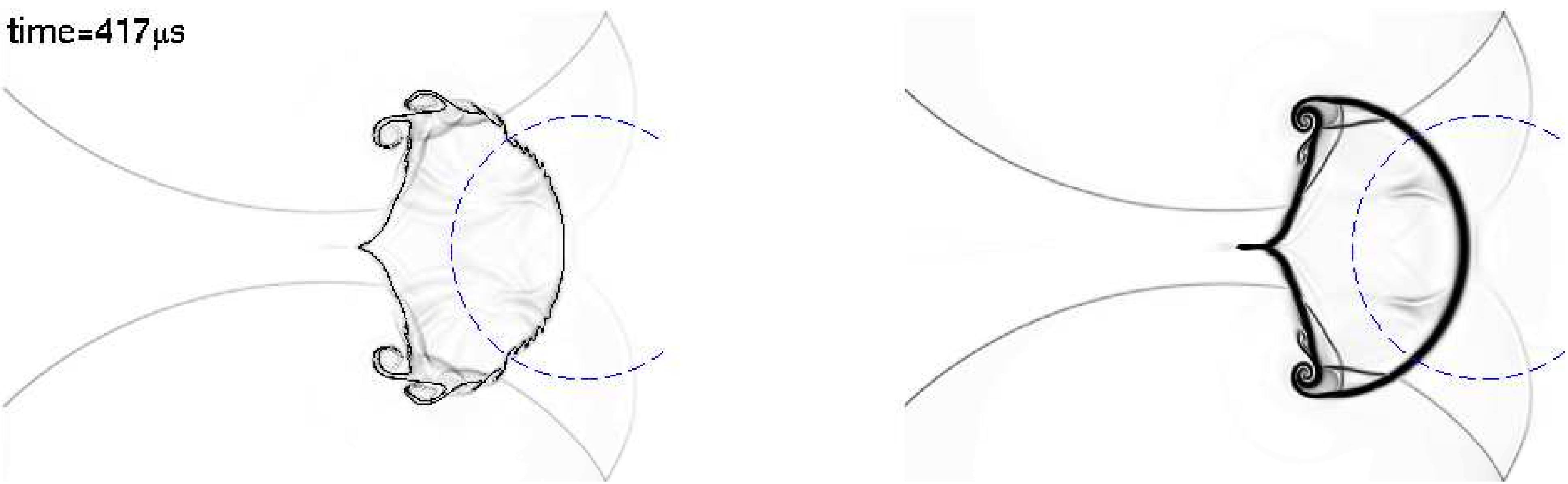
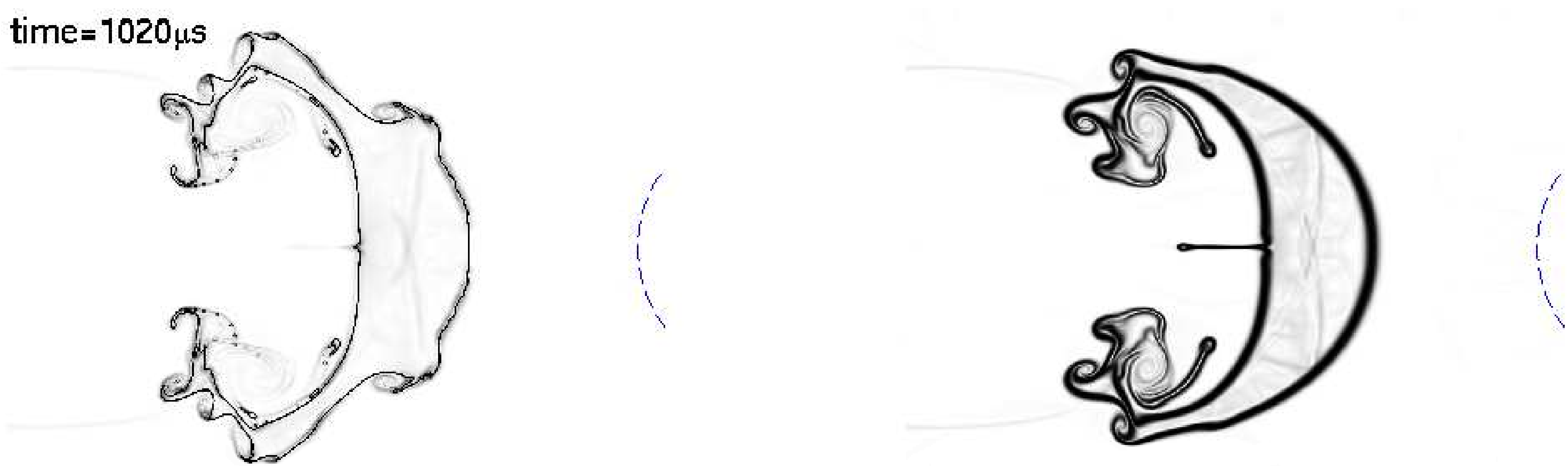


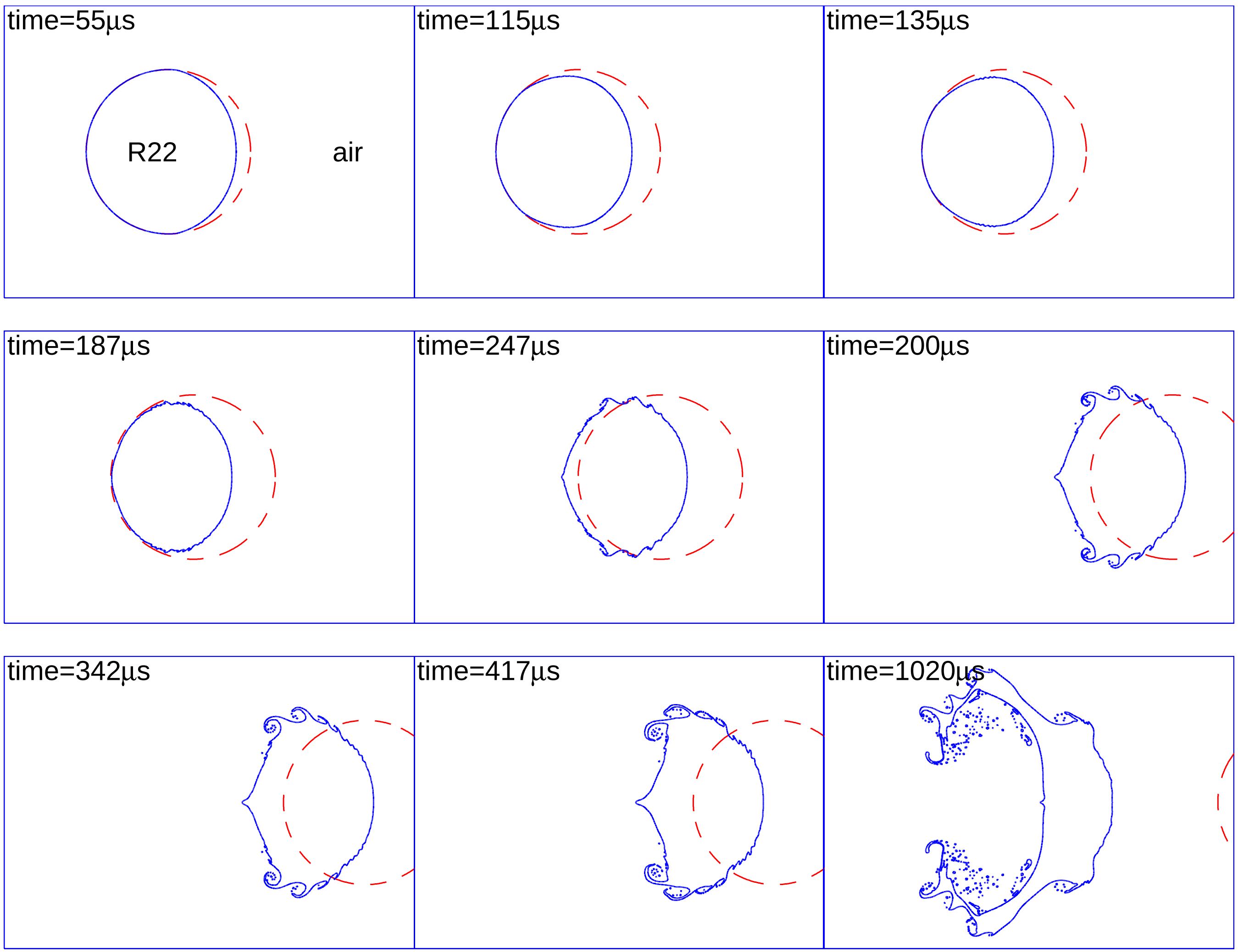
# Shock-Bubble Interaction Problem

- Cartesian grid results



# Shock-Bubble Interaction (cont.)

- Approximate locations of interfaces



# Cartesian cut-cell: Remarks

- Small cell problems
  - Stability
  - Accuracy
- Numerical implementation
  - Challenging task for embedded $3$D geometry
  - Challenging task for interface tracking in general geometry (even in $2$D)

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- Small cell problems
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  - Challenging task for embedded $3$D geometry
  - Challenging task for interface tracking in general geometry (even in $2$D)

This work is aimed at devising a more robust moving grid method than the aforementioned Cartesian cut-cell method

- To begin with, take unified coordinate method proposed by Hui & coworkers (JCP 1999, 2001)

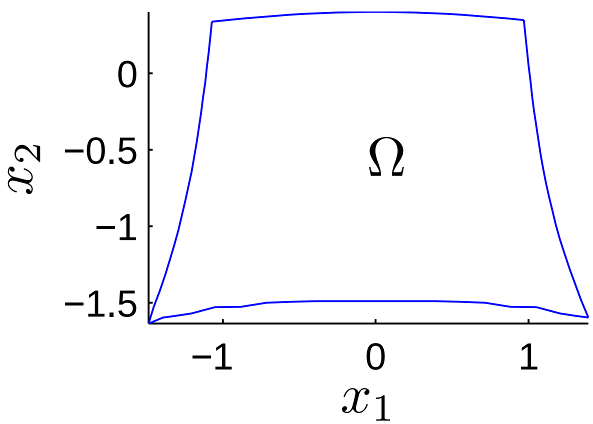
# Model system in unified coord.

To begin with, consider a general non-rectangular domain $\Omega$ ($N = 2$ shown below) & introduce coordinate change $(\vec{x},\ t) \mapsto (\vec{\xi},\ \tau)$ via

$$\vec{\xi} = (\xi_1, \xi_2, \ldots, \xi_N)\,, \qquad \xi_j = \xi_j(\vec{x}, t), \qquad \tau = t,$$

that maps a physical domain $\Omega$ to a logical one $\hat{\Omega}$

physical domain

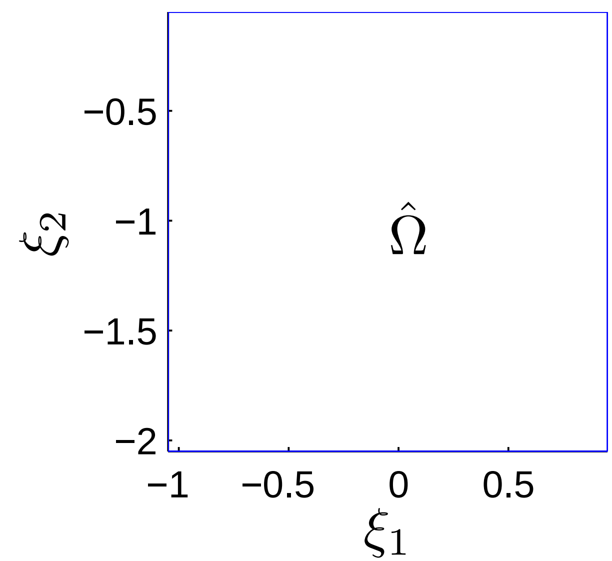



mapping

$$\longrightarrow$$

$$\xi_1 = \xi_1(x_1, x_2)$$
$$\xi_2 = \xi_2(x_1, x_2)$$

logical domain



# Unified coord. model (Cont.)

To derive hyperbolic conservation laws, for example, in this generalized coordinate $(\vec{\xi},\ \tau)$, using chain rule of partial differentiation, derivatives in physical space become

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \sum_{i=1}^{N} \frac{\partial \xi_i}{\partial t} \frac{\partial}{\partial \xi_i}, \qquad \frac{\partial}{\partial x_j} = \sum_{i=1}^{N} \frac{\partial \xi_i}{\partial x_j} \frac{\partial}{\partial \xi_i} \quad \text{for } j = 1, 2, \ldots, N,$$

yielding the equation

$$\frac{\partial q}{\partial \tau} + \sum_{j=1}^{N} \left( \frac{\partial \xi_j}{\partial t} \frac{\partial q}{\partial \xi_j} + \sum_{i=1}^{N} \frac{\partial \xi_i}{\partial x_j} \frac{\partial f_j}{\partial \xi_i} \right) = 0$$

Note this is not in divergence form, and hence is not conservative.

# Unified coord. model (Cont.)

To obtain a strong conservation-law form as

$$\frac{\partial \tilde{q}}{\partial \tau} + \sum_{j=1}^{N} \frac{\partial \tilde{f}_j}{\partial \xi_j} = \tilde{\psi}$$

for some $\tilde{q}$, $\tilde{f}_j$, & $\tilde{\psi}$, we first multiply $J = \det\left(\partial\vec{\xi}/\partial\vec{x}\right)^{-1}$ to the aforementioned non-conservative equations, and have

$$J\frac{\partial q}{\partial \tau} + \sum_{j=1}^{N} J \left( \frac{\partial \xi_j}{\partial t}\frac{\partial q}{\partial \xi_j} + \sum_{i=1}^{N} \frac{\partial \xi_i}{\partial x_j}\frac{\partial f_j}{\partial \xi_i} \right) = J\psi(q)$$

Then use differentiation by parts, $u\,dv = d(uv) - v\,du$, yielding

$$\frac{\partial \tilde{q}}{\partial \tau} + \sum_{j=1}^{N} \frac{\partial \tilde{f}_j}{\partial \xi_j} = \tilde{\psi} + \mathcal{G}$$

with $\tilde{q} = Jq$, $\quad \tilde{f}_j = J\left(q\frac{\partial \xi_j}{\partial t} + \sum_{k=1}^{N} f_k \frac{\partial \xi_j}{\partial x_k}\right)$, $\quad \tilde{\psi} = J\psi$, $\quad$ & $\mathcal{G}$ (see next)

# Unified coord. model (Cont.)

Here we have

$$\mathcal{G} = q\left[\frac{\partial J}{\partial \tau} + \sum_{j=1}^{N}\frac{\partial}{\partial \xi_j}\left(J\frac{\partial \xi_j}{\partial t}\right)\right] + \sum_{j=1}^{N} f_j\left[\sum_{k=1}^{N}\frac{\partial}{\partial \xi_k}\left(J\frac{\partial \xi_k}{\partial x_j}\right)\right]$$

With the use of basic grid-metric relations, it is known that

$$\frac{\partial J}{\partial \tau} + \sum_{j=1}^{N}\frac{\partial}{\partial \xi_j}\left(J\frac{\partial \xi_j}{\partial t}\right) = 0 \quad \text{(geometric conservation law)}$$

$$\sum_{k=1}^{N}\frac{\partial}{\partial \xi_k}\left(J\frac{\partial \xi_k}{\partial x_j}\right) = 0 \quad \forall\, j = 1, 2, \ldots, N \quad \text{(compatibility condition)}$$

and hence $\mathcal{G} = 0$

# Unified coord. model (Cont.)

- Shallow water equations

$$\frac{\partial}{\partial \tau}\begin{pmatrix} hJ \\ hJu_i \end{pmatrix} + \sum_{j=1}^{N} \frac{\partial}{\partial \xi_j} J \begin{pmatrix} hU_j \\ hu_i U_j + \frac{1}{2} g h^2 \delta_{ij} \frac{\partial \xi_j}{\partial x_i} \end{pmatrix} = \begin{pmatrix} 0 \\ -ghJ \frac{\partial B}{\partial x_i} \end{pmatrix}$$

- Compressible Euler equations

$$\frac{\partial}{\partial \tau}\begin{pmatrix} \rho J \\ \rho J u_i \\ JE \end{pmatrix} + \sum_{j=1}^{N} \frac{\partial}{\partial \xi_j} J \begin{pmatrix} \rho U_j \\ \rho u_i U_j + p \frac{\partial \xi_j}{\partial x_i} \\ EU_j + pU_j - p \frac{\partial \xi_j}{\partial t} \end{pmatrix} = \begin{pmatrix} 0 \\ -\rho J \frac{\partial \phi}{\partial x_i} \\ -\rho J \vec{u} \cdot \nabla \phi \end{pmatrix}$$

$U_j = \partial_t \xi_j + \sum_{i=1}^{N} u_i \partial_{x_i} \xi_j$: contravariant velocity in $\xi_j$-direction
$\phi$: gravitational potential

# Unified coord.: Geometric claw

With non-trivial $\partial_\tau \vec{x}$, we should impose conditions on grid metrics $\partial_t \vec{\xi}$ & $\nabla_{\vec{x}} \vec{\xi}$ to have the fulfillment of geometrical conservation law

$$\frac{\partial J}{\partial \tau} + \sum_{j=1}^{N} \frac{\partial}{\partial \xi_j} \left( J \frac{\partial \xi_j}{\partial t} \right) = 0$$

Here we are interested in an approach that is based on the compatibility condition of $\partial_\tau \partial_{\xi_j} x_i$ & $\partial_{\xi_j} \partial_\tau x_i$, *i.e.*,

$$\frac{\partial}{\partial \tau} \left( \frac{\partial x_i}{\partial \xi_j} \right) + \frac{\partial}{\partial \xi_j} \left( -\frac{\partial x_i}{\partial \tau} \right) = 0 \qquad \text{for } i, j = 1, 2, \ldots, N.$$

for unknowns $\partial x_i / \partial \xi_j$, yielding easy computation of $J$ & $\nabla \xi_j$

# Unified coord.: Grid movement

For fluid flow problems, to improve numerical resolution of interfaces (material or slip lines), it is popular to take $\partial_\tau \vec{x}$ as

- Lagrangian case: $\partial_\tau \vec{x} = \vec{u}$ (flow velocity)
- Lagrangian-like case: $\partial_\tau \vec{x} = h_0 \vec{u}$ (pseudo velocity)
  - $h_0 \in [0, 1]$ (fixed piecewise const.)
- Unified coordinate case: $\partial_\tau \vec{x} = h \vec{u}$
  - $h \in [0, 1]$ but is determined from a PDE constraint arising from such as grid-angle or grid-Jacobian preserving condition
- ALE-like case: $\partial_\tau \vec{x} = \vec{\mathcal{U}}$ (arbitrary velocity)

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- Unified coordinate case: $\partial_\tau \vec{x} = h \vec{u}$
  - $h \in [0, 1]$ but is determined from a PDE constraint arising from such as grid-angle or grid-Jacobian preserving condition
- ALE-like case: $\partial_\tau \vec{x} = \vec{\mathcal{U}}$ (arbitrary velocity)

For simplicity, we will focus on Lagrangian-like case

# Unified coord. model: Summary

With $\partial_\tau \vec{x} = h_0 \vec{u}$, unified coordinate model for single component compressible flow problems consists of

- Physical balance laws

$$\frac{\partial}{\partial \tau}\begin{pmatrix} \rho J \\ \rho J u_i \\ J E \end{pmatrix} + \sum_{j=1}^{N} \frac{\partial}{\partial \xi_j} J \begin{pmatrix} \rho U_j \\ \rho u_i U_j + p \frac{\partial \xi_j}{\partial x_i} \\ E U_j + p U_j - p \frac{\partial \xi_j}{\partial t} \end{pmatrix} = \begin{pmatrix} 0 \\ -\rho J \frac{\partial \phi}{\partial x_i} \\ -\rho J \vec{u} \cdot \nabla \phi \end{pmatrix}$$

- Geometrical conservation laws

$$\frac{\partial}{\partial \tau}\left(\frac{\partial x_i}{\partial \xi_j}\right) + \frac{\partial}{\partial \xi_j}\left(-\frac{\partial x_i}{\partial \tau}\right) = 0 \qquad \text{for } i, j = 1, 2, \ldots, N.$$

- pressure law $p(\rho, e)$

# Unified coord. model: Remarks

For unified coordinate models mentioned above, it is known that

- when $h_0 = 0$ (Eulerian case), the model is hyperbolic
- when $h_0 = 1$ (Lagrangian case), the model is weakly hyperbolic (do not possess complete eigenvectors)
- when $h_0 \in (0, 1)$ (Lagrangian-like case), the model is hyperbolic

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If a prescribed velocity $\vec{u}_b$ for a rigid body motion is included in the formulation *i.e.*, with $\partial_\tau \vec{x} = h_0 \vec{u} + \vec{u}_b$, we should be able to use the model to solve some moving body problems as well.

# Unified coord. model: Review

The work presented here is related to

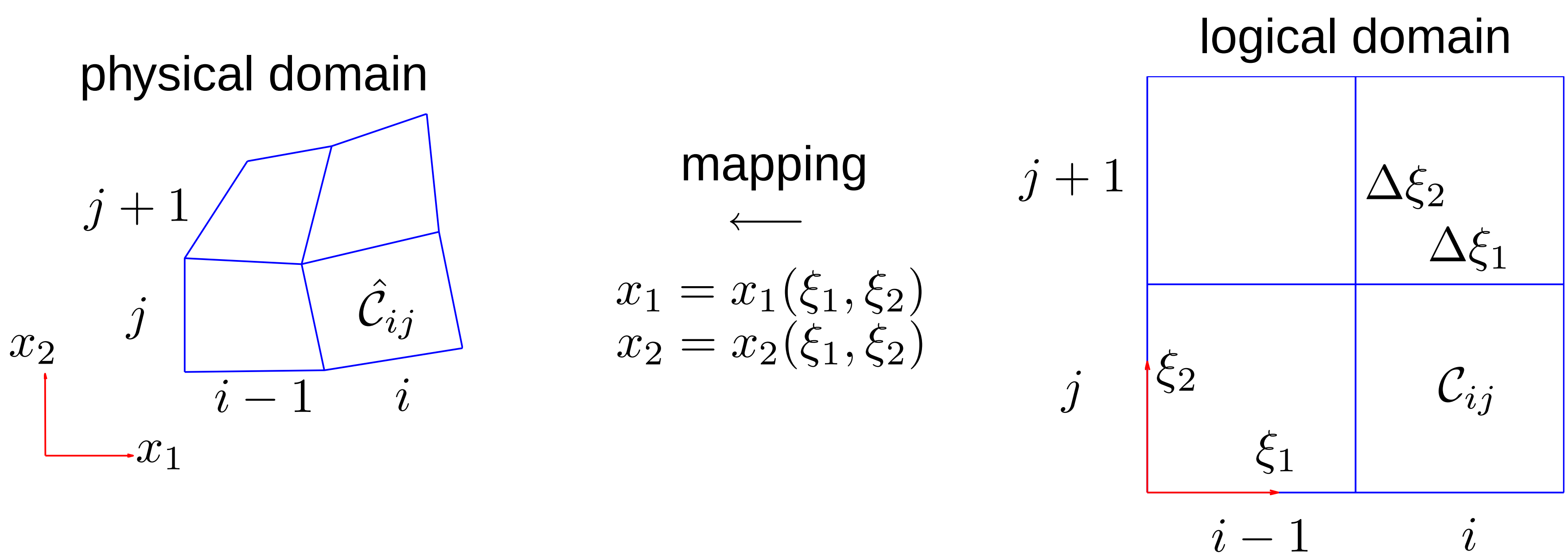
- W.H. Hui *et al.* (JCP 1999, 2001): Unified coordinated system for Euler equations
- W.H. Hui (Comm. Phys. Sci. 2007): Unified coordinate system in CFD
- C. Jin & K. Xu (JCP 2007): Moving grid gas-kinetic method for viscous flow
- P. Jia *et al.* (Computers and Fluids 2006) Unified coordinated system for compressible milti-material flow
- Z. Chen *et al.* (Int J. Numer. Meth Fluids 2007): Wave speed based moving coordinates for compressible flow equations

# Finite volume approximation

Employ finite volume formulation of numerical solution

$$Q_{ijk}^{n} \approx \frac{1}{\Delta\xi_1 \Delta\xi_2 \Delta\xi_3} \int_{C_{ijk}} q(\xi_1, \xi_2, \xi_3, \tau_n)\, dV$$

that gives approximate value of cell average of solution $q$ over cell $C_{ijk}$ at time $\tau_n$ (sample case in $2D$ shown below)



# Finite volume (Cont.)

In three dimensions $N = 3$, equations to be solved take

$$\frac{\partial}{\partial \tau} q\left(\vec{\xi},\ \tau\right) + \sum_{j=1}^{N} \frac{\partial}{\partial \xi_j} f_j\left(q,\ \vec{\xi}\right) = \psi\left(q,\ \vec{\xi}\right)$$

A simple dimensional-splitting method based on $f$-wave approach of LeVeque *et al.* is used for approximation, *i.e.*,

- Solve one-dimensional Riemann problem normal 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

# Finite volume (Cont.)

Basic steps of a dimensional-splitting scheme

- $\xi_1$-sweeps: solve

$$\frac{\partial q}{\partial \tau} + f_1\left(\frac{\partial}{\partial \xi}, q, \nabla\vec{\xi}\right) = 0 \quad \text{updating} \quad Q^n_{ijk} \text{ to } \quad Q^*_{ijk}$$

- $\xi_2$-sweeps: solve

$$\frac{\partial q}{\partial \tau} + f_2\left(\frac{\partial}{\partial \xi_2}, q, \nabla\vec{\xi}\right) = 0 \quad \text{updating} \quad Q^*_{ijk} \text{ to } \quad Q^{**}_{ijk}$$

- $\xi_3$-sweeps: solve

$$\frac{\partial q}{\partial \tau} + f_3\left(\frac{\partial}{\partial \xi_3}, q, \nabla\vec{\xi}\right) = 0 \quad \text{updating} \quad Q^{**}_{ijk} \text{ to } \quad Q^{n+1}_{ijk}$$

# Finite volume (Cont.)

Consider $\xi_1$-sweeps, for example,

- First order update is

$$Q^*_{ijk} = Q^n_{ijk} - \frac{\Delta\tau}{\Delta\xi_1}\left[\left(\mathcal{A}_1^+\Delta Q\right)^n_{i-1/2,jk} + \left(\mathcal{A}_1^-\Delta Q\right)^n_{i+1/2,jk}\right]$$

  with the fluctuations

$$(\mathcal{A}_1^+\Delta Q)^n_{i-1/2,jk} = \sum_{m:(\lambda_{1,m})^n_{i-1/2,jk}>0} (\mathcal{Z}_{1,m})^n_{i-1/2,jk}$$

  and

$$(\mathcal{A}_1^-\Delta Q)^n_{i+1/2,jk} = \sum_{m:(\lambda_{1,m})^n_{i+1/2,jk}<0} (\mathcal{Z}_{1,m})^n_{i+1/2,jk}$$

  $(\lambda_{1,m})^n_{\iota-1/2,jk}$ & $(\mathcal{Z}_{1,m})^n_{\iota-1/2,jk}$ are in turn wave speed and $f$-waves for the $m$th family of the $1$D Riemann problem solutions

# Finite volume (Cont.)

- High resolution correction is

$$Q^*_{ijk} := Q^*_{ijk} - \frac{\Delta\tau}{\Delta\xi_1}\left[\left(\tilde{\mathcal{F}}_1\right)^n_{i+1/2,jk} - \left(\tilde{\mathcal{F}}_1\right)^n_{i-1/2,jk}\right]$$

with $\quad (\tilde{\mathcal{F}}_1)^n_{i-1/2,jk} = \frac{1}{2}\sum_{m=1}^{m_w}\left[\text{sign}\left(\lambda_{1,m}\right)\left(1 - \frac{\Delta\tau}{\Delta\xi_1}\left|\lambda_{1,m}\right|\right)\tilde{\mathcal{Z}}_{1,m}\right]^n_{i-1/2,jk}$

$\tilde{\mathcal{Z}}_{\iota,m}$ is a limited value of $\mathcal{Z}_{\iota,m}$

It is clear that this method belongs to a class of upwind schemes, and is stable when the typical CFL (Courant-Friedrichs-Lewy) condition:

$$\nu = \frac{\Delta\tau \max_m\left(\lambda_{1,m}, \lambda_{2,m}, \lambda_{3,m}\right)}{\min\left(\Delta\xi_1, \Delta\xi_2, \Delta\xi_3\right)} \le 1,$$

# Finite volume: Riemann problem

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

$$\begin{cases} \dfrac{\partial q_{i-1,jk}}{\partial \tau} + f_1\left(\dfrac{\partial}{\partial \xi_1}, q_{i-1,jk}\right) = 0 & \text{if } \xi_1 < (\xi_1)_{i-1/2}, \\ \dfrac{\partial q_{ijk}}{\partial \tau} + f_1\left(\dfrac{\partial}{\partial \xi_1}, q_{ijk}\right) = 0 & \text{if } \xi_1 > (\xi_1)_{i-1/2}, \end{cases}$$

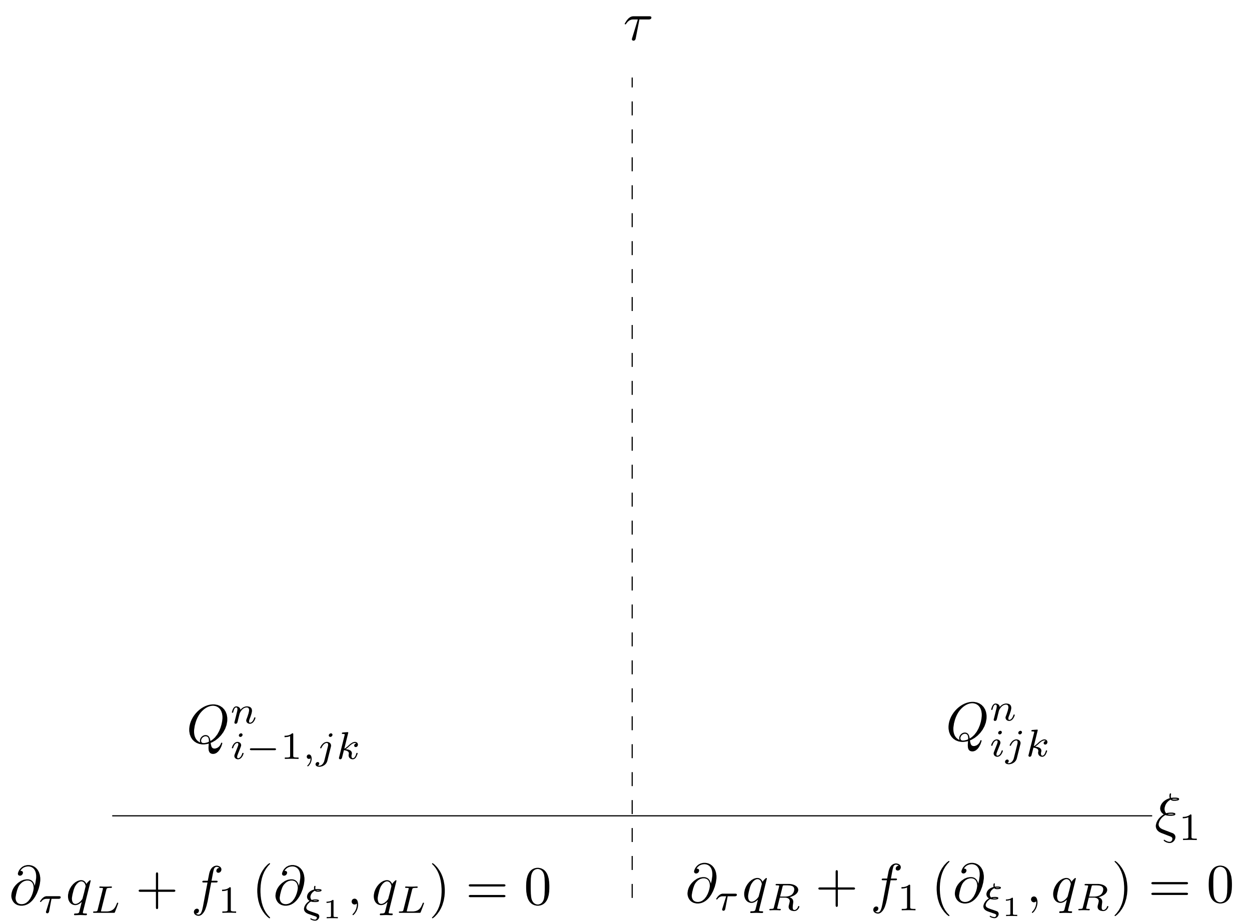
together with piecewise constant initial data

$$q(\xi_1, 0) = \begin{cases} Q^n_{i-1,jk} & \text{for} \quad \xi < \xi_{i-1/2} \\ Q^n_{ijk} & \text{for} \quad \xi > \xi_{i-1/2} \end{cases}$$

$$q_{ijk} = q\big|_{(\partial_{\xi_2}\vec{x},\, \partial_{\xi_3}\vec{x})_{ijk}} \qquad \& \qquad f_1(\partial_{\xi_1}, q_{ijk}) = f_1(\partial_{\xi_1}, q)\big|_{(\partial_{\xi_2}\vec{x},\, \partial_{\xi_3}\vec{x})_{ijk}}$$

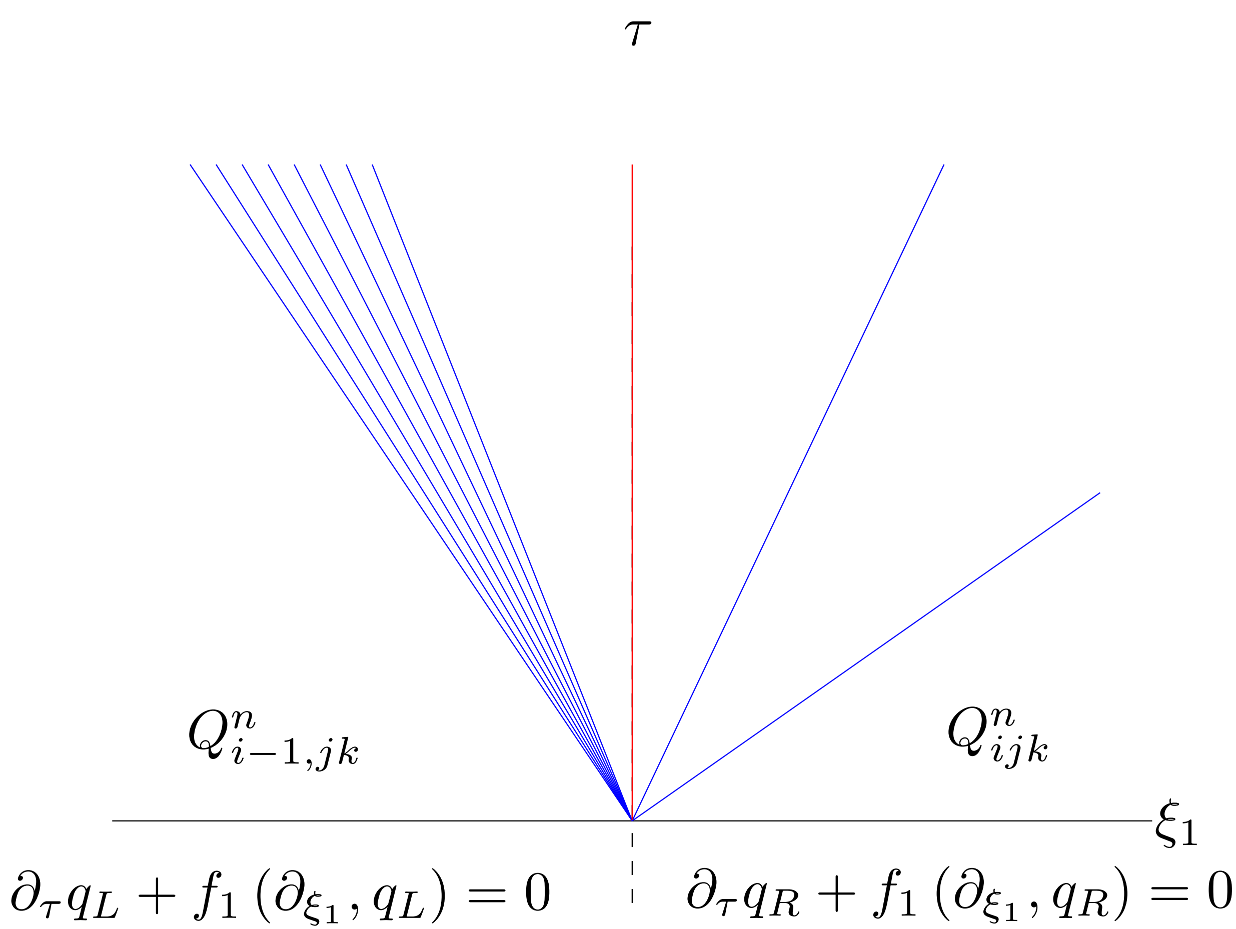
# Riemann problem

Riemann problem at time $\tau = 0$



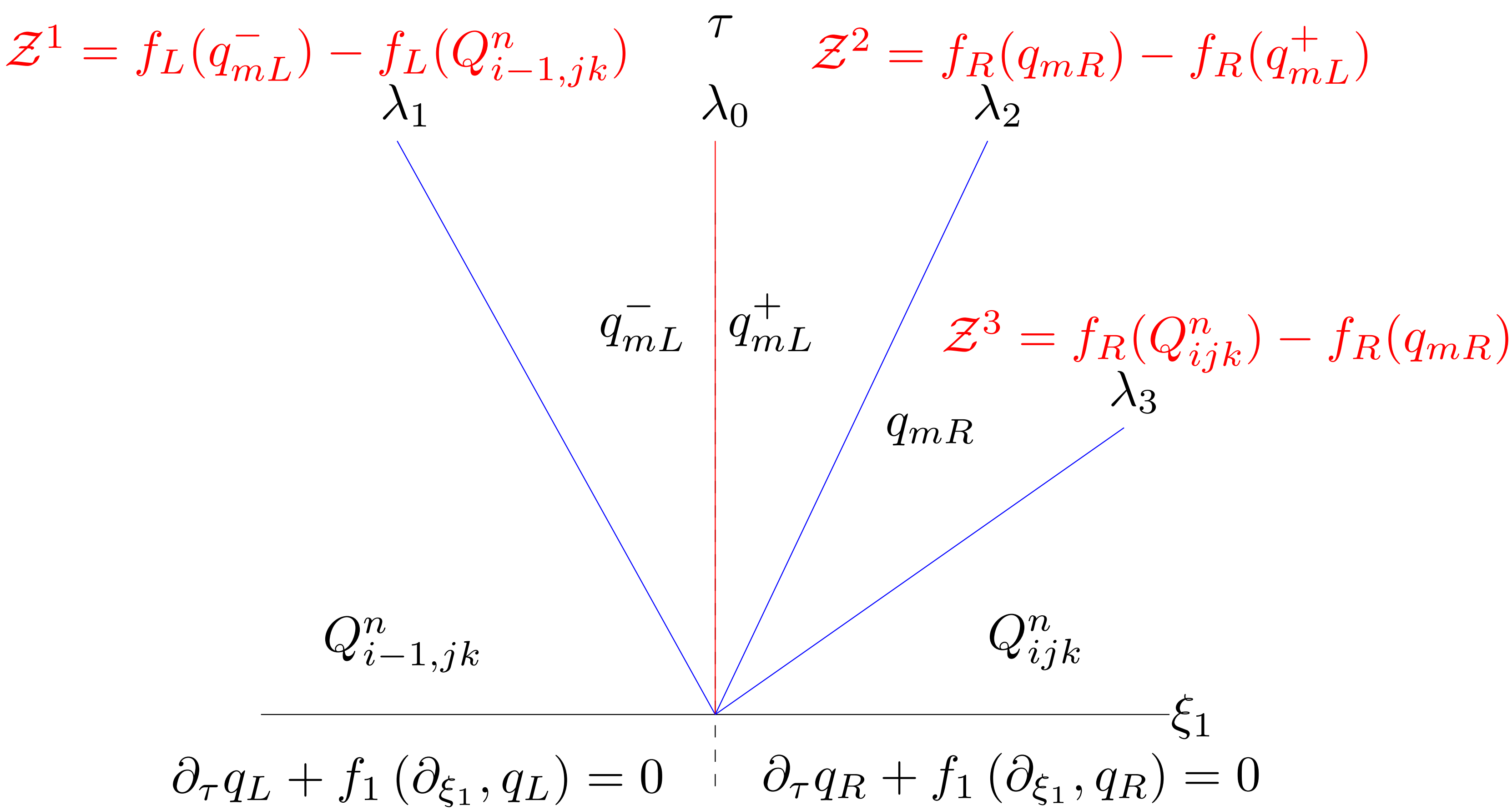
# Riemann problem

Exact Riemann solution: basic structure



# Riemann problem

Shock-only approximate Riemann solution: basic structure



# Shock-only Riemann solver

- Rotate velocity vector in Riemann data normal to each cell interface
- Find midstate velocity $\upsilon_m$ and pressure $p_m$ by solving

$$\phi(p_m) = \upsilon_{mR}(p_m) - \upsilon_{mL}(p_m) = 0$$

derived from Rankine-Hugoniot relation iteratively, where

$$\upsilon_{mL}(p) = \upsilon_L - \frac{p - p_L}{M_L(p)}, \qquad \upsilon_{mR}(p) = \upsilon_R + \frac{p - p_R}{M_R(p)}$$

- Propagation speed of each moving discontinuity is determined by

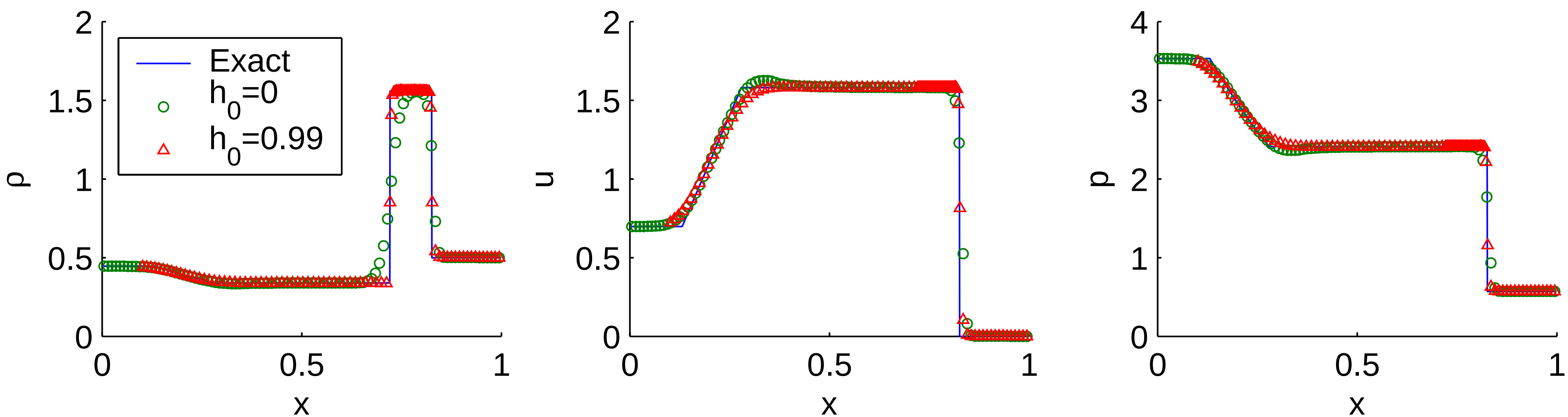
$$(\lambda_{1,1})_{i-1/2,jk} = \left[(1-h_0)\upsilon_m - \frac{M_L(p_m)}{\rho_{mL}(p_m)}\right] \left|\nabla_{\vec{X}}\xi_1\right|_{i-1/2,jk}$$

$$(\lambda_{1,2})_{i-1/2,jk} = (1-h_0)\upsilon_m \left|\nabla_{\vec{X}}\xi_1\right|_{i-1/2,jk}$$

$$(\lambda_{1,3})_{i-1/2,jk} = \left[(1-h_0)\upsilon_m + \frac{M_R(p_m)}{\rho_{mR}(p_m)}\right] \left|\nabla_{\vec{X}}\xi_1\right|_{i-1/2,jk}$$

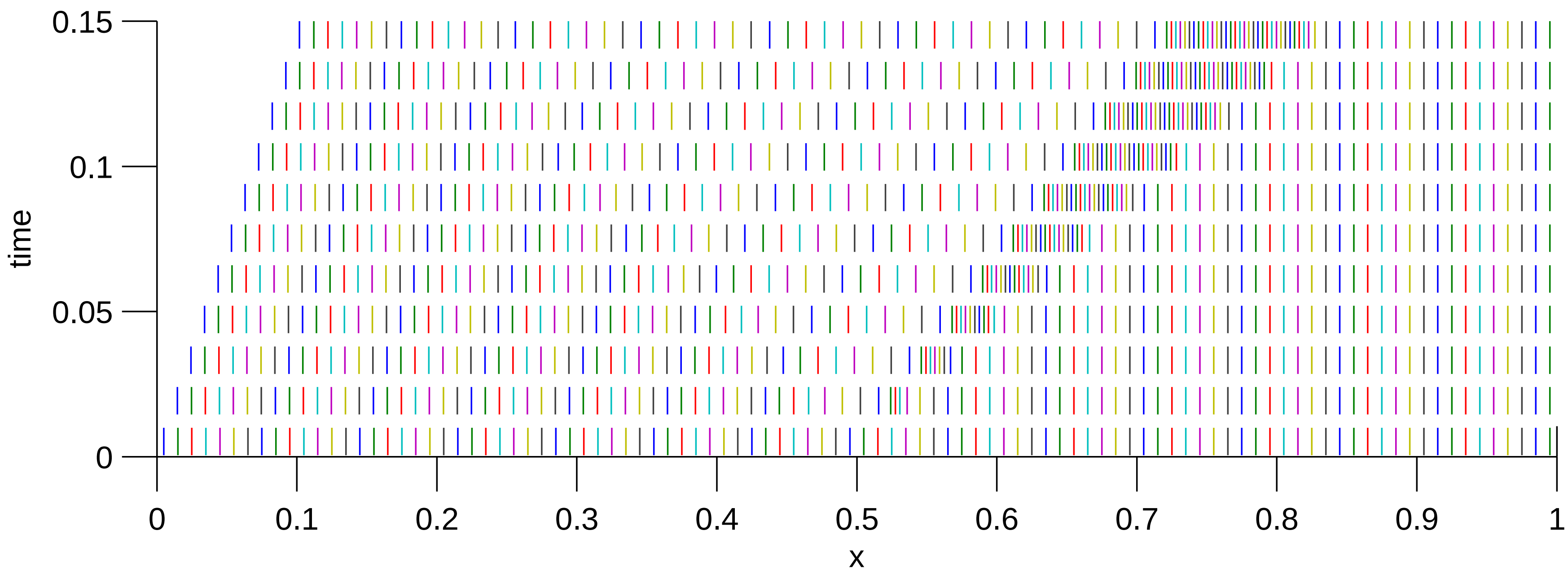
# Lax's Riemann problem

- Ideal gas EOS with $\gamma = 1.4$
- $h_0 = 0$ 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

- Ideal gas EOS with $\gamma = 1.4$
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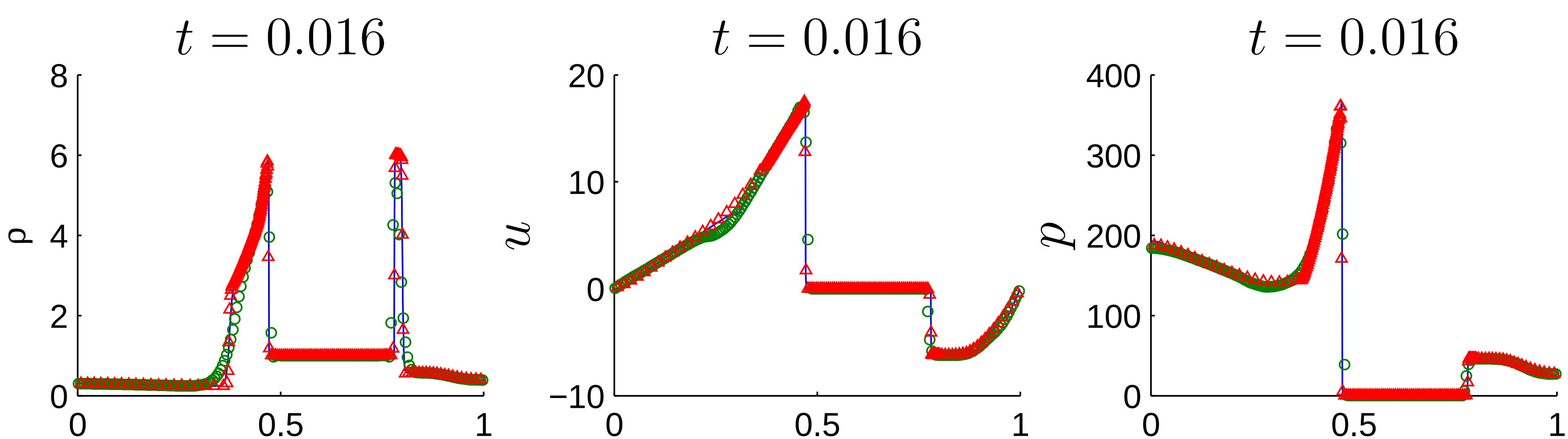

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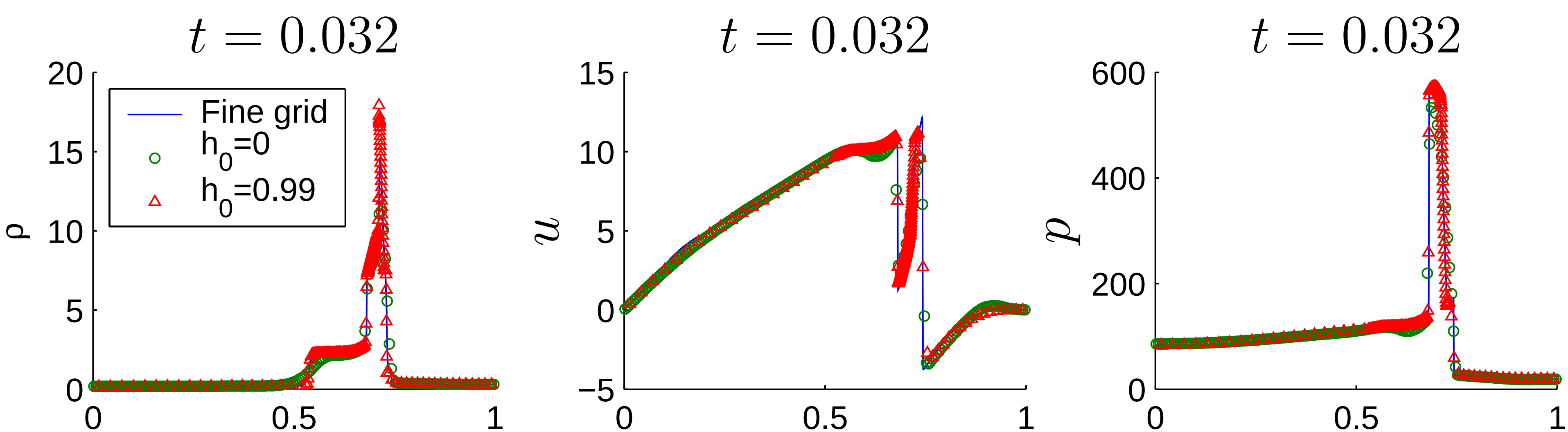

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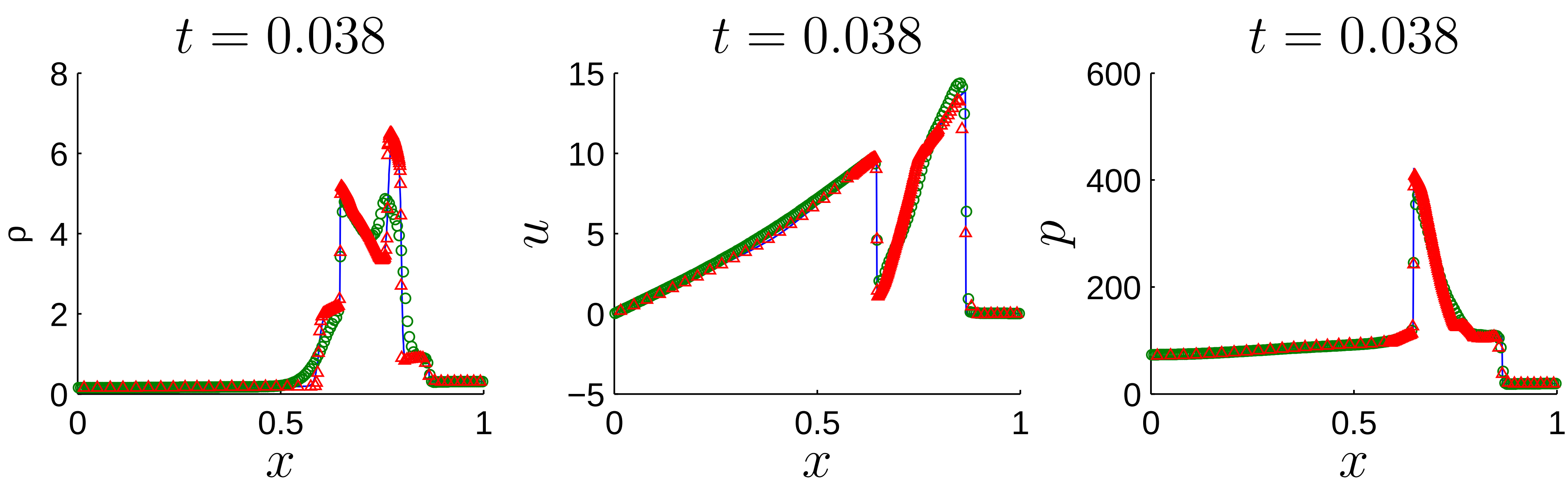

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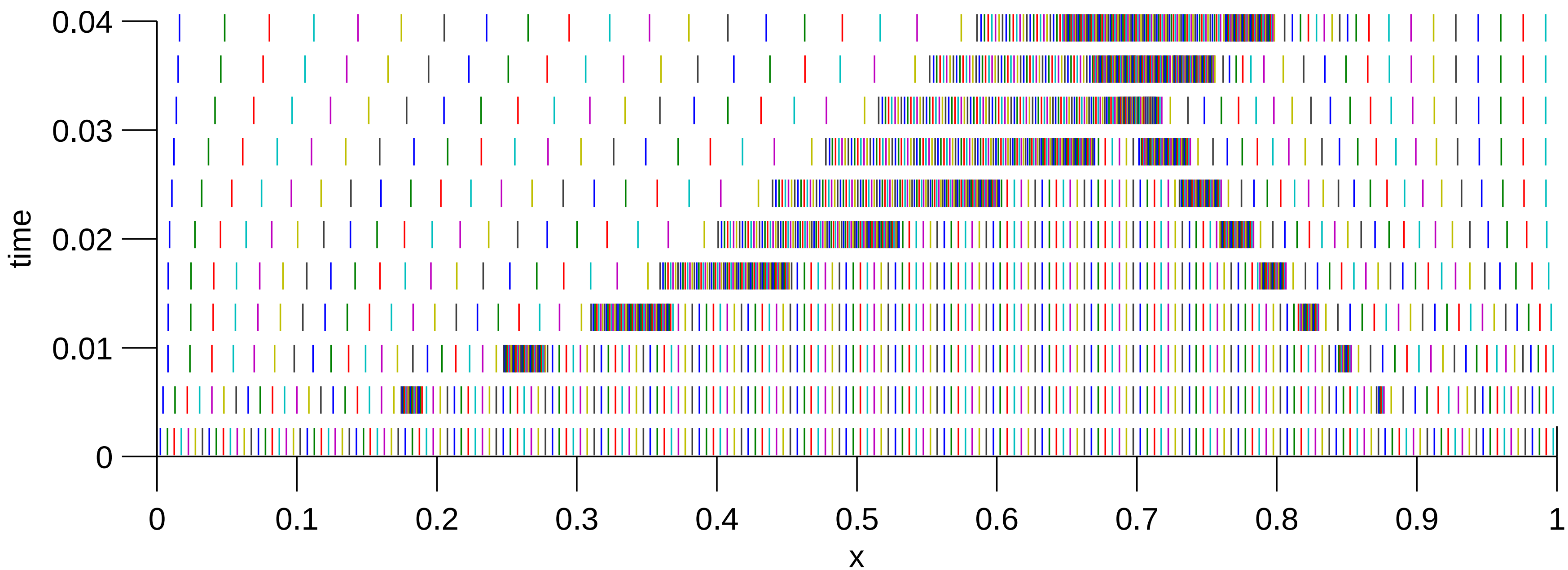
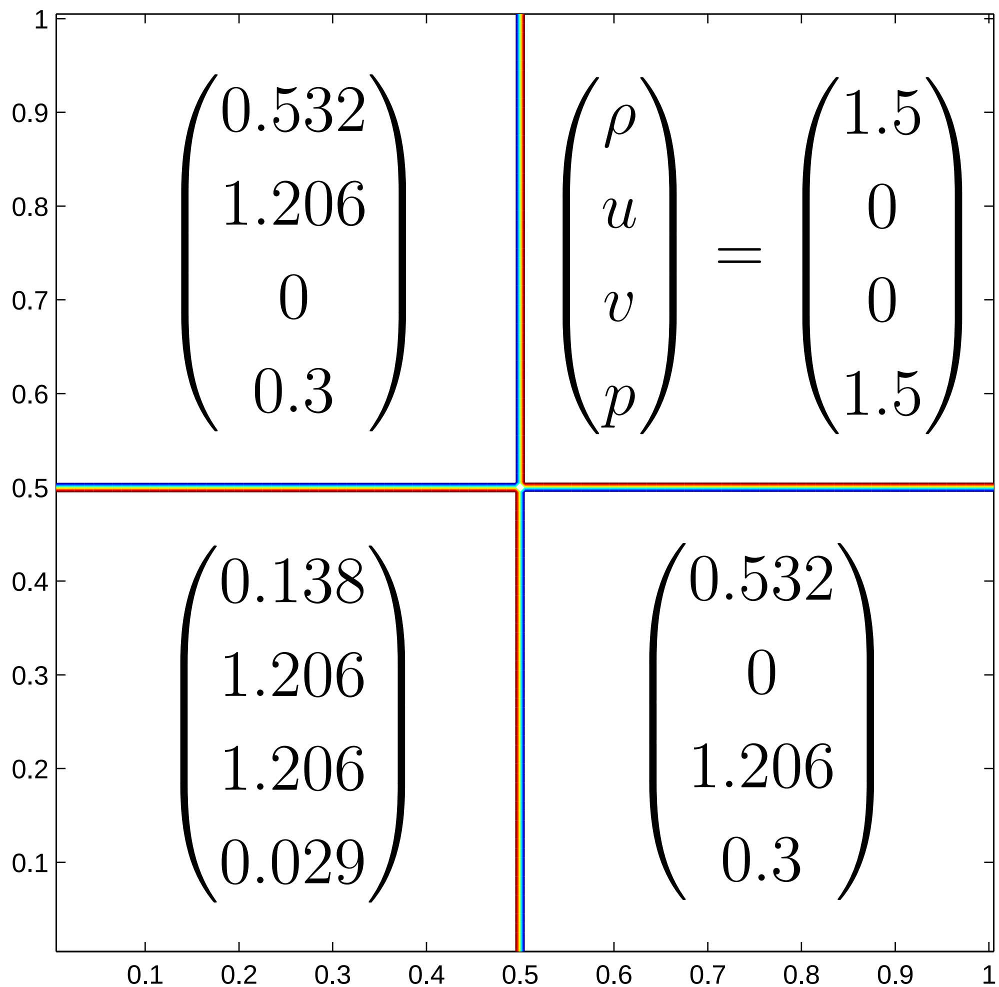


# 2D Riemann problem

With initial 4-shock wave pattern

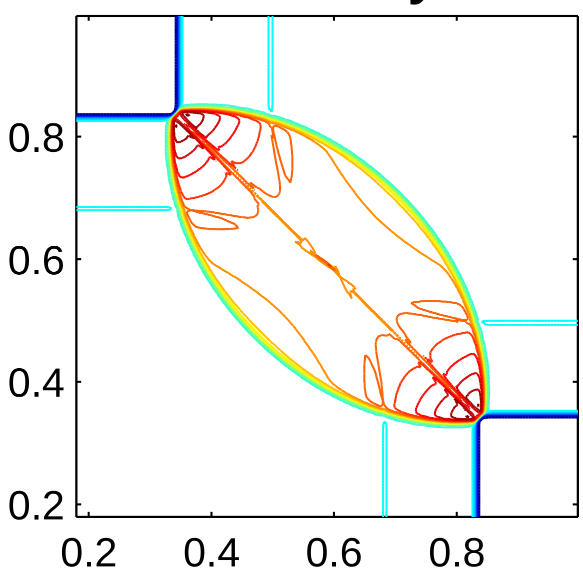


# $2$D Riemann problem

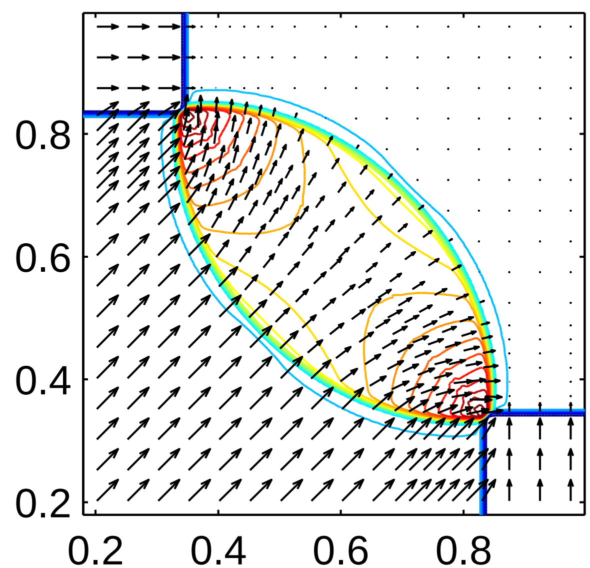
With initial $4$-shock wave pattern

- Lagrangian-like result
  - Occurrence of simple Mach reflection

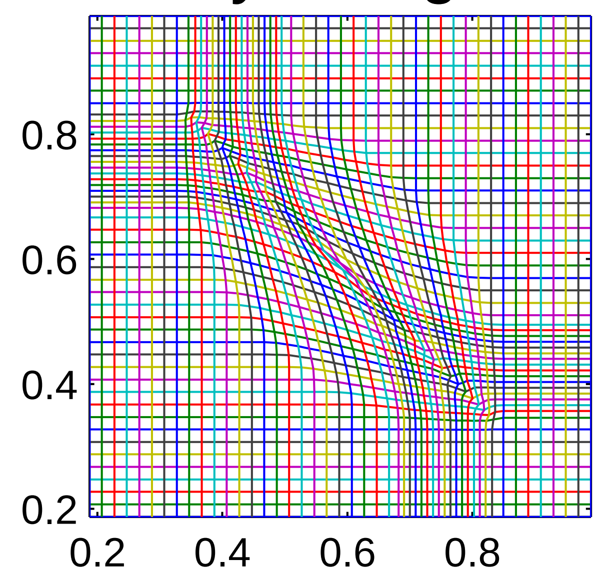
Density




Pressure



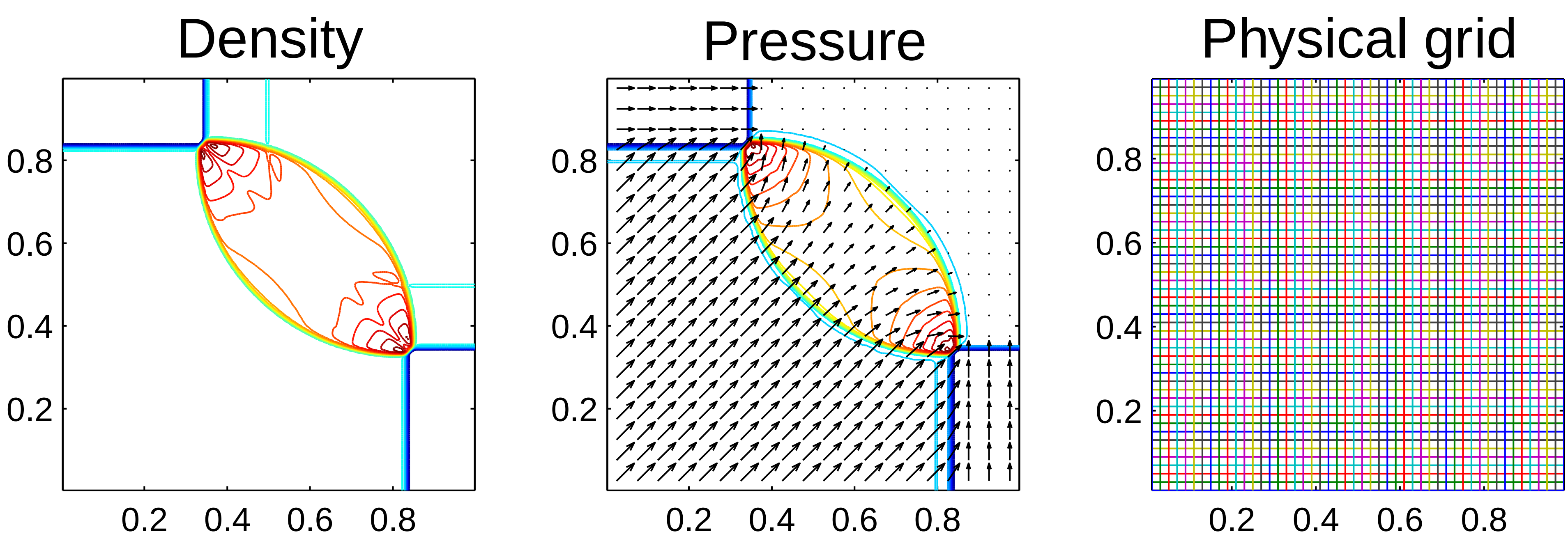

Physical grid



# $2$D Riemann problem

With initial $4$-shock wave pattern

- Eulerian result
  - Poor resolution around simple Mach reflection



# Reduced $2$-phase model

- Physical balance laws

$$\frac{\partial}{\partial \tau}\begin{pmatrix} \rho J \\ \rho J u_i \\ J E \end{pmatrix} + \sum_{j=1}^{N} \frac{\partial}{\partial \xi_j} J \begin{pmatrix} \rho U_j \\ \rho u_i U_j + p \frac{\partial \xi_j}{\partial x_i} \\ E U_j + p U_j - p \frac{\partial \xi_j}{\partial t} \end{pmatrix} = \begin{pmatrix} 0 \\ -\rho J \frac{\partial \phi}{\partial x_i} \\ -\rho J \vec{u} \cdot \nabla \phi \end{pmatrix}$$

- Geometric conservation laws

$$\frac{\partial}{\partial \tau}\left(\frac{\partial x_i}{\partial \xi_j}\right) + \frac{\partial}{\partial \xi_j}\left(-\frac{\partial x_i}{\partial \tau}\right) = 0 \qquad \text{for } i, j = 1, 2, \ldots, N.$$

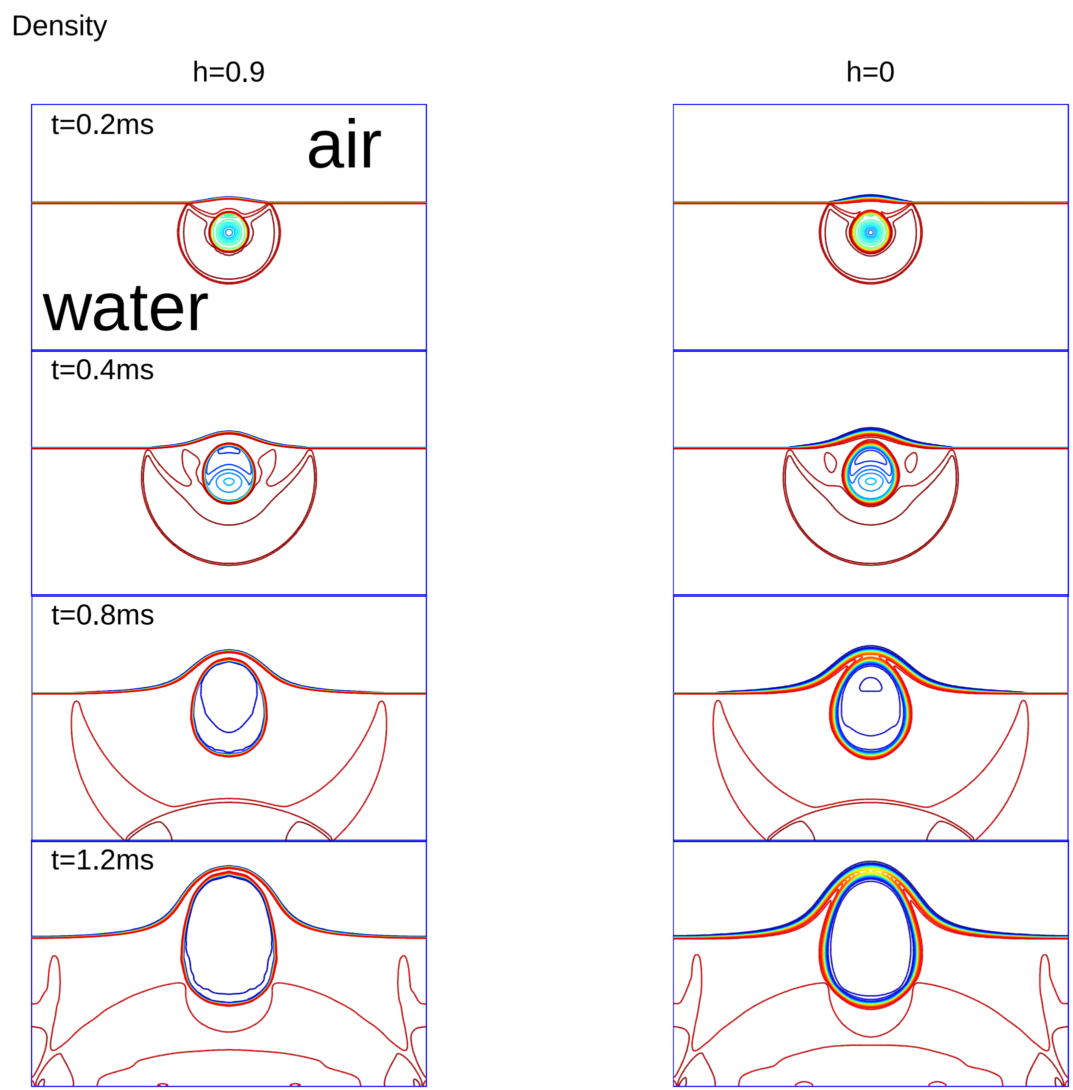
- Volume fraction transport equation

$$\frac{\partial \alpha}{\partial \tau} + \sum_{j=1}^{N} U_j \frac{\partial \alpha}{\partial \xi_j} = 0$$

- Moving grid condition $\partial_\tau \vec{x} = h_0 \vec{u}$ & pressure law $p(\rho, e, \alpha)$

# Underwater explosions

- Solution Comparison between $h_0 = 0.9$ & $h_0 = 0$



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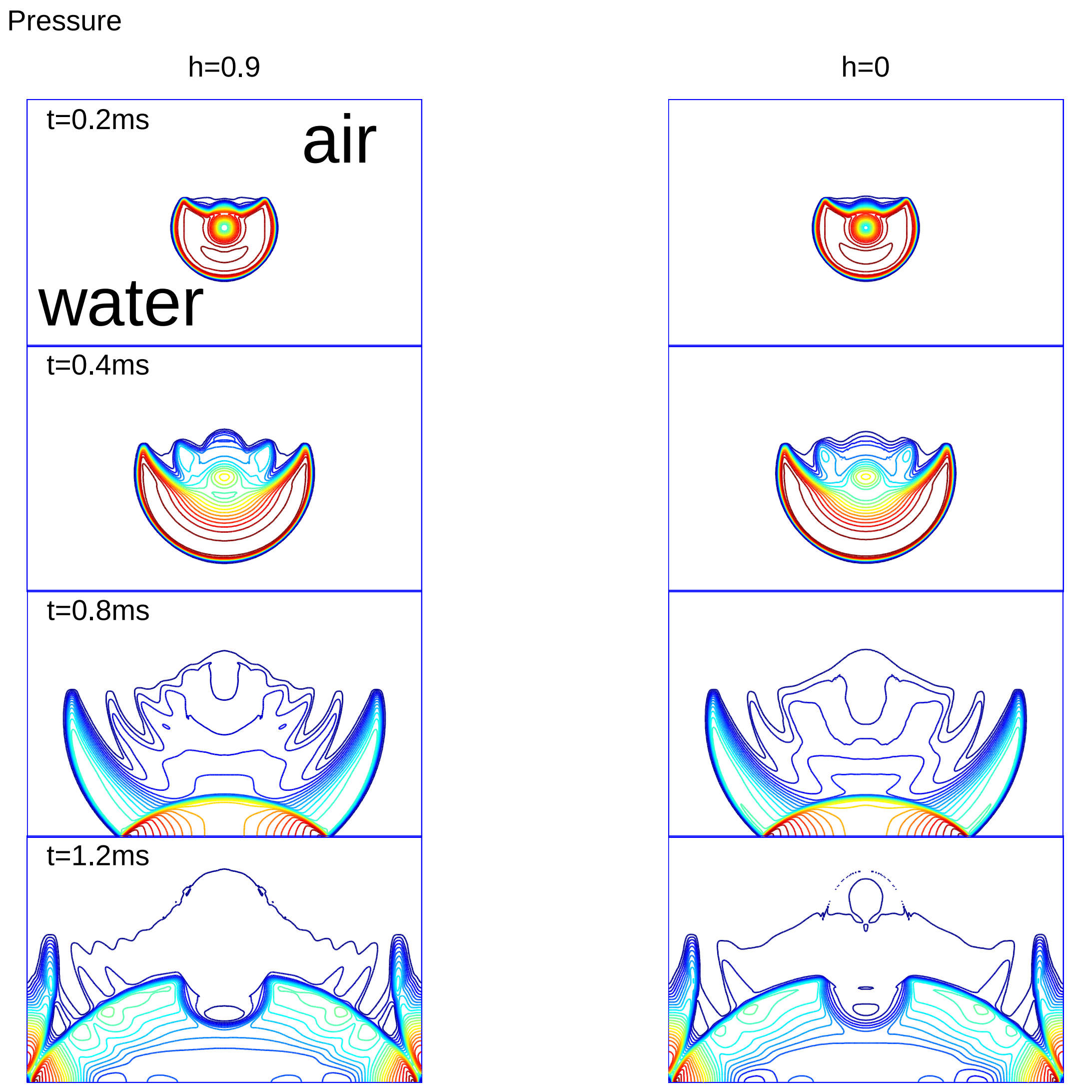
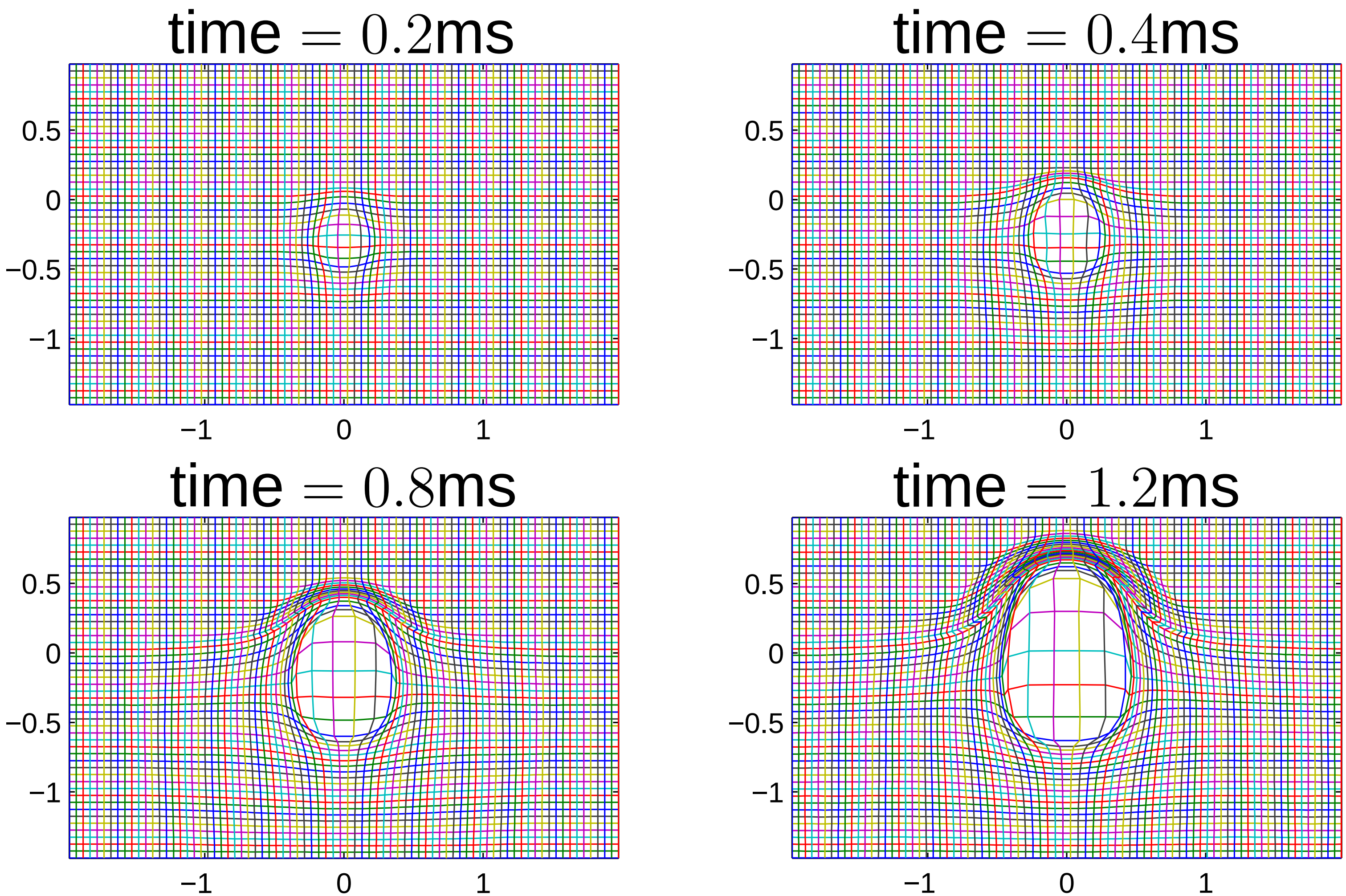


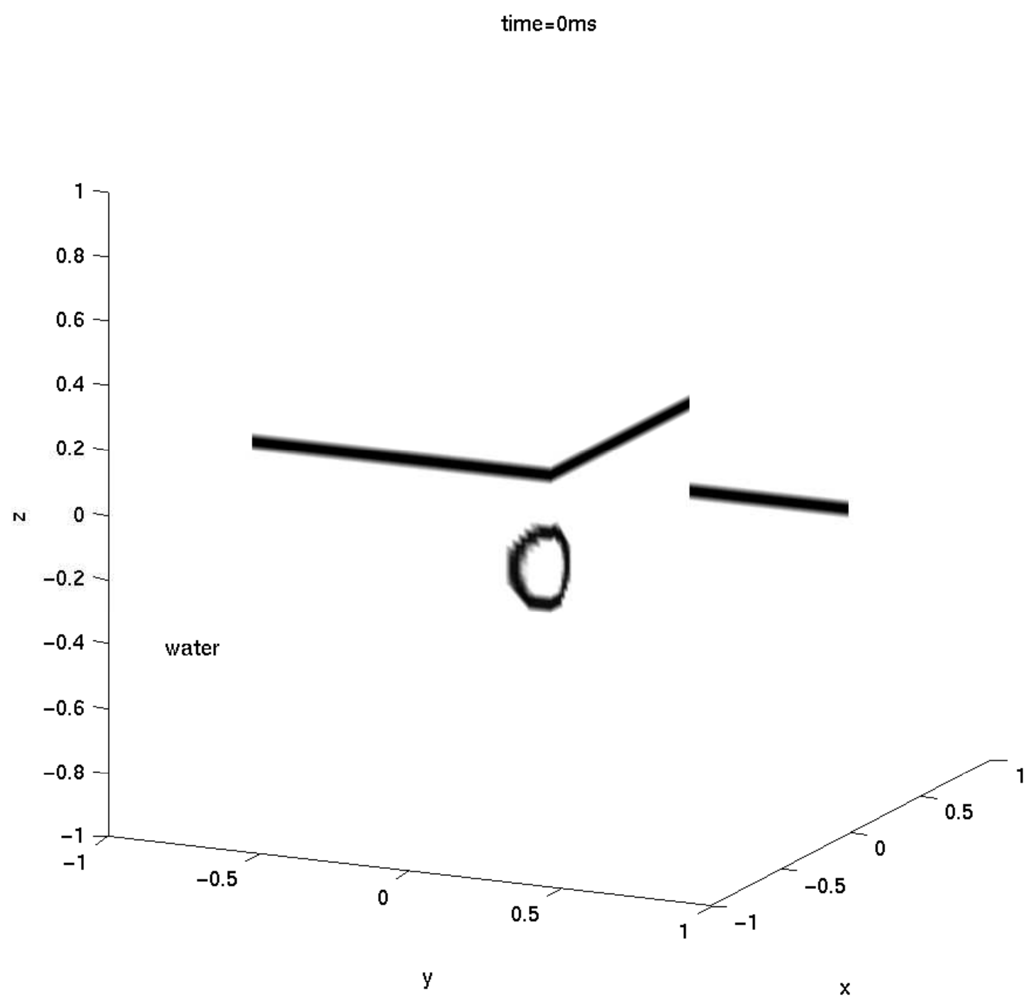
# Underwater explosions (Cont.)

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



# 3D underwater explosions

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



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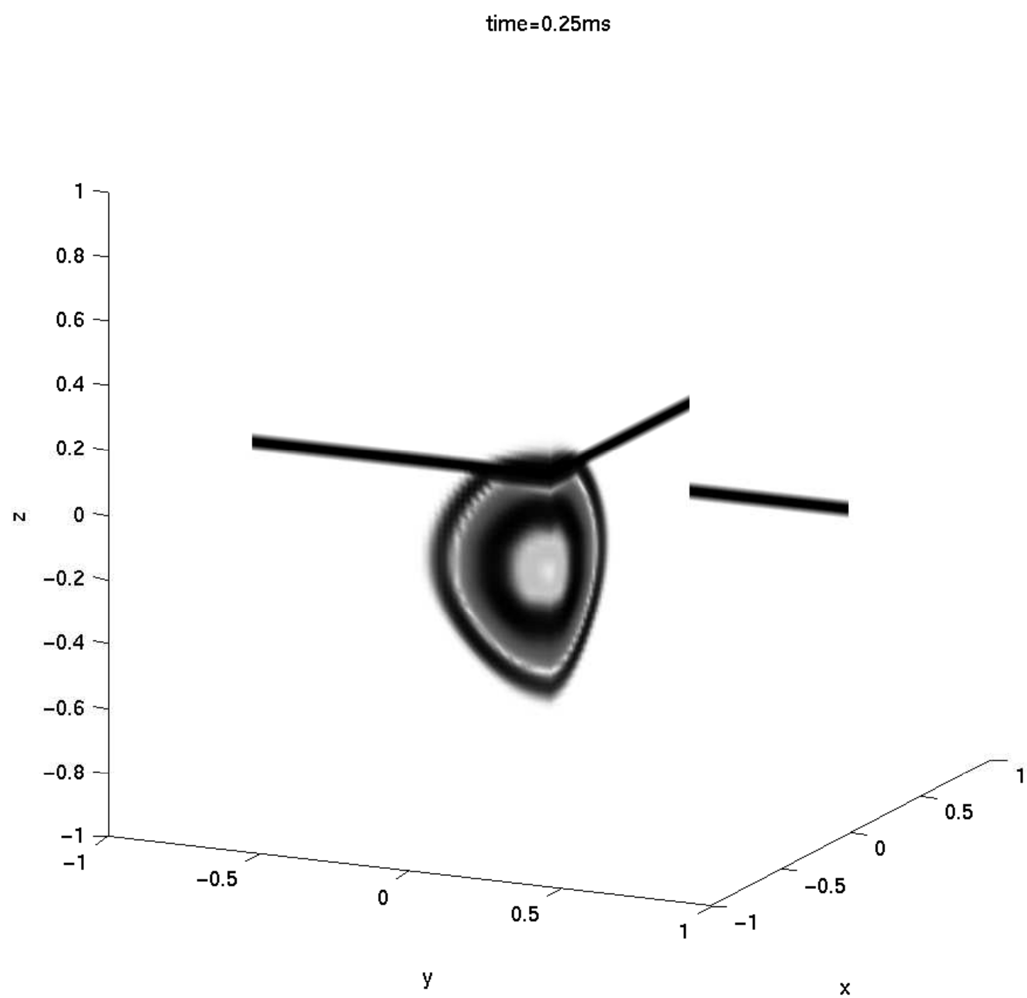

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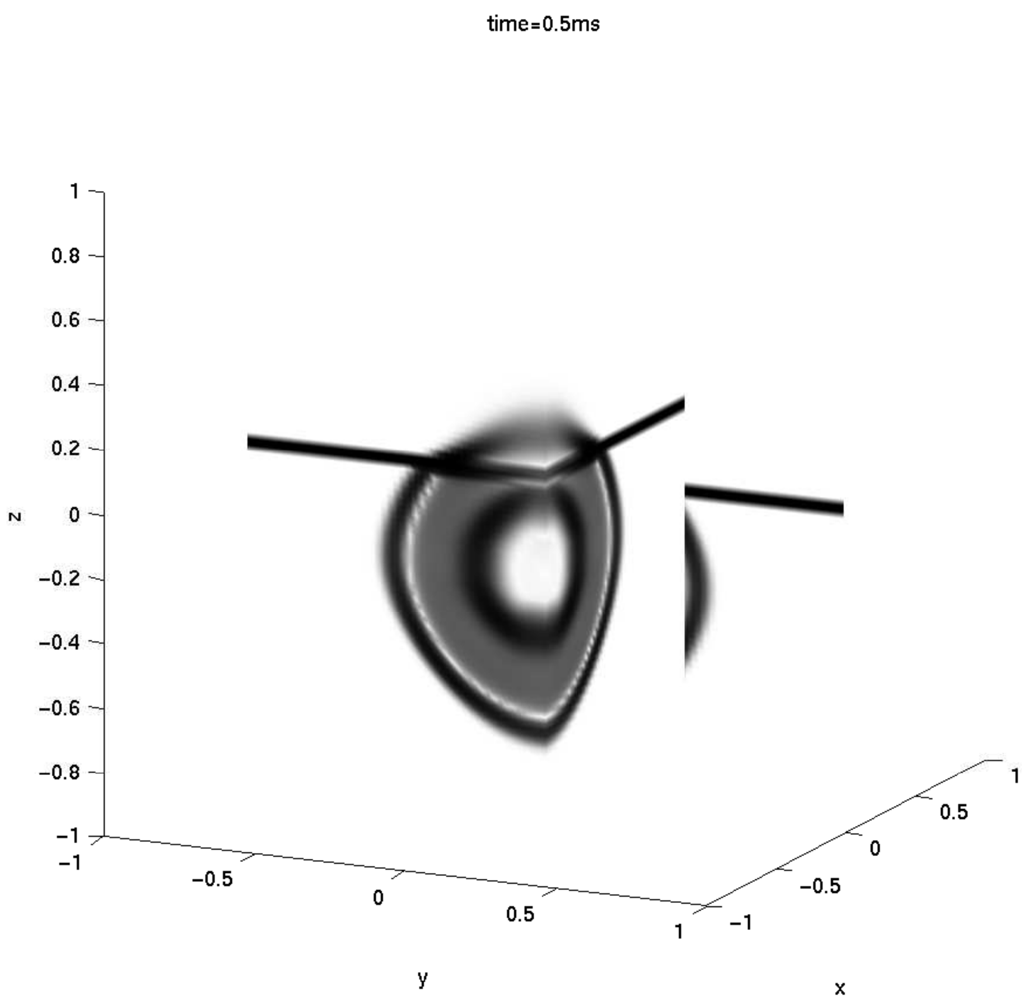

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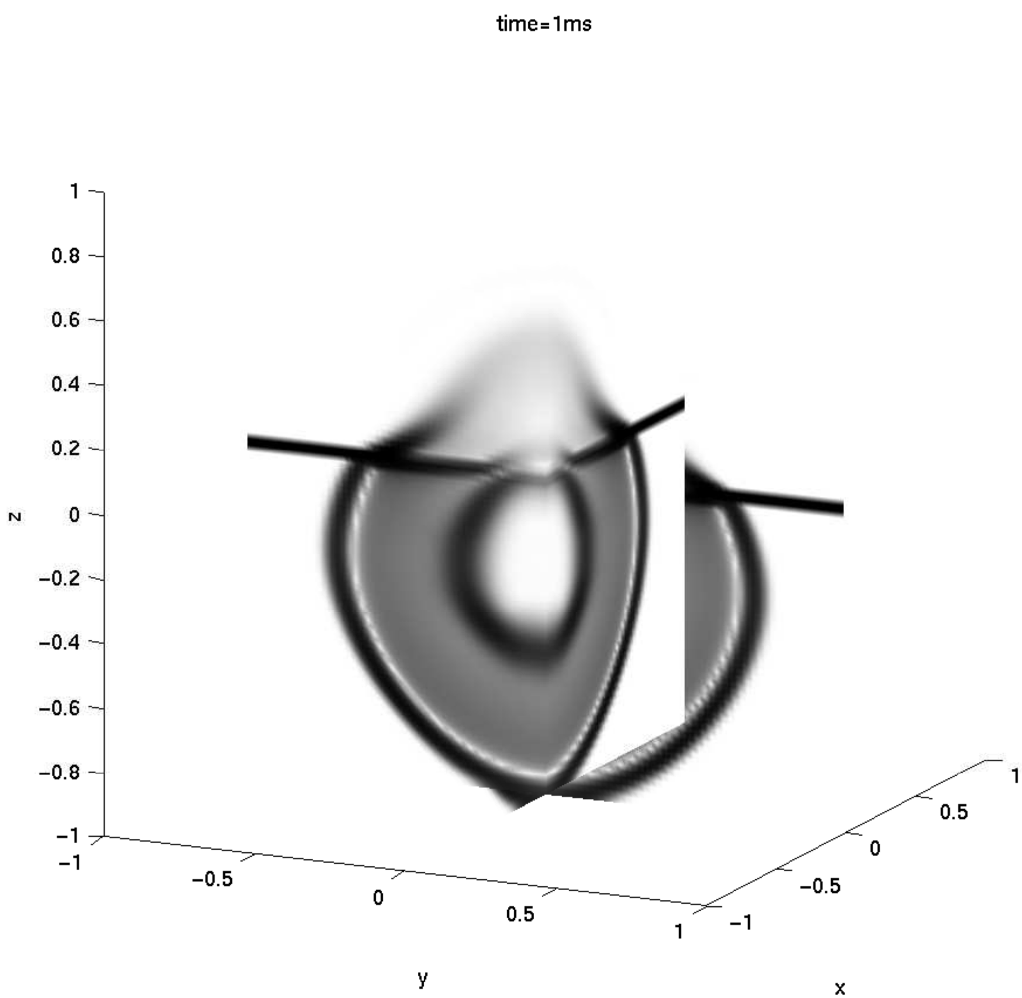

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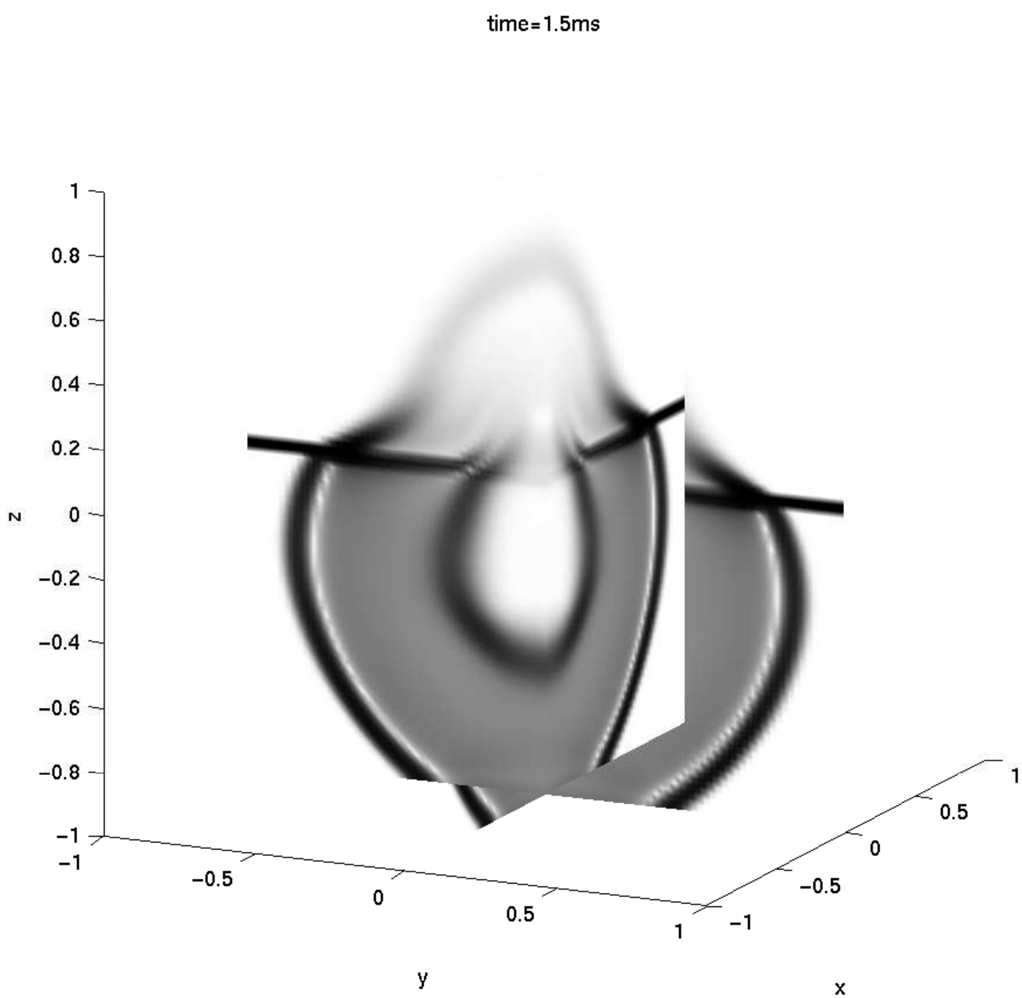
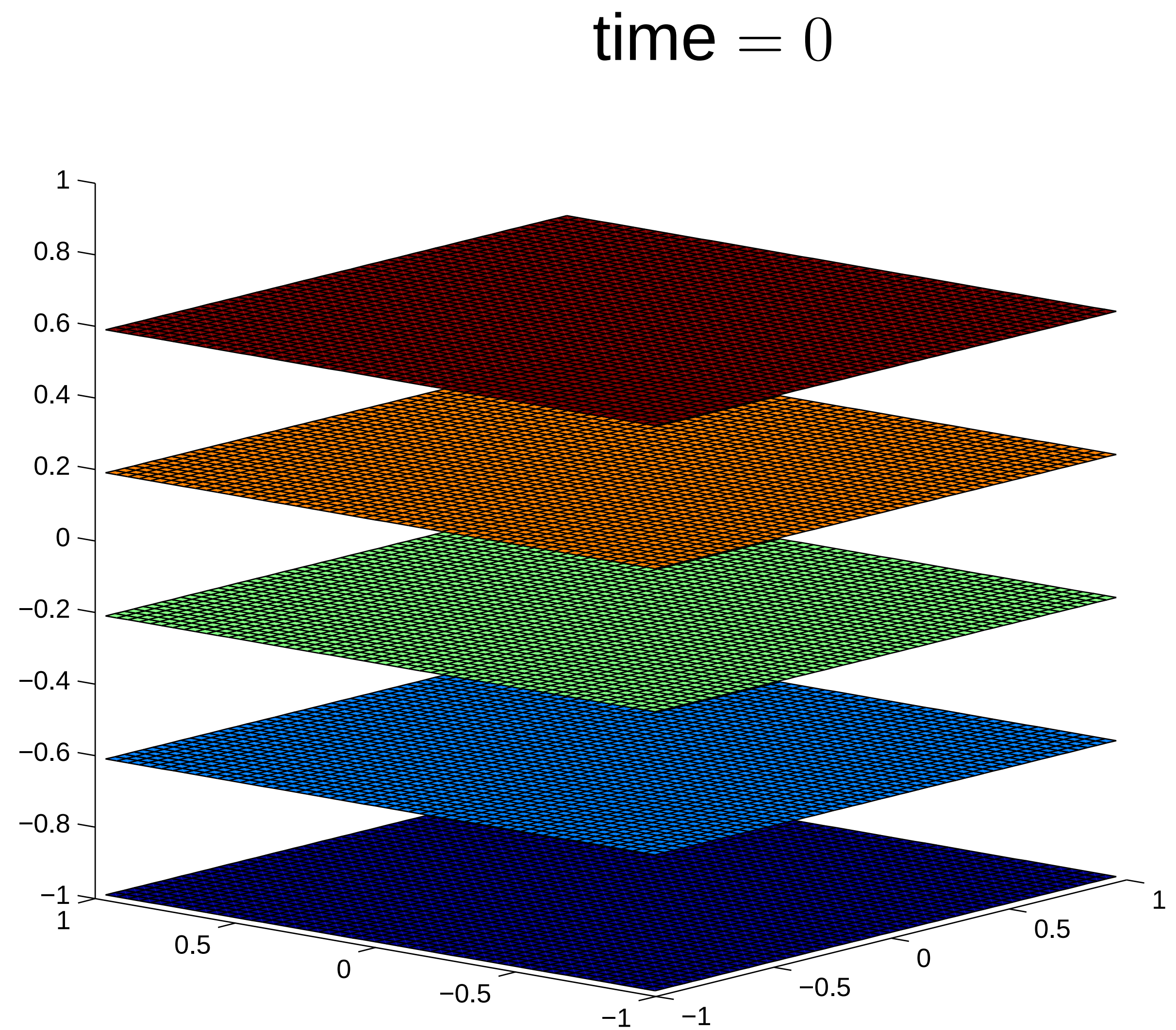


# 3D underwater explosions (Cont.)

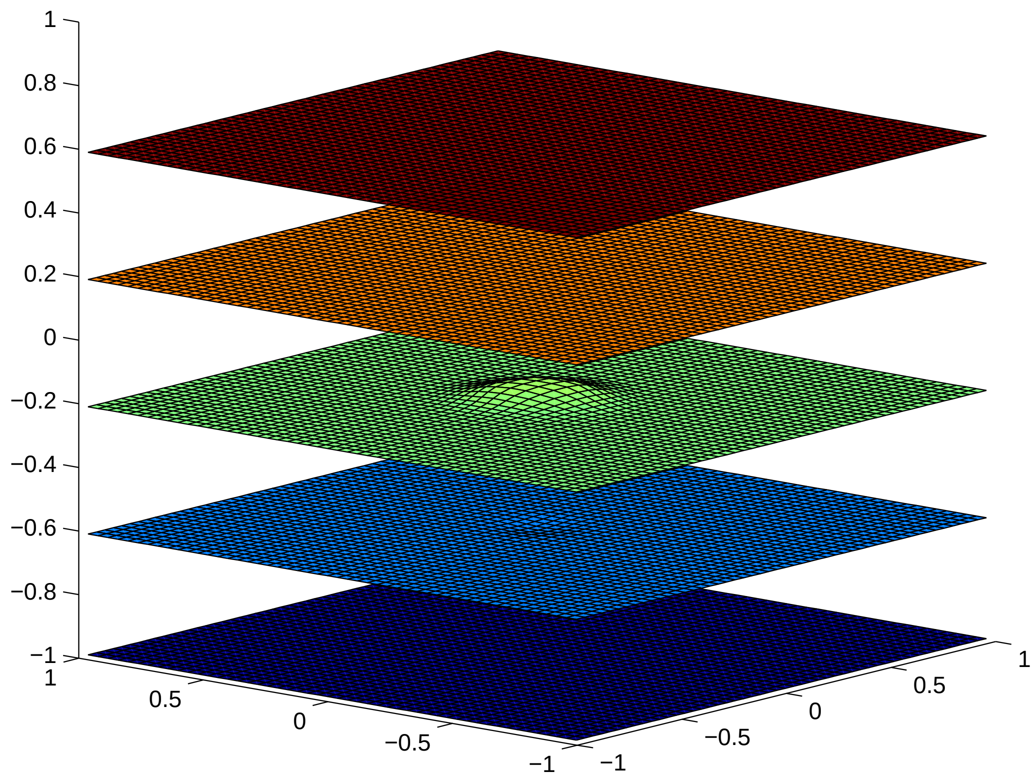
- Grid system (coarsen by factor $2$) with $h_0 = 0.6$



# 3D underwater explosions (Cont.)

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

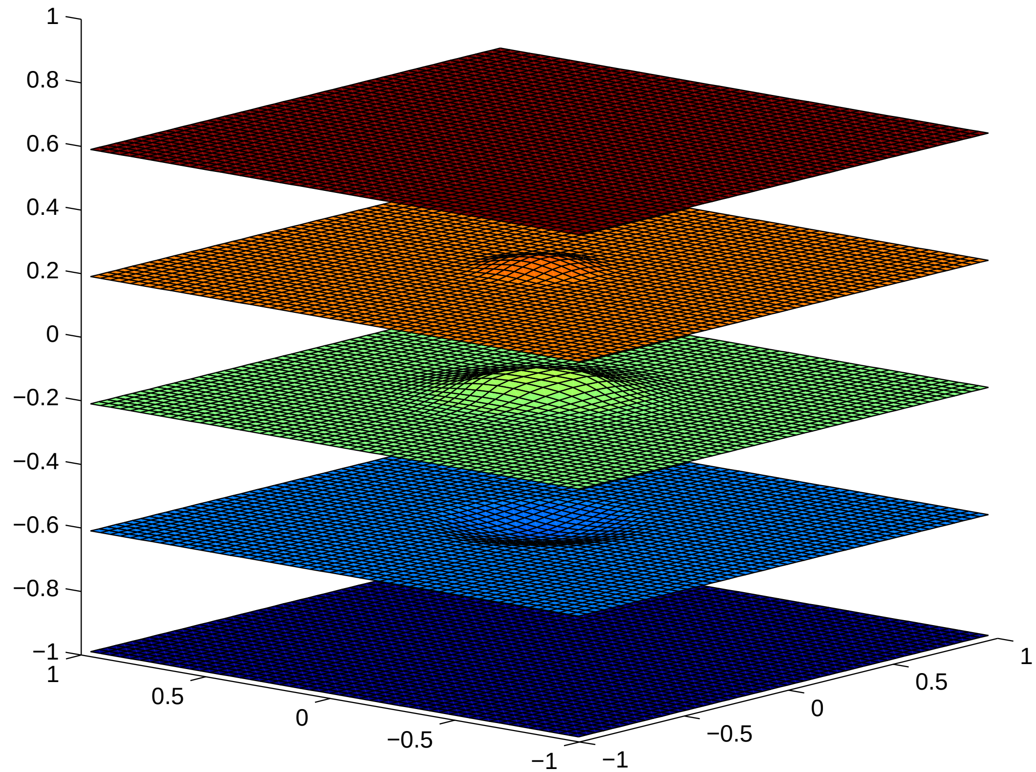
time $= 0.25$ms



# 3D underwater explosions (Cont.)

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

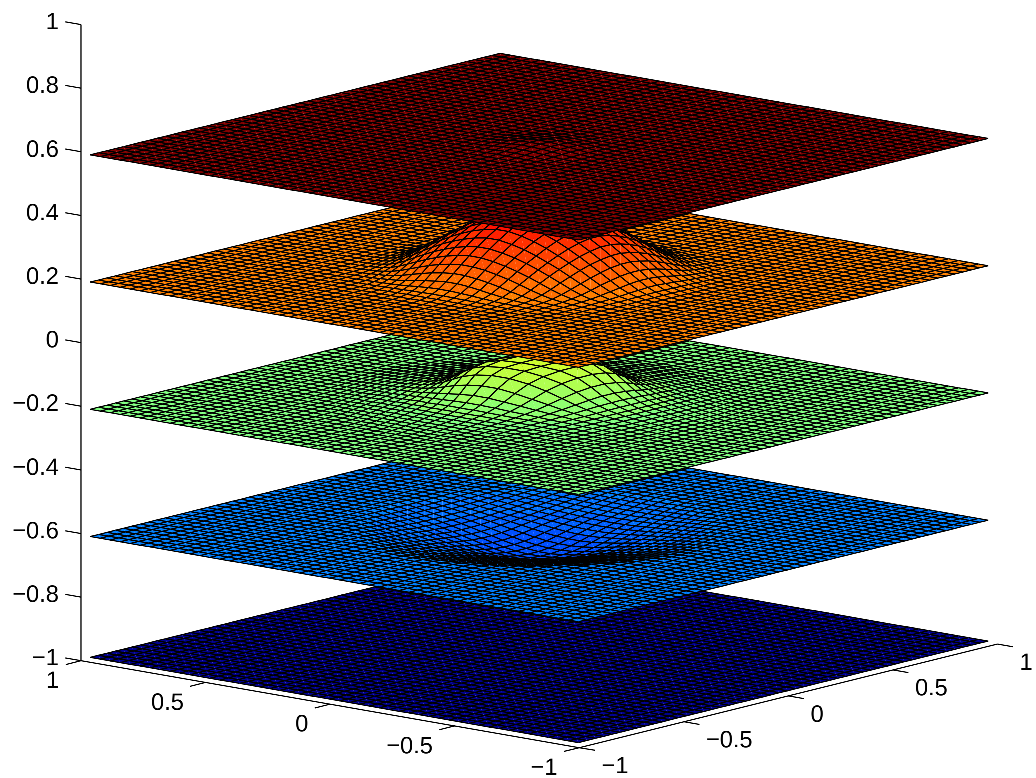
time $= 0.5$ms



# 3D underwater explosions (Cont.)

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

time $= 1.0$ms



# 3D underwater explosions (Cont.)

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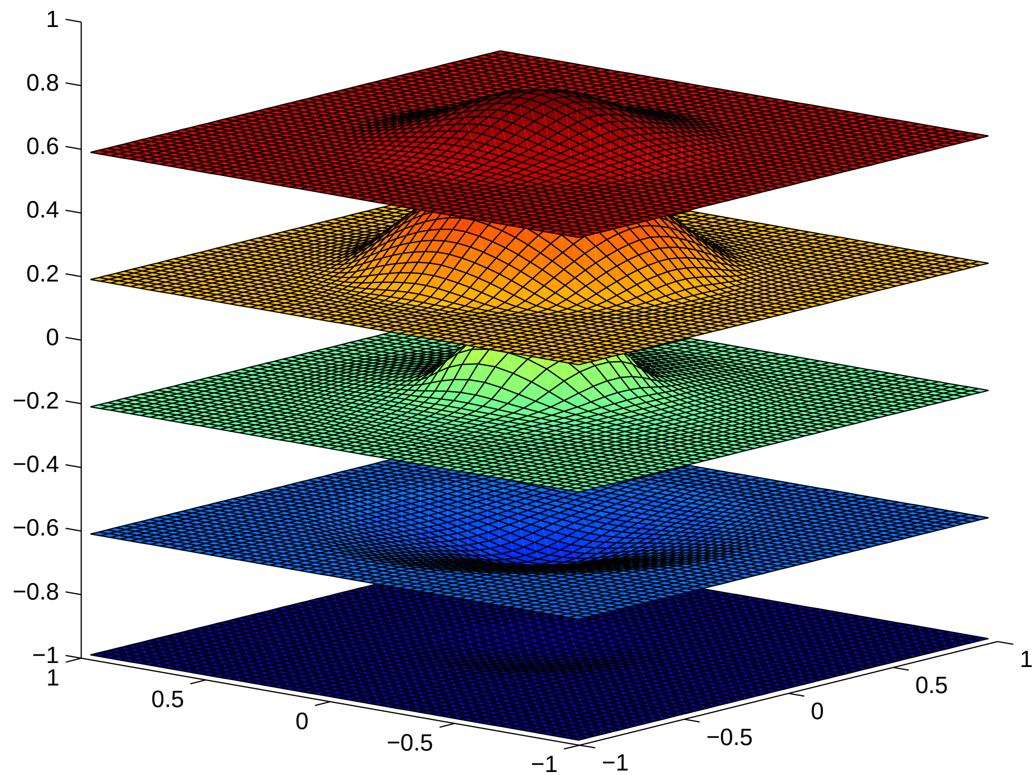
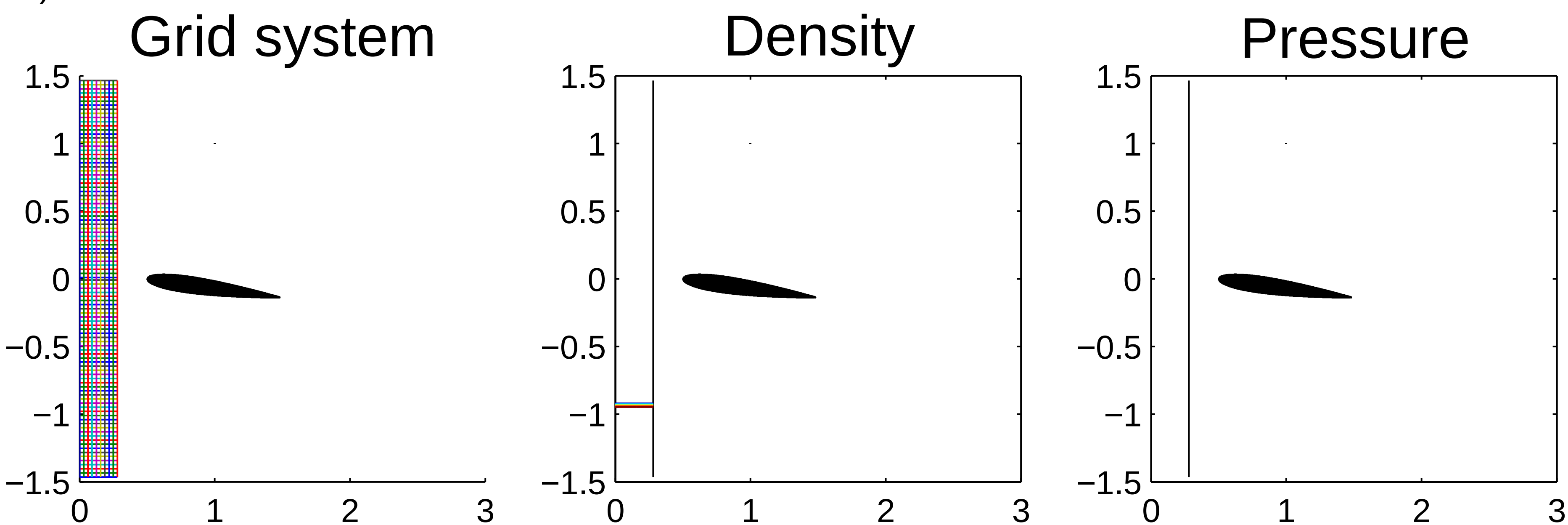
time $= 1.5$ms



# Automatic time-marching grid

- Supersonic NACA0012 over heavier gas

a)



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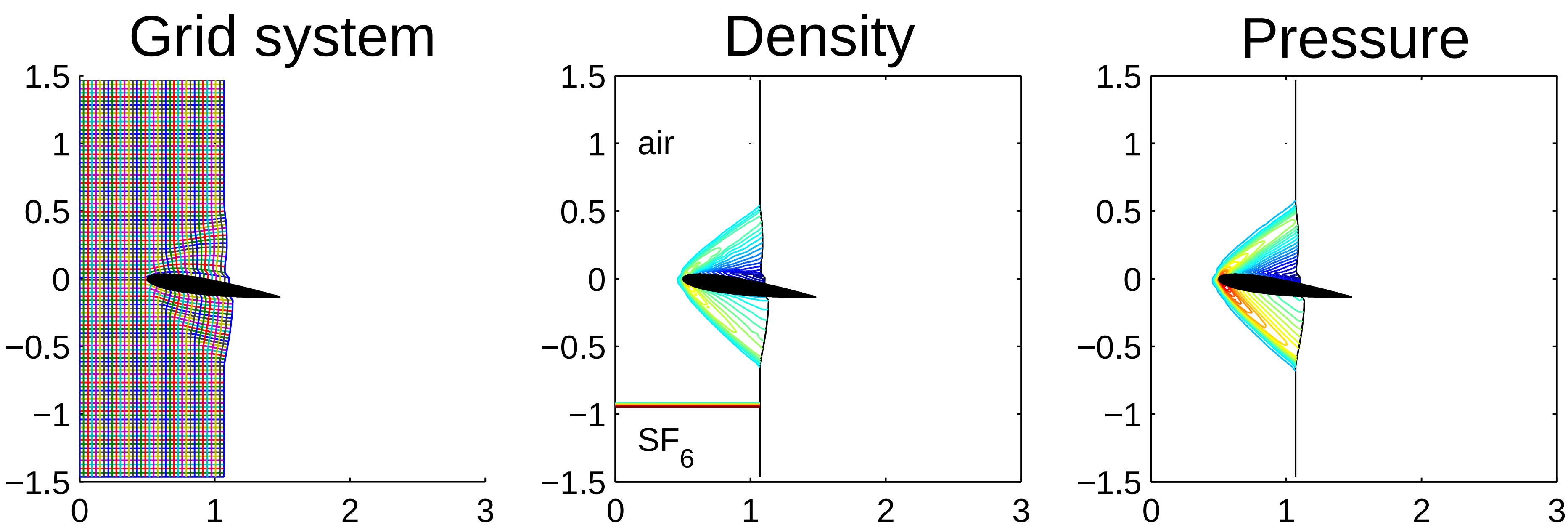
b)



# Automatic time-marching grid

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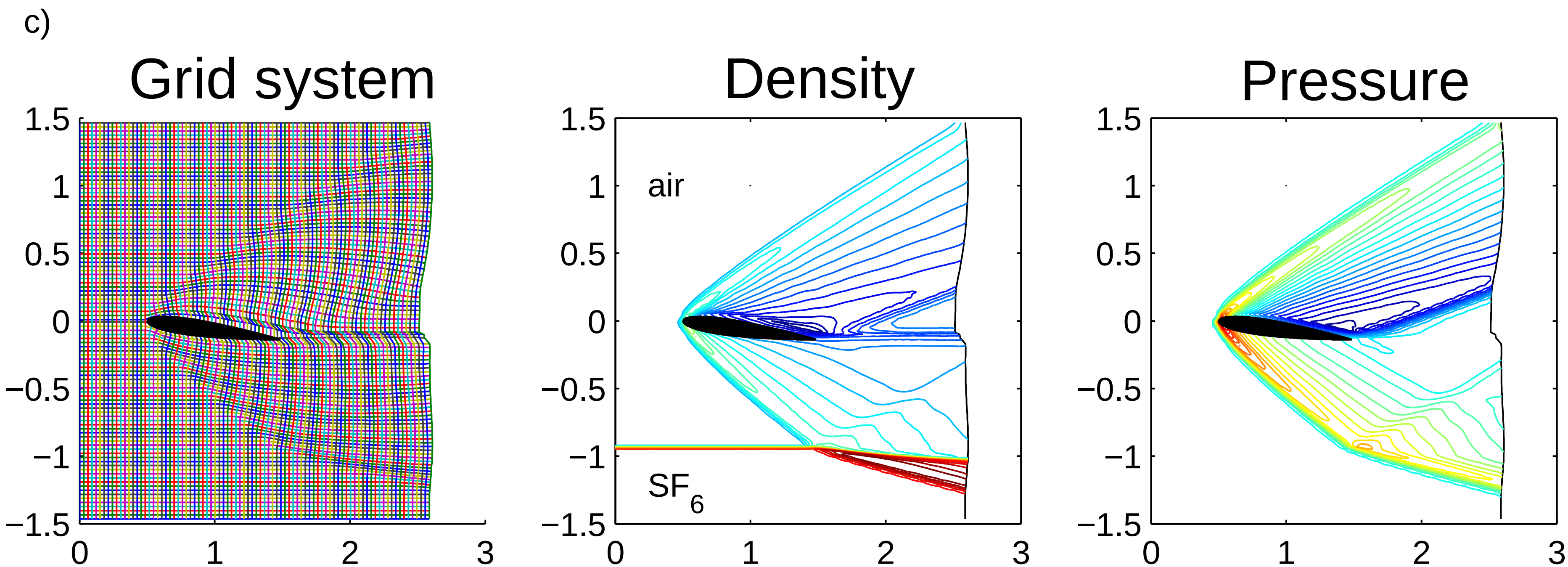

# Conclusion

- Have described a simple unified coordinate moving grid methods for hyperbolic PDEs
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  - Efficient & accurate grid movement strategy
  - Static & Moving $3$D geometry problems
  - Weakly compressible free-surface flow
  - Viscous flow extension
  - $\cdots$

# Conclusion

- Have described a simple unified coordinate moving grid methods for hyperbolic PDEs
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- Future direction
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  - Weakly compressible free-surface flow
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  - $\cdots$

Thank You

# 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
$\lambda$: velocity relaxation parameter, $\mu$: 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)
  - $p_0 = \sum_{k=1}^{2} \alpha_k p_k, \quad \vec{u}_0 = \sum_{k=1}^{2} \alpha_k \rho_k \vec{u}_k \Big/ \sum_{k=1}^{2} \alpha_k \rho_k$

$\lambda$ & $\mu$ (> 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 $\chi_k$ 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 $\psi$,

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

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 $\chi_k$ & 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 $\chi_k$ 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 fow model (Cont.)

In summary, averaged model system, we have, are

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

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

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

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

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

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

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

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

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

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

# 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 $\alpha_k = 0$, $\rho_k$ can not be recovered from $\alpha_k$ & $\alpha_k \rho_k$, 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

# 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: $p = p(\alpha_2,\ \alpha_1\rho_1,\ \alpha_2\rho_2,\ \rho e)$

# Grid-metric relations

Assume existence of inverse transformation

$$t = \tau, \qquad x_j = x_j(\vec{\xi}, t) \qquad \text{for} \quad j = 1, 2, \ldots, N,$$

To find basic grid-metric relations between different coordinates, employ elementary differential rule

$$\frac{\partial(\tau, \vec{\xi})}{\partial(t, \vec{x})} = \frac{\partial(t, \vec{x})}{\partial(\tau, \vec{\xi})}^{-1}$$

yielding in $N = 3$ case, for example, as

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ \partial_t \xi_1 & \partial_{x_1} \xi_1 & \partial_{x_2} \xi_1 & \partial_{x_3} \xi_1 \\ \partial_t \xi_2 & \partial_{x_1} \xi_2 & \partial_{x_2} \xi_2 & \partial_{x_3} \xi_2 \\ \partial_t \xi_3 & \partial_{x_1} \xi_3 & \partial_{x_2} \xi_3 & \partial_{x_3} \xi_3 \end{pmatrix} = \frac{1}{J} \begin{pmatrix} J & 0 & 0 & 0 \\ J_{01} & J_{11} & J_{21} & J_{31} \\ J_{02} & J_{12} & J_{22} & J_{32} \\ J_{03} & J_{13} & J_{23} & J_{33} \end{pmatrix}$$

# Grid-metric relations (Cont.)

Here

$$J = \left| \frac{\partial(x_1, x_2, x_3)}{\partial(\xi_1, \xi_2, \xi_3)} \right| = \text{det} \left( \frac{\partial(x_1, x_2, x_3)}{\partial(\xi_1, \xi_2, \xi_3)} \right),$$

$$J_{11} = \left| \frac{\partial(x_2, x_3)}{\partial(\xi_2, \xi_3)} \right|, \quad J_{21} = \left| \frac{\partial(x_1, x_3)}{\partial(\xi_3, \xi_2)} \right|, \quad J_{31} = \left| \frac{\partial(x_1, x_2)}{\partial(\xi_2, \xi_3)} \right|,$$

$$J_{12} = \left| \frac{\partial(x_2, x_3)}{\partial(\xi_3, \xi_1)} \right|, \quad J_{22} = \left| \frac{\partial(x_1, x_3)}{\partial(\xi_1, \xi_3)} \right|, \quad J_{32} = \left| \frac{\partial(x_1, x_2)}{\partial(\xi_3, \xi_1)} \right|,$$

$$J_{13} = \left| \frac{\partial(x_2, x_3)}{\partial(\xi_1, \xi_2)} \right|, \quad J_{23} = \left| \frac{\partial(x_1, x_3)}{\partial(\xi_2, \xi_1)} \right|, \quad J_{33} = \left| \frac{\partial(x_1, x_2)}{\partial(\xi_1, \xi_2)} \right|,$$

$$J_{0j} = -\sum_{i=1}^{N_d} J_{ij} \partial_\tau x_i, \qquad j = 1, 2, 3,$$

and so grid-metric relations between different coordinates

$$\nabla \xi_j = (\partial_t \xi_j,\ \nabla_{\vec{x}} \xi_j) = (\partial_t \xi_j,\ \partial_{x_1} \xi_j,\ \partial_{x_2} \xi_j,\ \partial_{x_3} \xi_j) = \frac{1}{J} (J_{0j},\ J_{1j},\ J_{2j},\ J_{3j})$$

# Grid-metric relations (Cont.)

Note in two dimensions $N = 2$, we have

$$\left(\frac{\partial \xi_1}{\partial t},\ \frac{\partial \xi_1}{\partial x_1},\ \frac{\partial \xi_1}{\partial x_2}\right) = \frac{1}{J}\left(-\frac{\partial x_1}{\partial \tau}\frac{\partial x_2}{\partial \xi_2} + \frac{\partial x_2}{\partial \tau}\frac{\partial x_1}{\partial \xi_2},\ \frac{\partial x_2}{\partial \xi_2},\ -\frac{\partial x_1}{\partial \xi_2}\right)$$

$$\left(\frac{\partial \xi_2}{\partial t},\ \frac{\partial \xi_2}{\partial x_1},\ \frac{\partial \xi_2}{\partial x_2}\right) = \frac{1}{J}\left(\frac{\partial x_1}{\partial \tau}\frac{\partial x_2}{\partial \xi_1} - \frac{\partial x_2}{\partial \tau}\frac{\partial x_1}{\partial \xi_1},\ -\frac{\partial x_2}{\partial \xi_1},\ \frac{\partial x_1}{\partial \xi_1}\right)$$

$$J = \frac{\partial x_1}{\partial \xi_1}\frac{\partial x_2}{\partial \xi_2} - \frac{\partial x_1}{\partial \xi_2}\frac{\partial x_2}{\partial \xi_1}$$

Thus to have $\mathcal{G} = 0$ fulfilled, grid-metrics should obey

$$\frac{\partial J}{\partial \tau} + \frac{\partial}{\partial \xi_1}\left(J\frac{\partial \xi_1}{\partial t}\right) + \frac{\partial}{\partial \xi_2}\left(J\frac{\partial \xi_2}{\partial t}\right) = 0$$

$$\frac{\partial}{\partial \xi_1}\left(J\frac{\partial \xi_1}{\partial x_1}\right) + \frac{\partial}{\partial \xi_2}\left(J\frac{\partial \xi_2}{\partial x_1}\right) = \frac{\partial}{\partial \xi_1}\left(\frac{\partial x_2}{\partial \xi_2}\right) + \frac{\partial}{\partial \xi_2}\left(-\frac{\partial x_2}{\partial \xi_1}\right) = 0$$

$$\frac{\partial}{\partial \xi_1}\left(J\frac{\partial \xi_1}{\partial x_2}\right) + \frac{\partial}{\partial \xi_2}\left(J\frac{\partial \xi_2}{\partial x_2}\right) = \frac{\partial}{\partial \xi_1}\left(\frac{-\partial x_1}{\partial \xi_2}\right) + \frac{\partial}{\partial \xi_2}\left(\frac{\partial x_1}{\partial \xi_1}\right) = 0$$

# Unified coord.: Grid movement

Consider $N = 2$ case, for example, and use simplified notation $\vec{x} = (x,\ y)$, $\vec{\xi} = (\xi,\ \eta)$. At given time instance, free parameter $h$ 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

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

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

# Unified coord.: Grid movement

Consider $N = 2$ case, for example, and use simplified notation $\vec{x} = (x,\ y)$, $\vec{\xi} = (\xi,\ \eta)$. Or alternatively, based on

- Grid-Jacobian preserving condition

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

with

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