

#### A generalized Lagrangian scheme for hyperbolic balance laws Application to compressible multifluid flow

Keh-Ming Shyue

**Department of Mathematics** 

National Taiwan University

Taiwan

# Outline



- Model scientific problem
- Previous work & current work motivation
- Mathematical formulation
  - Hyperbolic balance law in generalized coordinate
  - Grid movement conditions
  - Examples to shallow water/compressible flow model
- Numerical discretization
  - Generalized Riemann problem
  - Godunov-type flux-based wave propagation method
- Sample examples
- Future work

# **Model Scientific Problem**



Asteroid impact problem (a geophysical example)



# **Fundamental Challenges**



- Mathematical model aspect
  - Incompressible or compressible flow modelling
    - Equations of motion & constitutive laws
      - · Gas phase: air
      - · Liquid phase: ocean water
      - · Solid phase: asteroid, basalt crust, mantle
  - Interface conditions
    - Mass transfer, cavitation, fracture, ···
- Numerical method aspect
  - Multiphase, multiscale, Eulerian or Lagrangian solver
  - Discretization based on structured, unstructured, or overlapping grid

# **Previous Work**



- Fluid-mixture interface-capturing method (JCP 1998, 1999, 2001, 2004, Shock Waves 2006)
  - Shock over MORB (Mid-Ocean Ridge Basalt) liquid
  - Falling liquid drop problem
- Volume-of-fluid interface tracking method (JCP 2006)
   Shock-bubble interaction
- Surface tracking for moving boundaries (Hyp 2006)
  - Falling rigid object in water tank
  - Moving cylindrical vessel
- Unified coordinate method (2006, with Hui & Hu)
  - Supersonic NACA0012 over heavier gas

## **Current Work**



- Motivated by well-known facts that
  - Lagrangian method can resolve material or slip lines sharply if there is no grid tangling
  - Generalized curvilinear grid is often superior to Cartesian when employed in numerical methods for complex fixed or moving geometries

## **Current Work**



- Motivated by well-known facts that
  - Lagrangian method can resolve material or slip lines sharply if there is no grid tangling
  - Generalized curvilinear grid is often superior to Cartesian when employed in numerical methods for complex fixed or moving geometries
- Aim is to devise Lagrange-like moving grid approach for nonlinear hyperbolic system of balance law

$$\frac{\partial}{\partial t}q\left(\vec{x}, t\right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial x_j} f_j\left(q, \vec{x}\right) = \psi\left(q, \vec{x}\right)$$

in general  $N_d \ge 1$  space dimension that is more robust than aforementioned Eulerian-based method



Begin by considering canonical hyperbolic balance law

$$\frac{\partial}{\partial t}q\left(\vec{x}, t\right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial x_j} f_j\left(q, \vec{x}\right) = \psi\left(q, \vec{x}\right)$$

in Cartesian coordinate system

- Hyperbolic if  $\sum_{j=1}^{N_d} \alpha_j (\partial f_j / \partial q)$  is diagonalizable with real eigenvalues,  $\alpha_j \in \mathbb{R}$
- $q \in \mathbb{R}^m$ : vector of *m* state quantities
- $f_j \in \mathbb{R}^m$ : flux vector,  $j = 1, 2, \dots, N_d$ ,  $\psi \in \mathbb{R}^m$ : sources
- $\vec{x} = (x_1, x_2, \cdots, x_{N_d})$ : spatial vector,  $t \ge 0$ : time



Now consider a general non-rectangular domain  $\Omega$  in  $N_d = 2$  & introduce coordinate change  $(\vec{x}, t) \mapsto (\vec{\xi}, \tau)$  via

 $\vec{\xi} = (\xi_1, \xi_2, \cdots, \xi_{N_d}), \qquad \xi_j = \xi_j(\vec{x}, t), \qquad \tau = t,$ 

that maps  $\Omega$  to a logical domain  $\hat{\Omega}$  & also transforms balance law to a new form





That is, using chain rule of partial differentiation, derivatives in physical space become

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

yielding strong form of balance law in transformed space

$$\frac{\partial}{\partial \tau} \tilde{q} \left( \vec{\xi}, \tau \right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial \xi_j} \tilde{f}_j \left( \tilde{q}, \nabla \vec{\xi} \right) = \tilde{\psi} \left( \tilde{q}, \nabla \vec{\xi} \right)$$

with

$$\tilde{q} = Jq, \quad \tilde{f}_j = J\left(q\frac{\partial\xi_j}{\partial t} + \sum_{k=1}^{N_d} f_k\frac{\partial\xi_j}{\partial x_k}\right) \quad \tilde{\psi} = J\psi, \quad J = \det\left(\partial\vec{\xi}/\partial\vec{x}\right)^{-1}$$



Assume existence of inverse transformation

$$t = \tau, \qquad x_j = x_j(\vec{\xi}, t) \qquad \text{for } j = 1, 2, \cdots, N_d,$$

To find basic geometric-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  $N_d = 3$  case, for example, as

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



Here

$$\begin{split} J &= \left| \frac{\partial(x_1, x_2, x_3)}{\partial(\xi_1, \xi_2, \xi_3)} \right| = \det \left( \frac{\partial(x_1, x_2, x_3)}{\partial(\xi_1, \xi_2, \xi_3)} \right), \\ J_{11} &= \left| \frac{\partial(x_2, x_3)}{\partial(\xi_2, \xi_3)} \right|, \quad J_{21} = \left| \frac{\partial(x_1, x_3)}{\partial(\xi_3, \xi_2)} \right|, \quad J_{31} = \left| \frac{\partial(x_1, x_2)}{\partial(\xi_2, \xi_3)} \right|, \\ J_{12} &= \left| \frac{\partial(x_2, x_3)}{\partial(\xi_3, \xi_1)} \right|, \quad J_{22} = \left| \frac{\partial(x_1, x_3)}{\partial(\xi_1, \xi_3)} \right|, \quad J_{32} = \left| \frac{\partial(x_1, x_2)}{\partial(\xi_3, \xi_1)} \right|, \\ J_{13} &= \left| \frac{\partial(x_2, x_3)}{\partial(\xi_1, \xi_2)} \right|, \quad J_{23} = \left| \frac{\partial(x_1, x_3)}{\partial(\xi_2, \xi_1)} \right|, \quad J_{33} = \left| \frac{\partial(x_1, x_2)}{\partial(\xi_1, \xi_2)} \right|, \\ J_{0j} &= -\sum_{i=1}^{N_d} J_{ij} \partial_\tau x_i, \qquad j = 1, 2, 3, \end{split}$$

and so numerically computatable  $\nabla \xi_j$ , j = 1, 2, 3, as

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



Note that to complete the model

- When  $\partial_{\tau} \vec{x} = 0$  (stationary case)
  - $\partial_t \vec{\xi} = 0$  &  $\nabla_{\vec{x}} \vec{\xi}$  time-independent; no more condition



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- When  $\partial_{\tau} \vec{x} = \vec{u}_0$ ,  $\vec{u}_0$  is constant (quasi-stationary case)
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  - Both  $\partial_t \vec{\xi} \& \nabla_{\vec{x}} \vec{\xi}$  time-independent; no more condition
- Otherwise  $\partial_{\tau} \vec{x} \neq 0$  (genuine moving case)
  - Both  $\partial_t \vec{\xi} \& \nabla_{\vec{x}} \vec{\xi}$  time-dependent; require  $N_d$  degree of freedom for  $\partial_{\tau} \vec{x} \&$  numerical approach to compute  $\nabla_{\vec{\xi}} \vec{x}$  over time

# **Grid Movement Conditions**



Here we are interested in

- Lagrange-like condition  $\partial_{\tau} \vec{x} = h_0 \vec{u}$ ,  $\vec{u}$  velocity,  $h_0 \in [0, 1]$
- Compatibility conditions for  $\partial_{\tau}\partial_{\xi_j}x_i \& \partial_{\xi_j}\partial_{\tau}x_i$ , *i.e.*,

$$\frac{\partial}{\partial \tau} \left( \frac{\partial x_i}{\partial \xi_j} \right) + \frac{\partial}{\partial \xi_j} \left( -\frac{\partial x_i}{\partial \tau} \right) = 0 \quad \text{for} \quad i, j = 1, 2, \cdots, N_d$$

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- General 1-parameter  $\partial_{\tau} \vec{x} = h \vec{u}$  with  $h \in [0, 1]$  chosen by
  - J or grid-angle preserving, yielding

$$\mathcal{A}_0 h + \sum_{j=1}^{N_d} \mathcal{A}_j \partial_{\xi_j} h = 0$$
 (1st order PDE constraint)

• General *k*-parameter,  $k > 1, \cdots$ 

# **Shallow Water Equations**



With **bottom topography** included, for example

Cartesian coordinate case

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

Generalized coordinate case

$$\frac{\partial}{\partial \tau} \begin{pmatrix} hJ\\ hJu_i \end{pmatrix} + \sum_{j=1}^{N_d} \frac{\partial}{\partial \xi_j} J \begin{pmatrix} hU_j\\ hu_iU_j + \frac{1}{2}gh^2\frac{\partial \xi_j}{\partial x_i} \end{pmatrix} = \begin{pmatrix} 0\\ -ghJ\frac{\partial B}{\partial x_i} \end{pmatrix}$$

with  $U_j = \partial_t \xi_j + \sum_{i=1}^{N_d} u_i \partial_{x_i} \xi_j$ ,  $j = 1, 2, \cdots, N_d$ 

*h*: water height,  $u_i$ : velocity in  $x_i$ -direction *B*: bottom topography, *g*: gravitational constant

# **Shallow Water Equations**



With  $\partial_{\tau} \vec{x} = h_0 \vec{u}$  & grid-metric conditions, complete model system in  $N_d = 2$  transformed space, for example, takes

$$\frac{\partial}{\partial \tau} \begin{pmatrix} hJ \\ hJu_1 \\ hJu_2 \\ A \\ B \\ C \\ D \end{pmatrix} + \frac{\partial}{\partial \xi_1} \begin{pmatrix} hJU_1 \\ hJu_1U_1 + \frac{1}{2}gJh^2\frac{\partial\xi_1}{\partial x_1} \\ hJu_2U_1 + \frac{1}{2}gJh^2\frac{\partial\xi_1}{\partial x_2} \\ -h_0u_1 \\ -h_0u_2 \\ 0 \end{pmatrix} + \frac{\partial}{\partial \xi_2} \begin{pmatrix} hJU_2 \\ hJu_1U_2 + \frac{1}{2}gJh^2\frac{\partial\xi_2}{\partial x_1} \\ hJu_2U_2 + \frac{1}{2}gJh^2\frac{\partial\xi_2}{\partial x_2} \\ 0 \\ 0 \\ -h_0u_1 \\ -h_0u_1 \\ -h_0u_2 \end{pmatrix} =$$

Here  $A = \partial_{\xi_1} x_1$ ,  $B = \partial_{\xi_1} x_2$ ,  $C = \partial_{\xi_2} x_1$ ,  $D = \partial_{\xi_2} x_2$ 

# Remarks



#### Hyperbolicity

- In Cartesian coordinates, model is hyperbolic
- In generalized coord., model is hyperbolic when  $h_0 \neq 1$ , & is weakly hyperbolic when  $h_0 = 1$  &  $N_d > 1$
- Canonical form
  - In Cartesian coordinates

$$\frac{\partial}{\partial t}q\left(\vec{x}, t\right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial x_j} f_j\left(q\right) = \psi\left(q\right)$$

In generalized coordinates: spatially varying fluxes

$$\frac{\partial}{\partial t}q\left(\vec{x}, t\right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial x_j} f_j\left(q, \nabla \vec{\xi}\right) = \psi\left(q, \nabla \vec{\xi}\right)$$

# **Compressible Euler Equations**



With gravity effect included, for example

Cartesian coordinate case

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u_i \\ E \end{pmatrix} + \sum_{j=1}^{N_d} \frac{\partial}{\partial x_j} \begin{pmatrix} \rho u_j \\ \rho u_i u_j + p \delta_{ij} \\ E u_j + p u_j \end{pmatrix} = \begin{pmatrix} 0 \\ -\rho \frac{\partial \phi}{\partial x_i} \\ -\rho \vec{u} \cdot \nabla \phi \end{pmatrix}, \quad i = 1, \cdots, N_d$$

Generalized coordinate case

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

 $\rho$ : density,  $p = p(\rho, e)$ : pressure , e: internal energy  $E = \rho e + \rho \sum_{j=1}^{N_d} u_j^2/2$ : total energy,  $\phi$ : gravitational potential

### **Extension to Multifluid**



Assume homogeneous (1-pressure & 1-velocity) flow; *i.e.*, across interfaces  $p_{\iota} = p \& \vec{u}_{\iota} = \vec{u}$ ,  $\forall$  fluid phase  $\iota$ 



# **Extension to Multifluid**



Mathematical model: Fluid-mixture type

- Use basic conservation (or balance) laws for single & multicomponent fluid mixtures
- Introduce additional transport equations for problem-dependent material quantities near numerically diffused interfaces, yielding direct computation of pressure from EOS
- Model barotropic 2-phase flow problem with
   fluid component 1 & 2 characterized by Tait EOS

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

# **Barotropic** 2-Phase Flow



Define mixture pressure law (Shyue, JCP 2004)

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

Derived from  $de = -pd(1/\rho)$  using

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

Here  $\mathcal{A}(S) = e^{[(S-S_0)/C_V]}$ , *S*, *C<sub>V</sub>*: specific entropy & heat at constant vol.  $\alpha$ : volume fraction of one fluid component

# **Barotropic** 2-Phase Flow



Transport equations for material quantities γ, B, & ρ<sub>0</sub>
 γ-based equations

$$\frac{\partial}{\partial \tau} \left( \frac{1}{\gamma - 1} \right) + \sum_{j=1}^{N_d} U_j \frac{\partial}{\partial \xi_j} \left( \frac{1}{\gamma - 1} \right) = 0$$
$$\frac{\partial}{\partial \tau} \left( \frac{\gamma \mathcal{B}}{\gamma - 1} \right) + \sum_{j=1}^{N_d} U_j \frac{\partial}{\partial \xi_j} \left( \frac{\gamma \mathcal{B}}{\gamma - 1} \right) = 0$$
$$\frac{\partial}{\partial \tau} \left( J \frac{\mathcal{B}}{\rho_0} \rho \right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial \xi_j} \left( J \frac{\mathcal{B}}{\rho_0} \rho U_j \right) = 0$$

Above equations are derived from energy equation & make use of homogeneous equilibrium flow assumption together with mass conservation law

# **Barotropic** 2-Phase Flow



#### **\square** $\alpha$ -based equations

$$\frac{\partial \alpha}{\partial \tau} + \sum_{j=1}^{N_d} U_j \frac{\partial \alpha}{\partial \xi} = 0, \quad \text{with} \quad z = \sum_{\iota=1}^2 \alpha_\iota z_\iota, \quad z = \frac{1}{\gamma - 1} \& \frac{\gamma \mathcal{B}}{\gamma - 1}$$
$$\frac{\partial}{\partial \tau} \left( J \frac{\mathcal{B}}{\rho_0} \rho \right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial \xi_j} \left( J \frac{\mathcal{B}}{\rho_0} \rho U_j \right) = 0$$

**\square**  $\alpha$ -based equations (Allaire *et al.*, JCP 2002)

$$\frac{\partial \alpha}{\partial \tau} + \sum_{j=1}^{N_d} U_j \frac{\partial \alpha}{\partial \xi_j} = 0 \quad \text{with} \quad z = \sum_{\iota=1}^2 \alpha_{\iota} z_{\iota} , \quad z = \frac{1}{\gamma - 1} \& \frac{\gamma \mathcal{B}}{\gamma - 1}$$
$$\frac{\partial}{\partial \tau} \left( J \rho_1 \alpha \right) + \sum_{j=1}^{N_d} \frac{\partial}{\partial \xi_j} \left( J \rho_1 \alpha U_j \right) = 0$$

# **Multifluid Model**



With  $(x_{\tau}, y_{\tau}) = h_0(u, v)$  & sample EOS described above, our *\alpha*-based model for multifluid flow is



# **Multifluid Model**



For convenience, our multifluid model is written into

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

with

$$q = [J\rho, J\rho u, J\rho v, JE, x_{\xi}, y_{\xi}, x_{\eta}, y_{\eta}, J\rho_{1}\alpha, \alpha]^{T}$$

$$f_{1} = \left[\frac{\partial}{\partial\xi}(J\rho U), \frac{\partial}{\partial\xi}(J\rho u U + y_{\eta}p), \frac{\partial}{\partial\xi}(J\rho v U - x_{\eta}p), \frac{\partial}{\partial\xi}(JEU + (y_{\eta}u - x_{\eta}v)p), \frac{\partial}{\partial\xi}(-h_{0}u), \frac{\partial}{\partial\xi}(-h_{0}v), 0, 0, \frac{\partial}{\partial\xi}(J\rho_{1}\alpha U), U\frac{\partial\alpha}{\partial\xi}\right]^{T}$$

$$f_{2} = \left[\frac{\partial}{\partial\eta}(J\rho V), \frac{\partial}{\partial\eta}(J\rho u V - y_{\xi}p), \frac{\partial}{\partial\eta}(J\rho v V + x_{\xi}p), \frac{\partial}{\partial\eta}(JEV + (x_{\xi}v - y_{\xi}u)p), \frac{\partial}{\partial\eta}(-h_{0}u), \frac{\partial}{\partial\eta}(-h_{0}v), \frac{\partial}{\partial\eta}(J\rho_{1}\alpha V), V\frac{\partial\alpha}{\partial\eta}\right]^{T}$$

# Multifluid model: Remarks



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

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#### Numerical discretization?



# **Numerical Discretization**



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

# **Numerical Discretization**



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 qover cell  $C_{ij} = [\xi_i, \xi_{i+1}] \times [\eta_j, \eta_{j+1}]$  at time  $\tau_n$ 





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

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



Generalized Riemann problem at time  $\tau = 0$ 





Exact generalized Riemann solution: basic structure





Shock-only approximate Riemann solution: basic structure

$$\mathcal{Z}^{1} = f_{L}(q_{mL}^{-}) - f_{L}(Q_{i-1,j}^{n}) \qquad \mathcal{T} \qquad \mathcal{Z}^{2} = f_{R}(q_{mR}) - f_{R}(q_{mL}^{+}) \\ \lambda^{2} \qquad \qquad \lambda^{2}$$
#### **Numerical Discretization**

Basic steps of a dimensional-splitting scheme

•  $\xi$ -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  $Q_{i,j}^*$ 

•  $\eta$ -sweeps: solve

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

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



#### **Numerical Discretization**



That is to say,

•  $\xi$ -sweeps: we use

$$\begin{aligned} Q_{ij}^* &= Q_{ij}^n - \frac{\Delta \tau}{\Delta \xi} \left( \mathcal{F}_{i+\frac{1}{2},j}^- - \mathcal{F}_{i-\frac{1}{2},j}^+ \right) - \frac{\Delta \tau}{\Delta \xi} \left( \tilde{\mathcal{Z}}_{i+\frac{1}{2},j} - \tilde{\mathcal{Z}}_{i-\frac{1}{2},j} \right) \\ \text{with} \quad \tilde{\mathcal{Z}}_{i-\frac{1}{2},j} &= \frac{1}{2} \sum_{p=1}^{m_w} \operatorname{sign} \left( \lambda_{i-\frac{1}{2},j}^p \right) \left( 1 - \frac{\Delta \tau}{\Delta \xi} \left| \lambda_{i-\frac{1}{2},j}^p \right| \right) \tilde{\mathcal{Z}}_{i-\frac{1}{2},j}^p \end{aligned}$$

•  $\eta$ -sweeps: we use

$$\begin{split} Q_{ij}^{n+1} &= Q_{ij}^* - \frac{\Delta\tau}{\Delta\eta} \left( \mathcal{G}_{i,j+\frac{1}{2}}^- - \mathcal{G}_{i,j-\frac{1}{2}}^+ \right) - \frac{\Delta\tau}{\Delta\eta} \left( \tilde{\mathcal{Z}}_{i,j+\frac{1}{2}}^- - \tilde{\mathcal{Z}}_{i,j-\frac{1}{2}}^- \right) \\ \text{with} \quad \tilde{\mathcal{Z}}_{i,j-\frac{1}{2}}^- &= \frac{1}{2} \sum_{p=1}^{m_w} \operatorname{sign} \left( \lambda_{i,j-\frac{1}{2}}^p \right) \left( 1 - \frac{\Delta\tau}{\Delta\eta} \left| \lambda_{i,j-\frac{1}{2}}^p \right| \right) \tilde{\mathcal{Z}}_{i,j-\frac{1}{2}}^p \end{split}$$

#### **Numerical Discretization**



Flux-based wave decomposition

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

- Some care should be taken on the limited jump of fluxes  $\tilde{W}^p$ , 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





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





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Physical grid coordinates at selected times

 Each little dashed line gives a cell-center location of the proposed Lagrange-like grid system



#### 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



#### **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



#### Conclusion



- Have described fluid-mixture type algorithm in generalized moving-curvilinear grid
- Have shown results in 1, 2 & 3D to demonstrate feasibility of method for practical problems

### Conclusion



- Have described fluid-mixture type algorithm in generalized moving-curvilinear grid
- Have shown results in 1, 2 & 3D to demonstrate feasibility of method for practical problems
- Future direction
  - Efficient & accurate grid movement strategy
  - Static & Moving 3D geometry problems
  - Weakly compressible flow
  - Viscous flow extension
  - **\_** •

### Conclusion



- Have described fluid-mixture type algorithm in generalized moving-curvilinear grid
- Have shown results in 1, 2 & 3D to demonstrate feasibility of method for practical problems
- Future direction
  - Efficient & accurate grid movement strategy
  - Static & Moving 3D geometry problems
  - Weakly compressible flow
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  - **\_** ..

# Thank You

#### **Euler in General. Coord.**



Model system in quasi-linear form

$$\begin{aligned} \frac{\partial \tilde{q}}{\partial \tau} + A \frac{\partial \tilde{q}}{\partial \xi} + B \frac{\partial \tilde{q}}{\partial \eta} &= \tilde{\psi} \\ A &= \frac{\partial \tilde{f}}{\partial \tilde{q}} = \begin{bmatrix} \xi_t & \xi_x & \xi_y & 0\\ \xi_x p_\rho - u\mathcal{U} & \xi_x u(1 - p_E) + U & \xi_y u - \xi_x v p_E & \xi_x p_E\\ \xi_y p_\rho - v\mathcal{U} & \xi_x v - \xi_y u p_E & \xi_y v(1 - p_E) + U & \xi_y p_E\\ (p_\rho - H)\mathcal{U} & \xi_x H - u\mathcal{U} p_E & \xi_y H - v\mathcal{U} p_E & U + p_E \mathcal{U} \end{bmatrix} \\ B &= \frac{\partial \tilde{g}}{\partial \tilde{q}} = \begin{bmatrix} \eta_t & \eta_x & \eta_y & 0\\ \eta_x p_\rho - u\mathcal{V} & \eta_x u(1 - p_E) + V & \eta_y u - \eta_x v p_E & \eta_x p_E\\ \eta_y p_\rho - v\mathcal{V} & \eta_x v - \eta_y u p_E & \eta_y v(1 - p_E) + V & \eta_y p_E\\ (p_\rho - H)\mathcal{V} & \eta_x H - u\mathcal{V} p_E & \eta_y H - v\mathcal{V} p_E & V + p_E \mathcal{V} \end{bmatrix} \end{aligned}$$

with  $H = (E+p)/\rho$ ,  $\mathcal{U} = U - \xi_t = \xi_x u + \xi_y v$ ,  $\mathcal{V} = V - \eta_t = \eta_x u + \eta_y v$ 

#### Euler in General. Coord. (Cont.)



**Eigen-structure** of matrix *A* is

$$\begin{split} \Lambda_{A} &= \operatorname{diag} \left( U - c\sqrt{\xi_{x}^{2} + \xi_{y}^{2}}, \ U, \ U, \ U + c\sqrt{\xi_{x}^{2} + \xi_{y}^{2}} \right) \\ R_{A} &= \begin{bmatrix} 1 & 1 & 0 & 1 \\ u - \alpha_{1}c & u & \alpha_{2} & u + \alpha_{1}c \\ v - \alpha_{2}c & v & -\alpha_{1} & v + \alpha_{2}c \\ H - \mathcal{U}_{1}c & H - c^{2}/p_{E} & -\mathcal{U}_{2} & H + \mathcal{U}_{1}c \end{bmatrix} \\ L_{A} &= \begin{bmatrix} (p_{\rho} + c\mathcal{U}_{1})/2c^{2} & -(\alpha_{1}c + up_{E})/2c^{2} & -(\alpha_{2}c + vp_{E})/2c^{2} & p_{E}/2c^{2} \\ 1 - p_{\rho}/c^{2} & up_{E}/c^{2} & vp_{E}/c^{2} & -p_{E}/c^{2} \\ \mathcal{U}_{2} & \alpha_{2} & -\alpha_{1} & 0 \\ (p_{\rho} - c\mathcal{U}_{1})/2c^{2} & (\alpha_{1}c - up_{E})/2c^{2} & (\alpha_{2}c - vp_{E})/2c^{2} & p_{E}/2c^{2} \end{bmatrix} \\ \text{with } (\alpha_{1}, \alpha_{2}) &= (\xi_{x}, \xi_{y})/\sqrt{\xi_{x}^{2} + \xi_{y}^{2}}, \quad \mathcal{U}_{1} = \alpha_{1}u + \alpha_{2}v, \quad \mathcal{U}_{2} = -\alpha_{2}u + \alpha_{1}v \end{bmatrix}$$

#### Euler in General. Coord. (Cont.) (



#### **Eigen-structure** of matrix *B* is

$$\begin{split} \Lambda_B &= \operatorname{diag} \left( V - c \sqrt{\eta_x^2 + \eta_y^2}, \, V, \, V, \, V + c \sqrt{\eta_x^2 + \eta_y^2} \right) \\ R_B &= \begin{bmatrix} 1 & 1 & 0 & 1 \\ u - \beta_1 c & u & \beta_2 & u + \beta_1 c \\ v - \beta_2 c & v & -\beta_1 & v + \beta_2 c \\ H - \mathcal{V}_1 c & H - c^2 / p_E & -\mathcal{V}_2 & H + \mathcal{V}_1 c \end{bmatrix} \\ L_B &= \begin{bmatrix} (p_\rho + c\mathcal{V}_1)/2c^2 & -(\beta_1 c + up_E)/2c^2 & -(\beta_2 c + vp_E)/2c^2 & p_E/2c^2 \\ 1 - p_\rho/c^2 & up_E/c^2 & vp_E/c^2 & -p_E/c^2 \\ \mathcal{V}_2 & \beta_2 & -\beta_1 & 0 \\ (p_\rho - c\mathcal{V}_1)/2c^2 & (\beta_1 c - up_E)/2c^2 & (\beta_2 c - vp_E)/2c^2 & p_E/2c^2 \end{bmatrix} \\ \text{with } (\beta_1, \beta_2) &= (\eta_x, \eta_y)/\sqrt{\eta_x^2 + \eta_y^2}, \quad \mathcal{V}_1 = \beta_1 u + \beta_2 v, \quad \mathcal{V}_2 = -\beta_2 u + \beta_1 v \end{split}$$

#### **Grid Movement (Cont.)**



- General 1-parameter case:  $(x_{\tau}, y_{\tau}) = h(u, v)$ ,  $h \in [0, 1]$ 
  - At given time instance, *h* can be chosen based on Grid-angle preserving condition (Hui *et al.* JCP 1999)

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

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

with

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

#### **Grid Movement (Cont.)**



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

Or alternatively, based onMesh-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

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

#### Grid Movement (Cont.)



To ensure  $h \in [0, 1]$ , transformed variable  $\tilde{h} = \kappa(h)$  is used, *e.g.*, Hui *et al.* employed  $\kappa = \ln(\varepsilon h |\vec{u}|)$ ,  $\varepsilon$  normalized constant, yielding

 $\tilde{\mathcal{A}}\tilde{h}_{\xi} + \tilde{\mathcal{B}}\tilde{h}_{\eta} + \tilde{\mathcal{C}} = 0$ 

Grid-angle preserving case

$$\tilde{\mathcal{A}} = \sqrt{x_{\eta}^2 + y_{\eta}^2} \left( x_{\xi} \sin \theta - y_{\xi} \cos \theta \right), \quad \tilde{\mathcal{B}} = \sqrt{x_{\xi}^2 + y_{\xi}^2} \left( y_{\eta} \cos \theta - x_{\eta} \sin \theta \right) \\ \tilde{\mathcal{C}} = \sqrt{x_{\xi}^2 + y_{\xi}^2} \left[ y_{\eta} (\cos \theta)_{\eta} - x_{\eta} (\sin \theta)_{\eta} \right] - \sqrt{x_{\eta}^2 + y_{\eta}^2} \left[ y_{\xi} (\cos \theta)_{\xi} - x_{\xi} (\sin \theta)_{\xi} \right]$$

Mesh-area preserving case

$$\begin{split} \tilde{\mathcal{A}} &= y_{\eta} \cos \theta - x_{\eta} \sin \theta, \quad \tilde{\mathcal{B}} = x_{\xi} \sin \theta - y_{\xi} \cos \theta \\ \tilde{\mathcal{C}} &= y_{\eta} (\cos \theta)_{\xi} - x_{\eta} (\sin \theta)_{\xi} + x_{\xi} (\sin \theta)_{\eta} - y_{\xi} (\cos \theta)_{\eta} \end{split}$$
where  $\vec{u} = (u, v) = |\vec{u}| (\cos \theta, \sin \theta)$ 

#### **Grid Movement: Remarks**



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

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

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



- 2-parameter case of Hui *et al.* (2005):  $(x_{\tau}, y_{\tau}) = (U_g, V_g)$ 
  - Imposed conditions
    - 1. Grid-angle preserving
    - 2. Specialized grid-material line matching (see next)



- 2-parameter case of Hui *et al.* (2005):  $(x_{\tau}, y_{\tau}) = (U_g, V_g)$ 
  - Imposed conditions
    - 1. Grid-angle preserving
    - 2. Specialized grid-material line matching (see next)
  - Good results are shown for steady-state problems



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    - 2. Specialized grid-material line matching (see next)
  - Good results are shown for steady-state problems
  - Little results for time-dependent problems with rapid transient solution structures



- **2**-parameter case of Hui *et al.* (2005):  $(x_{\tau}, y_{\tau}) = (U_g, V_g)$ 
  - Imposed conditions
    - 1. Grid-angle preserving
    - 2. Specialized grid-material line matching (see next)
  - Good results are shown for steady-state problems
  - Little results for time-dependent problems with rapid transient solution structures
- Other 2-parameter case:  $(x_{\tau}, y_{\tau}) = (hu, kv)$ 
  - Novel imposed conditions for  $h \in [0,1]$  &  $k \in [0,1]$  ?



- 2-parameter case of Hui *et al.* (2005):  $(x_{\tau}, y_{\tau}) = (U_g, V_g)$ 
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- Other 2-parameter case:  $(x_{\tau}, y_{\tau}) = (hu, kv)$ 
  - Novel imposed conditions for  $h \in [0,1]$  &  $k \in [0,1]$  ?

Roadmap of current work:

$$(x_{\tau}, y_{\tau}) = \frac{h_0(u, v)}{||} \rightarrow (x_{\tau}, y_{\tau}) = \frac{h(u, v)}{||} \rightarrow \cdots$$

#### Novel Conditions for $h\ \&\ k$



Mesh-area preserving case

$$\begin{aligned} \frac{\partial J}{\partial \tau} &= \frac{\partial}{\partial \tau} \left( x_{\xi} y_{\eta} - x_{\eta} y_{\xi} \right) \\ &= x_{\xi\tau} \ y_{\eta} + x_{\xi} \ y_{\eta\tau} - x_{\eta\tau} \ y_{\xi} - x_{\eta} \ y_{\xi\tau} \\ &= \cdots \\ &= \left( \mathcal{A}_{1} h_{\xi} + \mathcal{B}_{1} h_{\eta} + \mathcal{C}_{1} h \right) + \left( \mathcal{A}_{2} k_{\xi} + \mathcal{B}_{2} k_{\eta} + \mathcal{C}_{2} k \right) = 0, \end{aligned}$$

yielding, for example,

$$\mathcal{A}_1 h_{\xi} + \mathcal{B}_1 h_{\eta} + \mathcal{C}_1 h = 0$$
$$\mathcal{A}_2 k_{\xi} + \mathcal{B}_2 k_{\eta} + \mathcal{C}_2 k = 0$$

with

$$\mathcal{A}_1 = uy_{\eta}, \qquad \mathcal{B}_1 = uy_{\xi}, \quad \mathcal{C}_1 = u_{\xi}y_{\eta} - u_{\eta}y_{\xi}$$
$$\mathcal{A}_2 = -vx_{\eta}, \quad \mathcal{B}_2 = vx_{\xi}, \quad \mathcal{C}_2 = v_{\eta}x_{\xi} - v_{\xi}x_{\eta}$$

# Shock in molybdenum over MORB







#### Interface capturing with gravity









Interface diffused badily











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Volume tracking for material interface



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Small moving irregular cells: stability & accuracy





Moving boundary tracking & interface capturing



# Falling Rigid Object in Water Tank



#### Falling Rigid Object in Water Tank Density Volume fraction Pressure 3 3 3 = 2msair 2 2 2 1 1 1 0 0 0

0

-1

-2

-3

-2

-1

-2

-3

water

0

2

-2

-1

-2

-3

-2

2

0

2



Small moving irregular cells: stability & accuracy









Two sample grid systems used in computation





#### Cartesian grid results with embedded moving boundary







Cartesian grid results with embedded stationary boundary



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#### NACA0012 over heavier gas



Automatic time-marching grid



#### NACA0012 over heavier gas



Automatic time-marching grid



#### NACA0012 over heavier gas



Automatic time-marching grid



### **Radially Symmetric Problem**





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#### Radially Symmetric Prob. (Cont.)













































#### Volume tracking & interface capturing results

Tracking time=0.2ms air water time=0.4ms time=0.8ms time=1.2ms

a) Density



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- Generalized curvilinear grid: single bubble animation
- Cartesian grid: multiple bubble animation



#### **Shock-Bubble (Helium)**






















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

















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

























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





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





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





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









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





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





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





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





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



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

time = 0



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

time = 0.25ms



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

time = 0.5ms



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

time = 1.0ms



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

time = 1.5ms





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

t=0

























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

time = 0.02


# **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.)**



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

time = 0.35



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

t=0





















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





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





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





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





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

