Computing Interface Motion in Hyperbolic Problems

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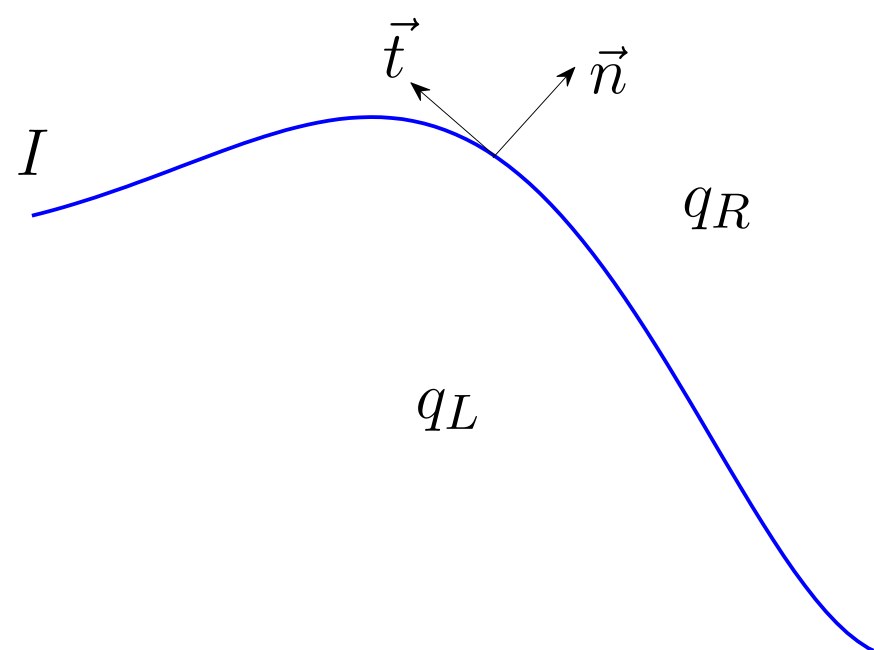
Problem Setup

Consider an interface I in 2D (shown below) that separate the domain into two parts with different states q_L and q_R

Motion and dynamics of interface depends, clearly, on

- Mathematical model
- Interface conditions
- Initial & boundary cond.
- Discretization scheme



Mathematical Model

As an example, we consider problems governed by compressible Euler equations in $N \geq 1$ dimension

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho u_i \\ E \end{bmatrix} + \sum_{j=1}^{N} \frac{\partial}{\partial x_j}\begin{bmatrix} \rho u_j \\ \rho u_i u_j + p\delta_{ij} \\ E u_j + p u_j \end{bmatrix} = \begin{bmatrix} 0 \\ -\rho \partial_{x_i}\phi \\ -\rho \vec{u}\cdot\nabla\phi \end{bmatrix}, \qquad i = 1, \ldots, N$$

ρ	$p = p(\rho, e)$	e	$E = \rho e + \rho \sum_{j=1}^{N} u_j^2/2$	ϕ
density	pressure	int. energy	total energy	gr. potential

Mathematical Model (Cont.)

For the ease of the latter reference, we write the above compressible flow model as

$$\frac{\partial q}{\partial t} + \sum_{j=1}^{N} \frac{\partial f_j(q)}{\partial x_j} = \psi(q),$$

where

$$q = [\rho, \rho u_1, \ldots, \rho u_N, E]^T,$$

$$f_j = \left[\rho u_j, \rho u_1 u_j + p\delta_{j1}, \ldots, \rho u_N u_j + p\delta_{jN}, E u_j + p u_j\right]^T,$$

$$\psi = [0, -\rho \partial_{x_1} \phi, \ldots, -\rho \partial_{x_N} \phi, -\rho \vec{u} \cdot \nabla \phi]^T$$

Interface Conditions

Interface conditions of interest are such as

- Dynamic condition

$$p_R - p_L = 0 \quad (\text{or } = f(\kappa_I))$$

- Kinematic condition

$$(\vec{u}_R - \vec{u}_L) \cdot \vec{n} = 0, \qquad (\vec{u}_R - \vec{u}_L) \cdot \vec{t} = 0 \quad (\text{or } \neq 0)$$

- Vacuum (or called cavitation) condition

$$(\vec{u}_R - \vec{u}_L) \cdot \vec{n} < \int_{\rho_{vL}}^{\rho_L} \frac{c}{\rho}\, d\rho + \int_{\rho_{vR}}^{\rho_R} \frac{c}{\rho}\, d\rho$$

κ_I	ρ_v	c
curvature at interface	density at vacuum	sound speed

Aim of Talk

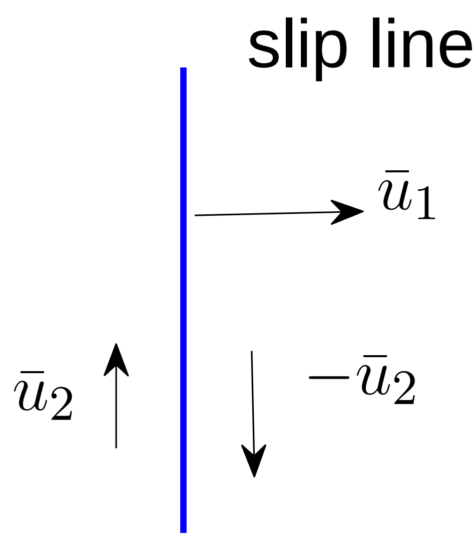
With the above compressible flow model & interface conditions in mind, the plan of this talk is to:

- Discuss anomales of state-of-the-art methods for solving the following interface problems:
  - Slip line (shear flow) problem
  - Material line problem
  - Cavitation problem
- Discuss mapped grid approach for problems with complex geometries

Slip Line (Shear Flow) Problem

For simplicity, we consider a plane interface moving vertically from the left to right in x_1-direction as shown in $N = 2$ below. Interface conditions for this problem are

- Dynamic condition: $p_R = p_L$
- Kinematic condition: $u_{1,R} = u_{1,L}$ & $\left(u_{2,R} - u_{2,L}\right) \neq 0$



Slip Line Problem (Cont.)

Ignore gravitational-potential term, we may derive following transport equations for motion of ρ, ρu_2, & $\rho e + \rho u_2^2/2$, respectively, as

$$\frac{\partial \rho}{\partial t} + \bar{u}_1 \frac{\partial \rho}{\partial x_1} = 0 \quad (\text{from mass conservation law})$$

$$\frac{\partial}{\partial t}\left(\rho u_2\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\rho u_2\right) = 0 \quad (\text{from momentum in } x_2\text{-dir})$$

$$\frac{\partial}{\partial t}\left(\rho e\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\rho e\right) + \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_2^2\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\frac{1}{2}\rho u_2^2\right) = 0 \quad (\text{from total energy})$$

Slip Line Problem (Cont.)

Assume a single phase ideal gas flow with EOS
$p(\rho, e) = (\gamma - 1)\rho e$; $\gamma > 1$ is ratio of specific heats

In this instance, to ensure pressure equilibrium, as it should be for this slip line problem, from

$$\frac{\partial}{\partial t}\left(\frac{p}{\gamma - 1}\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\frac{p}{\gamma - 1}\right) + \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_2^2\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\frac{1}{2}\rho u_2^2\right) = 0,$$

we should have

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_2^2\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\frac{1}{2}\rho u_2^2\right) = 0$$

Slip Line Problem (Cont.)

Note that when the problem is solved numerically by an interface-capturing method, it is common to compute pressure, p, based on conservative variables as

$$p = (\gamma - 1)\left(E - \frac{\sum_{i=1}^{2}(\rho u_i)^2}{2\rho}\right),$$

while generally $(\rho u_2)^2/2\rho \neq \rho u_2^2/2$ when a slip line is smeared out

Immediate consequence of this is loss of pressure equilibrium, and so incorrect solution of other state variables (see below)

Slip Line Problem (Cont.)

Suppose a first order Godunov method of the form

$$Q_{ij}^{n+1} = Q_{ij}^{n} - \frac{\Delta t}{\Delta x_1}\left[F_1\left(Q_{i,j}^{n}, Q_{i+1,j}^{n}\right) - F_1\left(Q_{i-1,j}^{n}, Q_{ij}^{n}\right)\right]$$

is used for numerical discretization of this slip line problem Here Q_{ij}^n denotes approximate value of cell average of solution q over cell C_{ij} at time t_n, *i.e.*,

$$Q_{ij}^{n} = \frac{1}{\Delta x_1 \Delta x_2}\int\int_{C_{ij}} q(x_1, x_2, t_n)\,dx_1 dx_2,$$

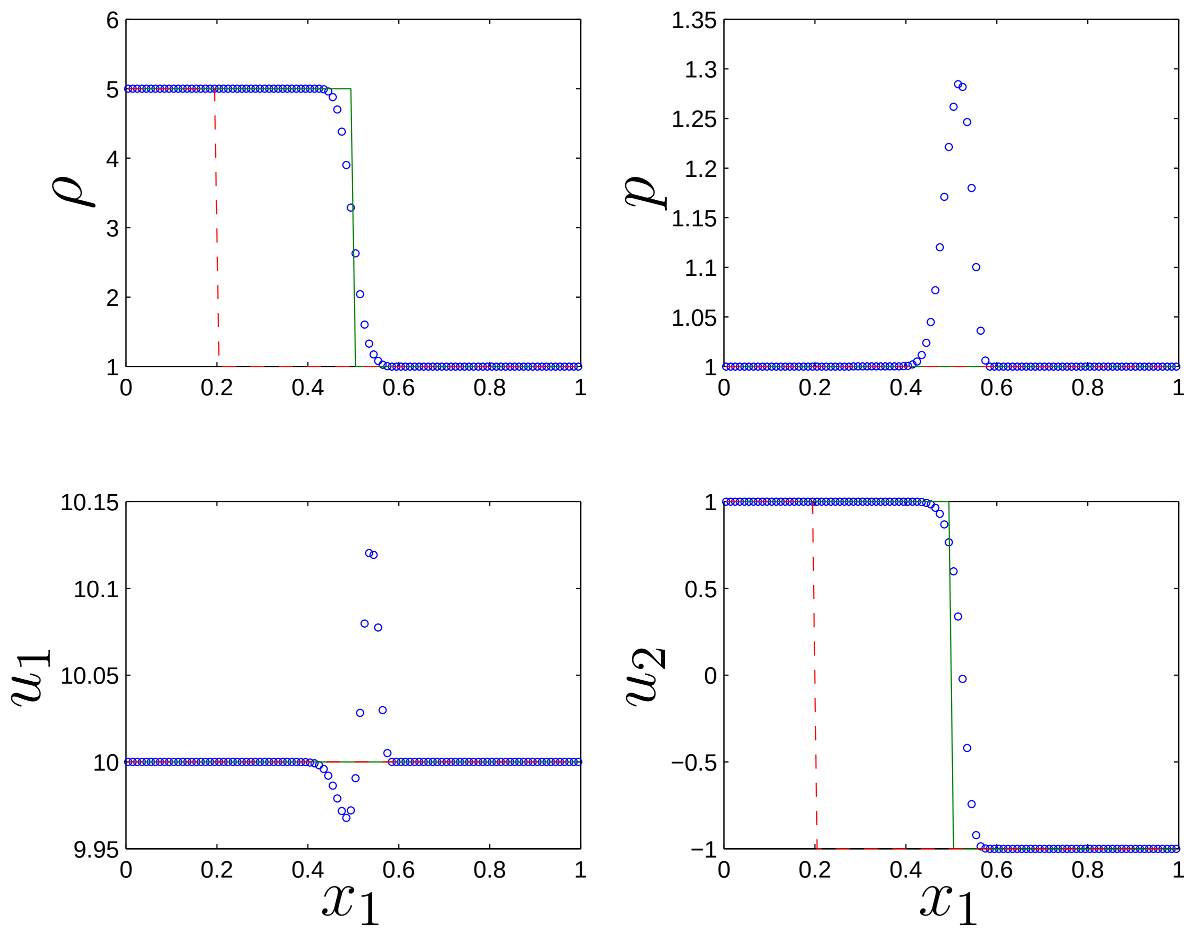
and $F_1(Q_{i\pm 1,j}, Q_{ij})$ denotes numerical flux, say, defined by

$$F_1(Q_{i\pm 1,j}, Q_{ij}) = f_1\left(q^*_{i\pm 1/2,j}\right) \qquad (q^*_{i\pm 1/2,j} \text{ Riemann solution})$$

Slip Line Problem (Cont.)

An example obtained by using a Godunov-type method

- Errors depend strongly on transverse velocity jump



Slip Line Problem (Cont.)

To devise a more accurate method for numerical resolution of slip lines, we may use

- Diffuse interface approach
  - Include transverse kinetic energy equation in the model & use its solution for pressure update

$$p = (\gamma - 1)\left(E - \frac{(\rho u_1)^2}{2\rho} + \frac{\rho u_2^2}{2}\right)$$

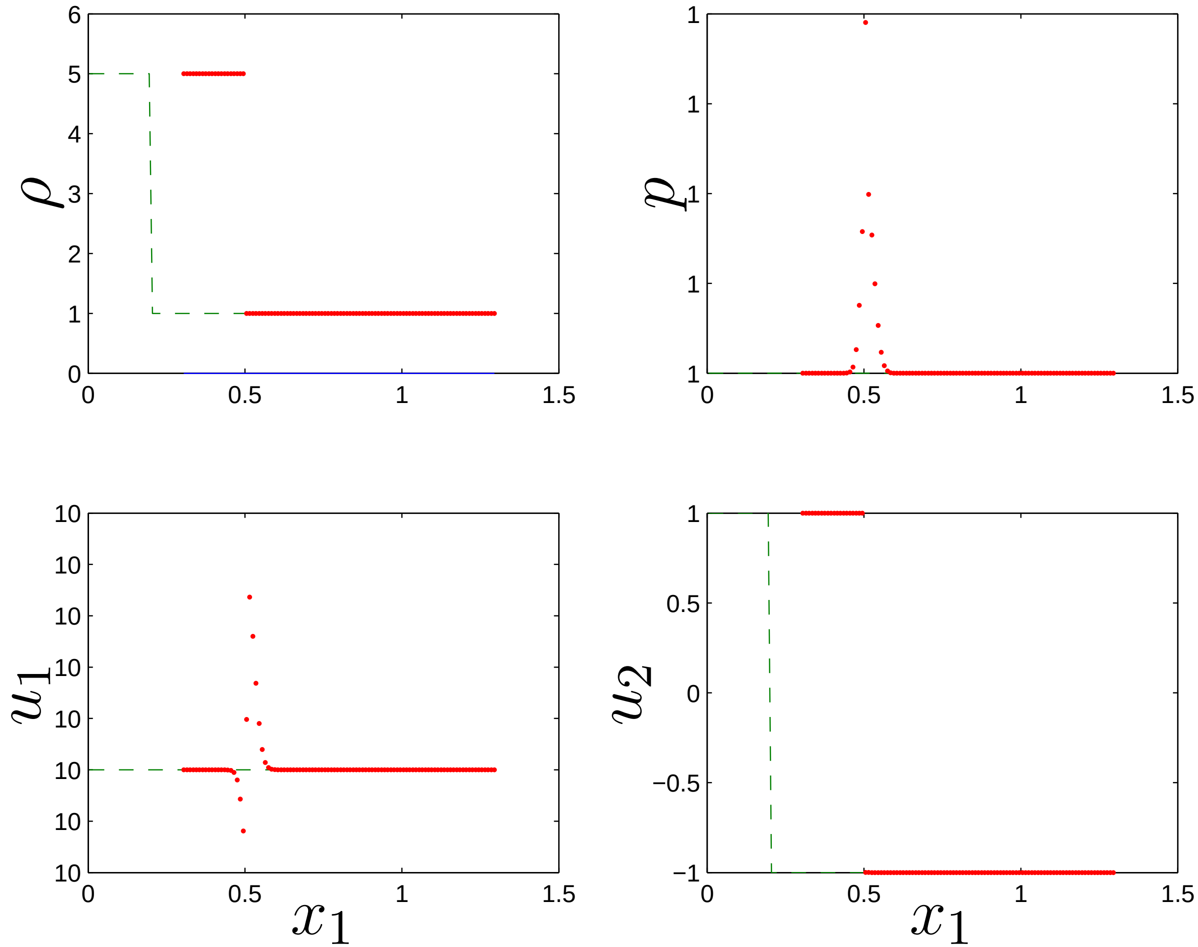
  This transverse kinetic equation should be modified so that there is no difficulty to work with shock waves

- Sharp interface approach
  - Front tracking or Lagrangian moving grid method

Slip Line Problem (Cont.)

Result obtained using a Lagrangian-like method

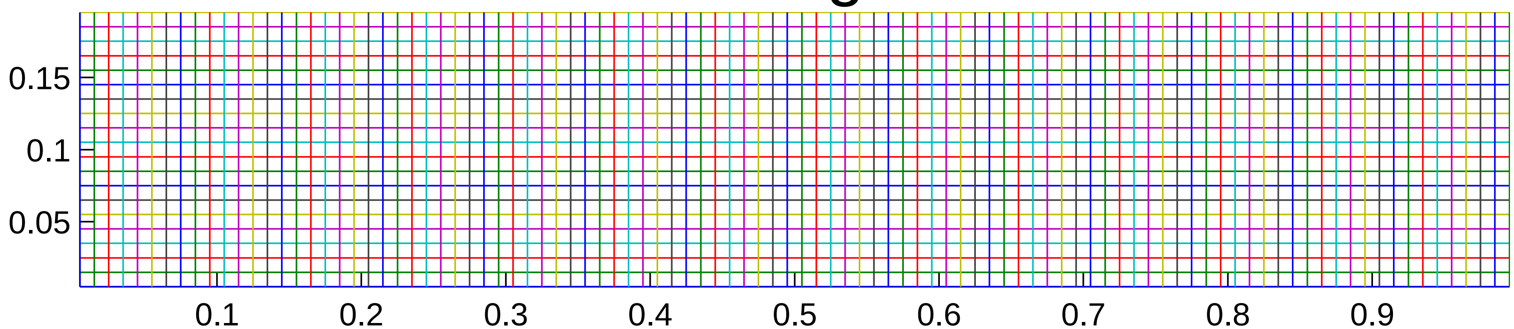
- Errors are on the order of machine epsilon



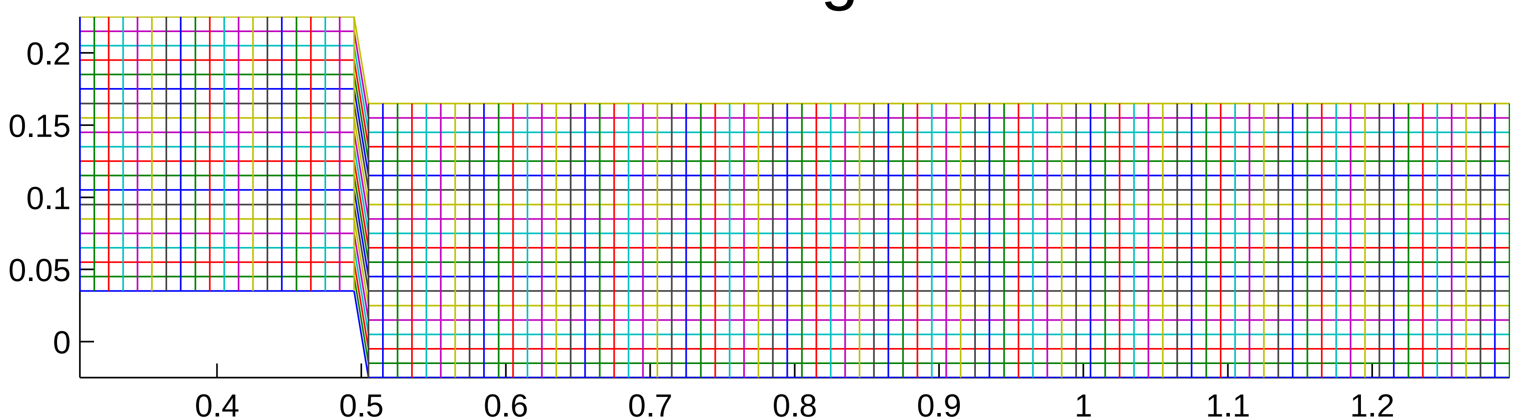
Slip Line Problem (Cont.)

Grid system for a Lagrangian run of slip line problem

Initial grid



Final grid



Euler Equations in Generalized Coord.

Lagrangian results shown above is based on solving Euler equations in generalized coordinates of the form

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

which is as a result of coordinate change $(\vec{x},\ t) \mapsto (\vec{\xi},\ \tau)$ via

$$\begin{aligned} dt &= d\tau, \\ dx_1 &= u_1^g \, d\tau + a_1 \, d\xi_1 + a_2 \, d\xi_2 + a_3 \, d\xi_3, \\ dx_2 &= u_2^g \, d\tau + b_1 \, d\xi_1 + b_2 \, d\xi_2 + b_3 \, d\xi_3, \\ dx_3 &= u_3^g \, d\tau + c_1 \, d\xi_1 + c_2 \, d\xi_2 + c_3 \, d\xi_3. \end{aligned}$$

Euler in Generalized Coord. (Cont.)

For convenience, we write

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

where

$$\tilde{q} = [\rho J, \rho u_1 J, \ldots, \rho u_N J, EJ]^T,$$

$$\tilde{f}_j = J\left[\rho U_j, \rho u_1 U_j + p\partial_{x_1}\xi_j, \ldots, \rho u_N U_j + p\partial_{x_N}\xi_j, EU_j + pU_j - p\partial_t \xi_j\right]^T,$$

$$\tilde{\psi} = [0, -\rho J \partial_{x_1}\phi, \ldots, -\rho J \partial_{x_N}\phi, -\rho J \vec{u}\cdot\nabla\phi]^T$$

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

$\vec{u}^g = h\vec{u}$: speed of grid motion, $\quad h \approx 1$

Material Line Problem

Now let us move on to our second interface-only problem that concerns a material line, separating regions of two different fluid phases

Again for simplicity, we consider a plane interface moving vertically from the left to right in x_1-direction.

Interface conditions for this problem are the same as in slip line case.

- Dynamic condition: $p_R = p_L$ (but there is jump in material quantities)
- Kinematic condition: $u_{1,R} = u_{1,L}$ & $\left(u_{2,R} - u_{2,L}\right) \neq 0$

Material Line Problem (Cont.)

Assume ideal gas law $p(\rho, e) = (\gamma - 1)\rho e$ for each fluid phase, where γ takes different quantities for each phase

In this instance, to ensure pressure equilibrium, from

$$\begin{aligned}\frac{\partial}{\partial t}\left(\frac{p}{\gamma - 1}\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\frac{p}{\gamma - 1}\right) + \\ \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_2^2\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\frac{1}{2}\rho u_2^2\right) = 0,\end{aligned}$$

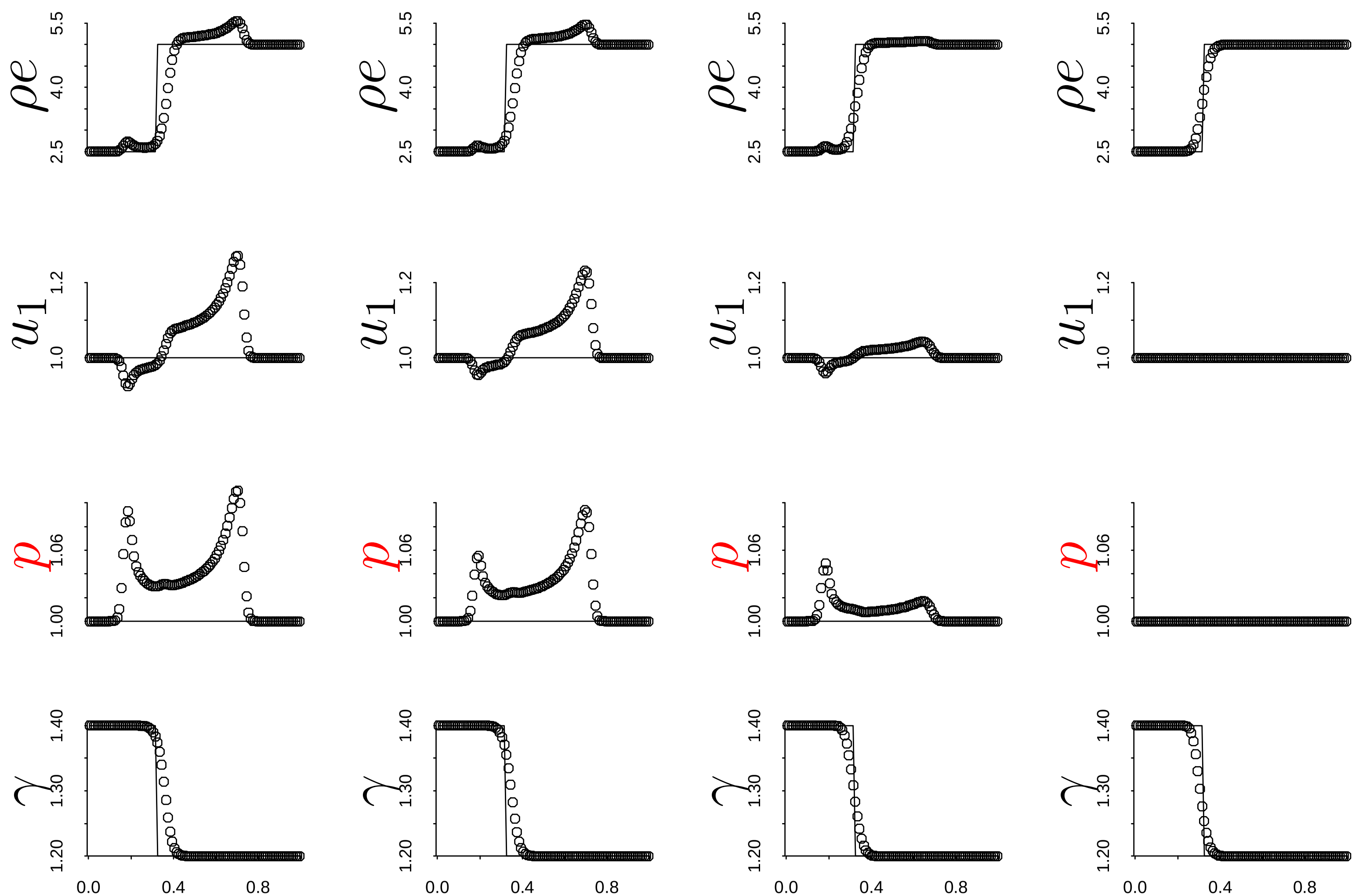
we should have

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_2^2\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\frac{1}{2}\rho u_2^2\right) = 0 \quad \& \quad \frac{\partial}{\partial t}\left(\frac{1}{\gamma - 1}\right) + \bar{u}_1 \frac{\partial}{\partial x_1}\left(\frac{1}{\gamma - 1}\right) = 0$$

Material Line Problem (Cont.)

Comparison with different γ model (no u_2 jump)

with $\rho\gamma$ | with $\rho/(\gamma-1)$ | with γ | with $1/(\gamma-1)$



Material Line Problem (Cont.)

Comments on problems with complex equation of state

- Even for single phase flow case, standard method will fail to attain pressure equilibrium, say, for example, van der Waals gas

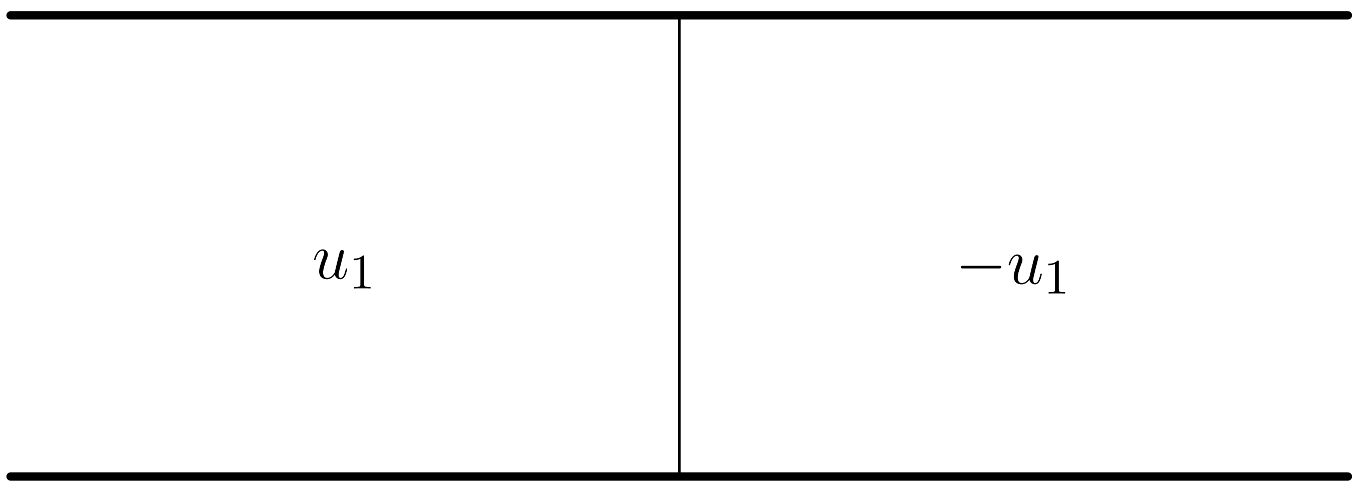
$$p(\rho, e) = \frac{\gamma - 1}{1 - b\rho} \left(\rho e + a\rho^2\right) - a\rho^2$$

- For multiphase flow case, suitable transport equations for characterizing numerical fluid mixing can be derived (see in a later)

Cavitation Problem: 1D

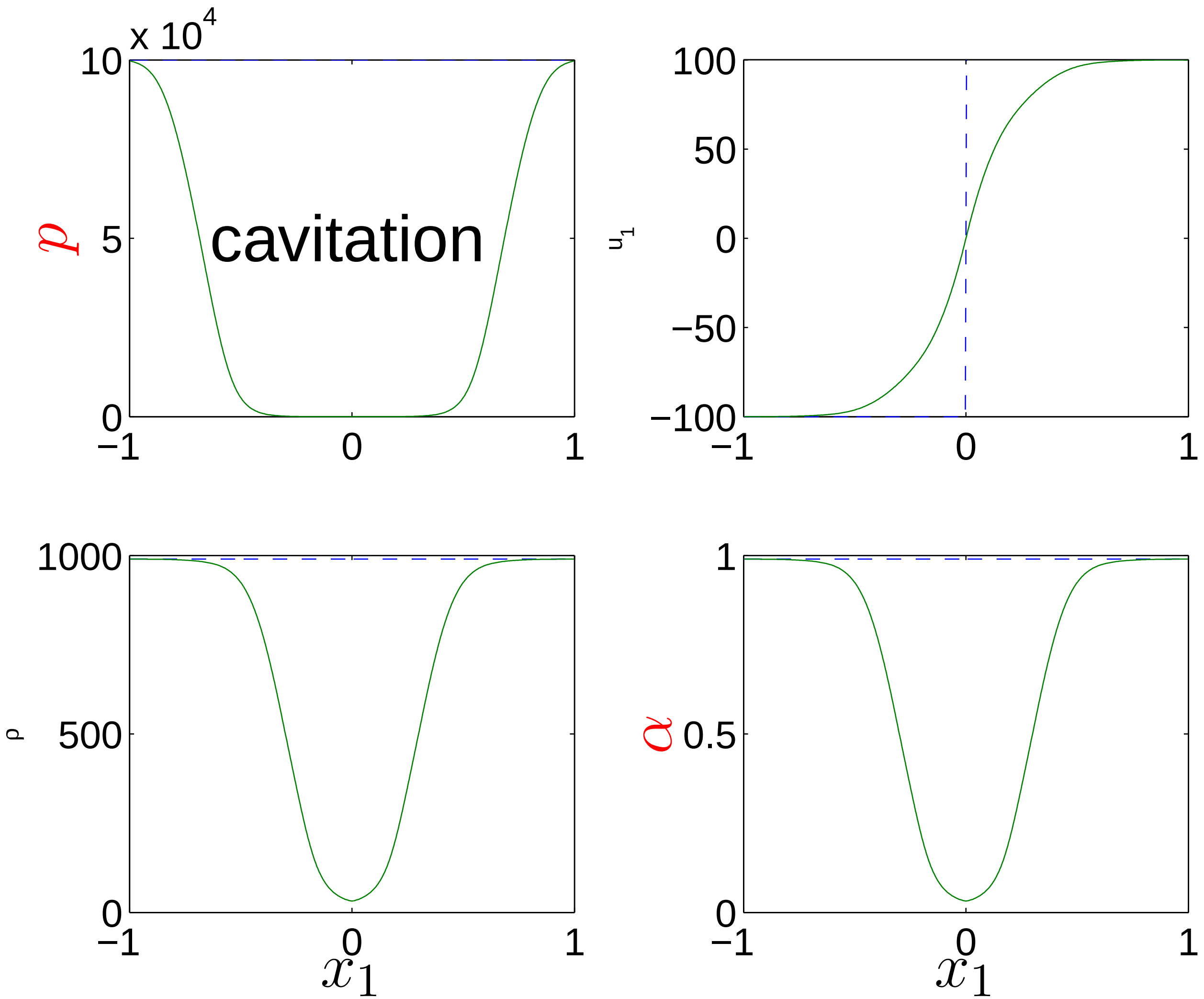
Homogeneous flow with standard atmospheric condition

- Due to opposite flow motion, pressure drop & formation of cavitation zone



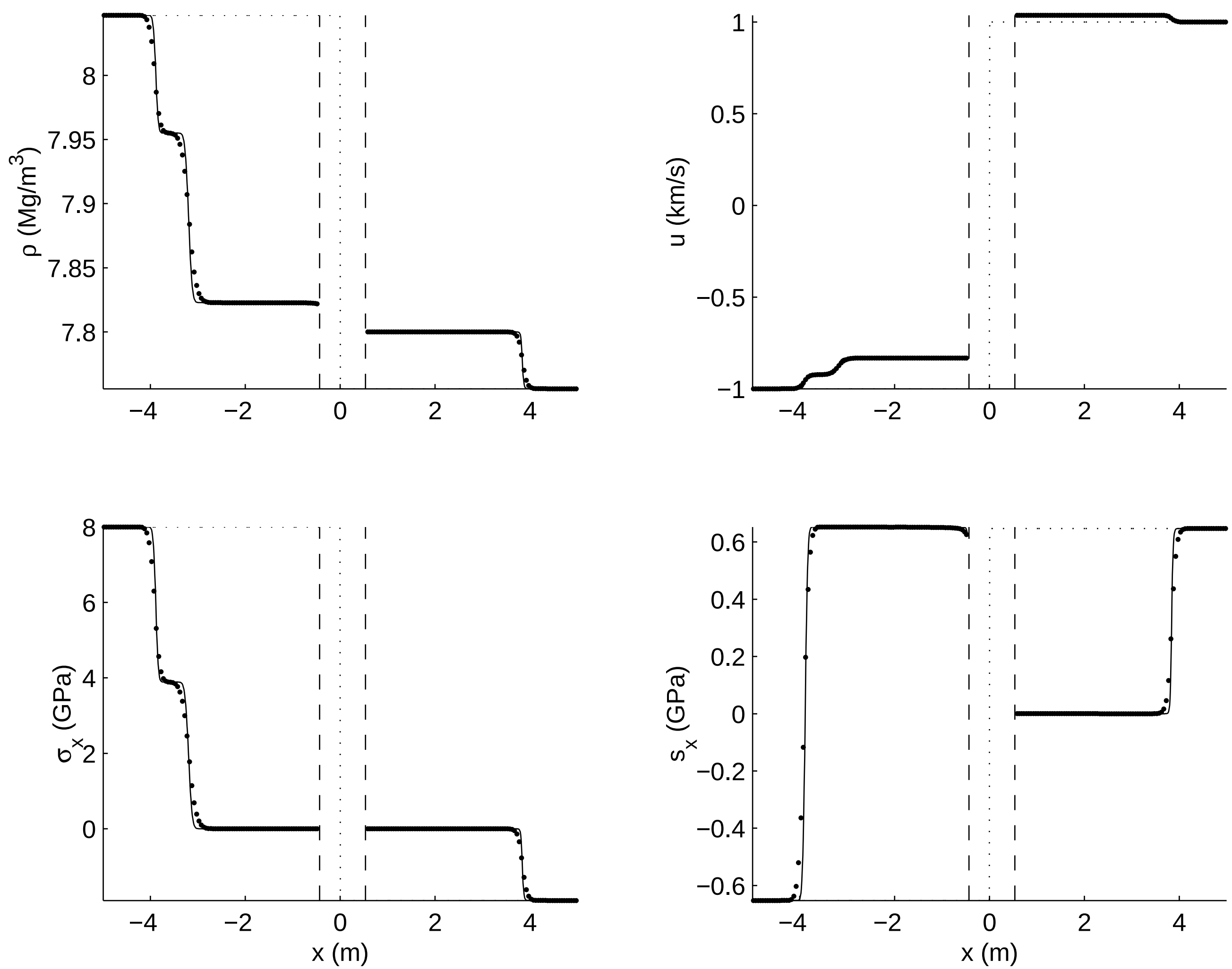
Cavitation test: $1D$

Dynamic cavitation formation (gas-liquid mixture case)



Cavitation test: 1D

Cavitation formation after $t = 0^+$ (elastic-plastic case)



Cavitating Problem (Cont.)

- Isentropic relaxation model (Saurel *et al.* JCP '09)

$$\frac{\partial}{\partial t}(\alpha_1\rho_1)+\sum_{j=1}^{N}\frac{\partial}{\partial x_j}(\alpha_1\rho_1 u_j)=0,$$

$$\frac{\partial}{\partial t}(\alpha_2\rho_2)+\sum_{j=1}^{N}\frac{\partial}{\partial x_j}(\alpha_2\rho_2 u_j)=0,$$

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

$$\frac{\partial \alpha_1}{\partial t}+\sum_{j=1}^{N}u_j\frac{\partial \alpha_1}{\partial x_j}=\mu\left(p_1\left(\rho_1\right)-p_2\left(\rho_2\right)\right)$$

Each phasic pressure p_ι satisfies $p_\iota(\rho)=(p_0+\mathcal{B})\left(\rho/\rho_0\right)^\gamma-\mathcal{B}$
Mixture pressure p satisfies $p=\alpha_1 p_1+\alpha_2 p_2, \quad \mu$: parameter

Cavitating Problem (Cont.)

There are some funadmental issues for numerical resolution cavitating problems that I do not show here. But in general the following two things are important for the problem

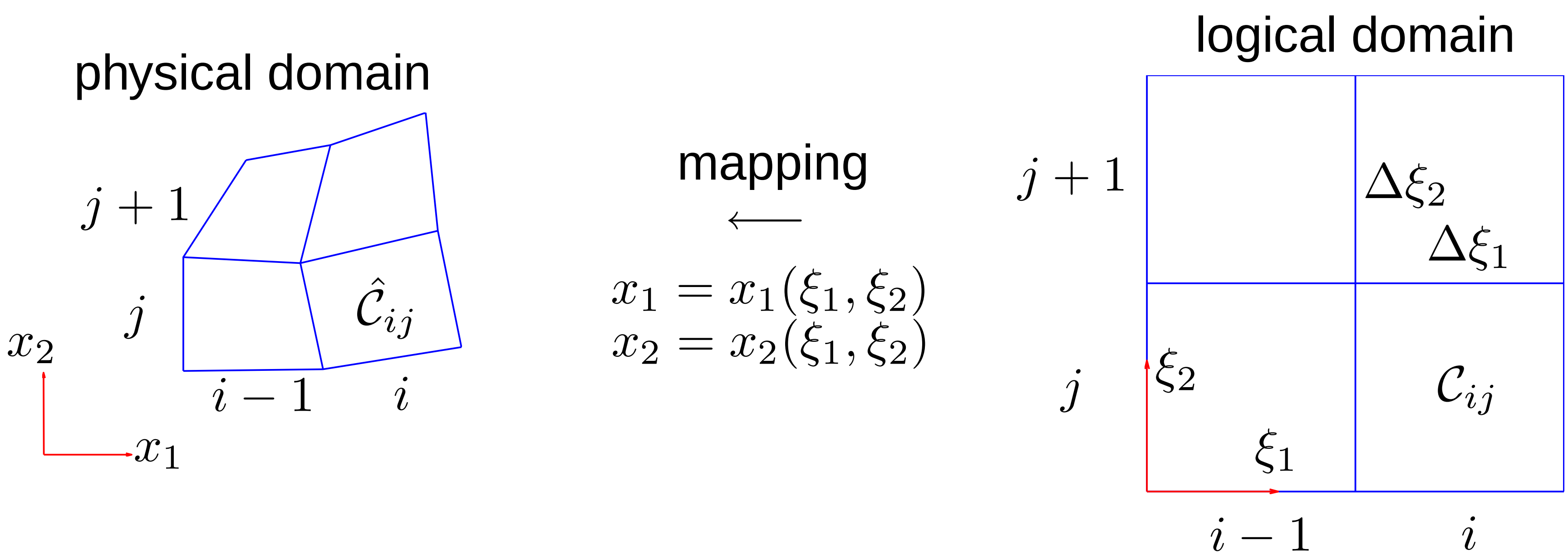
- Devise of general cavitation-capturing method ?
- Relaxation model to elastic-plastic & to other physical laws

Mapped Grid Method

To solve problem with complex geometries, here we consider body-fitted mapped grid method for its easy extension to three dimensions

Employ finite volume formulation of numerical solution

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



Mapped Grid Method (Cont.)

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

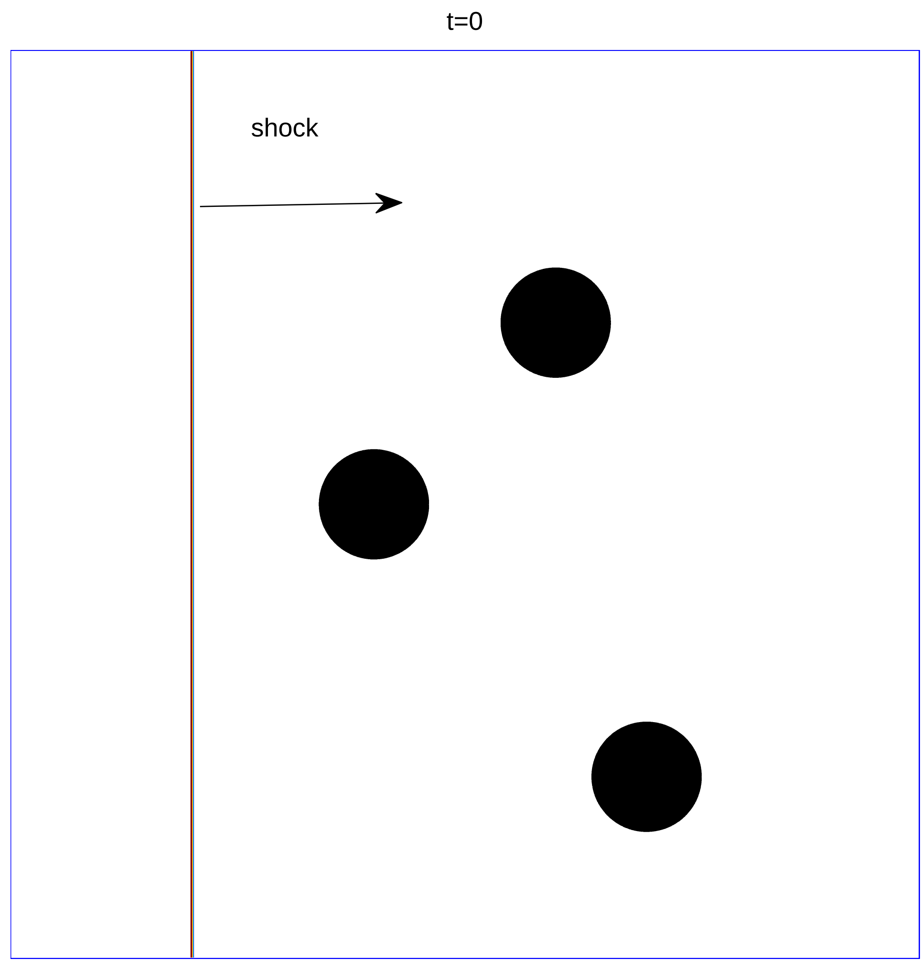
$$\frac{\partial q}{\partial t} + \sum_{j=1}^{N} \frac{\partial \tilde{f}_j}{\partial \xi_j} = \psi(q)$$

A simple dimensional-splitting method based on wave propagation approach of LeVeque *et al.* is used, *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

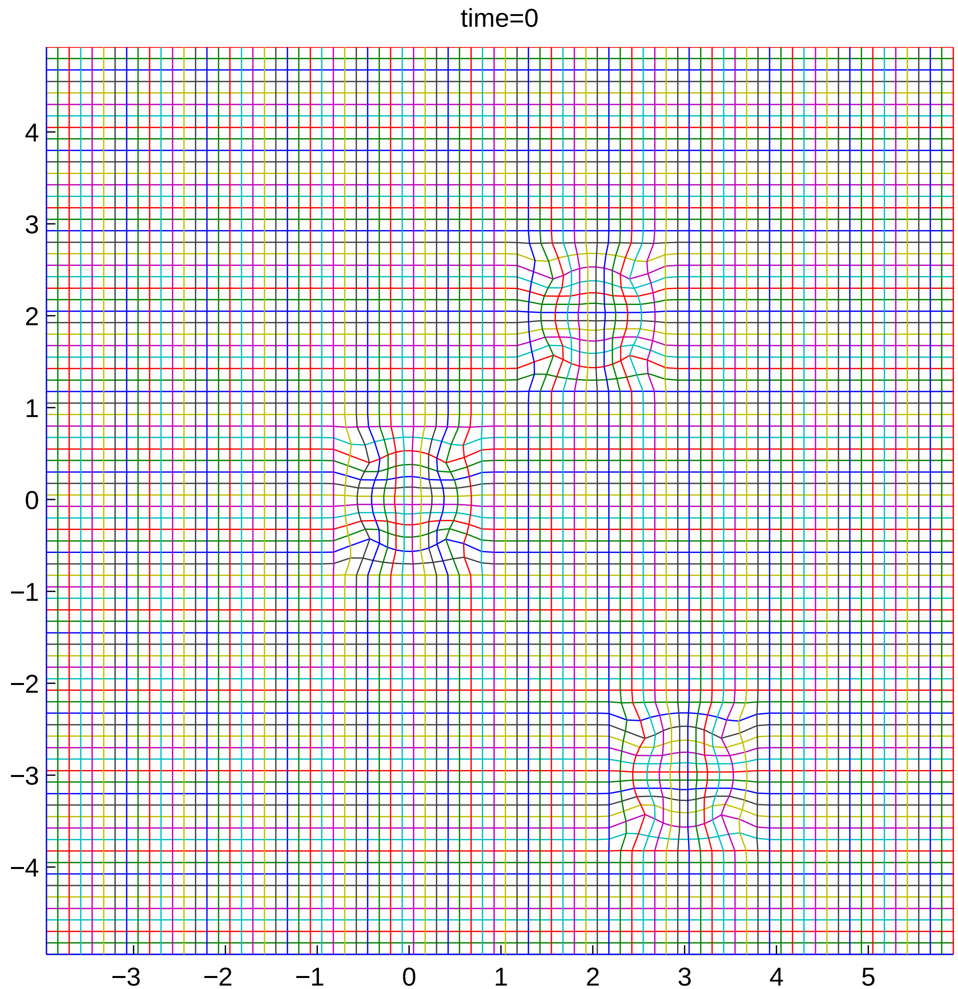
Shock waves over circular array

- A Mach 1.42 shock wave in water over a circular array



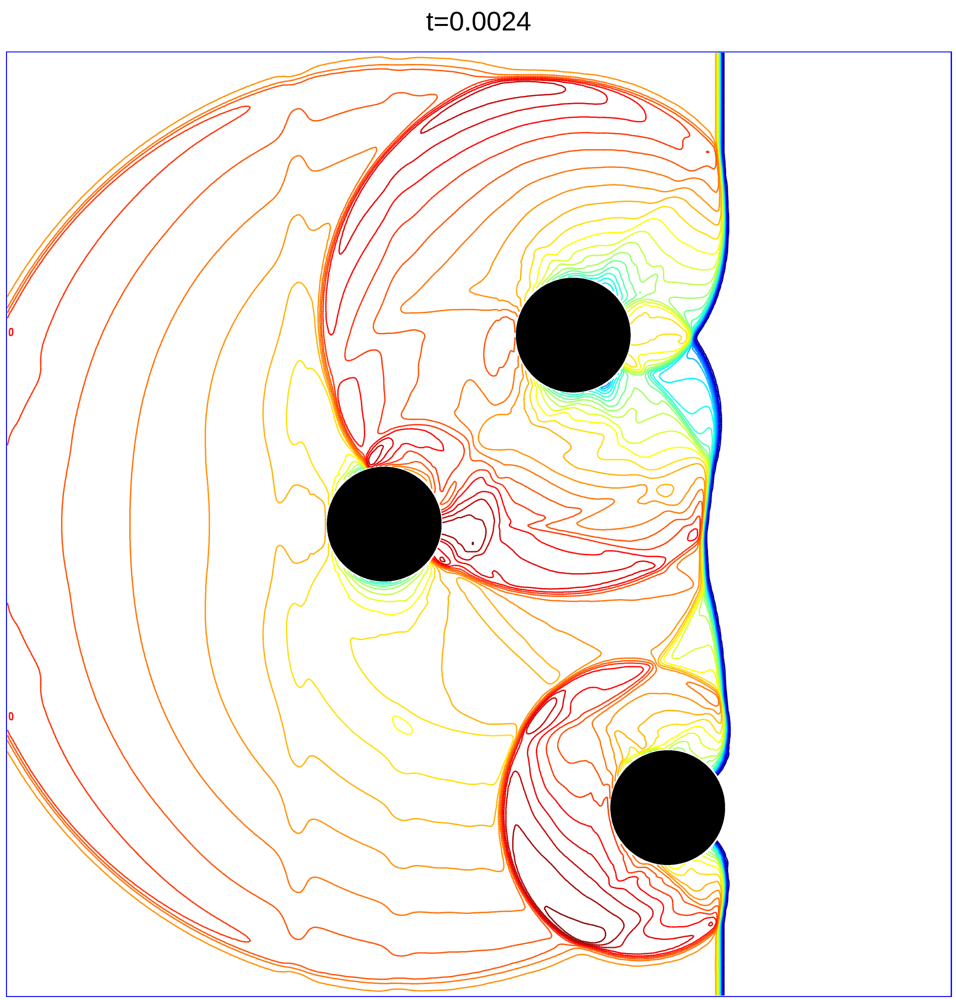
Shock waves over circular array

- Grid system



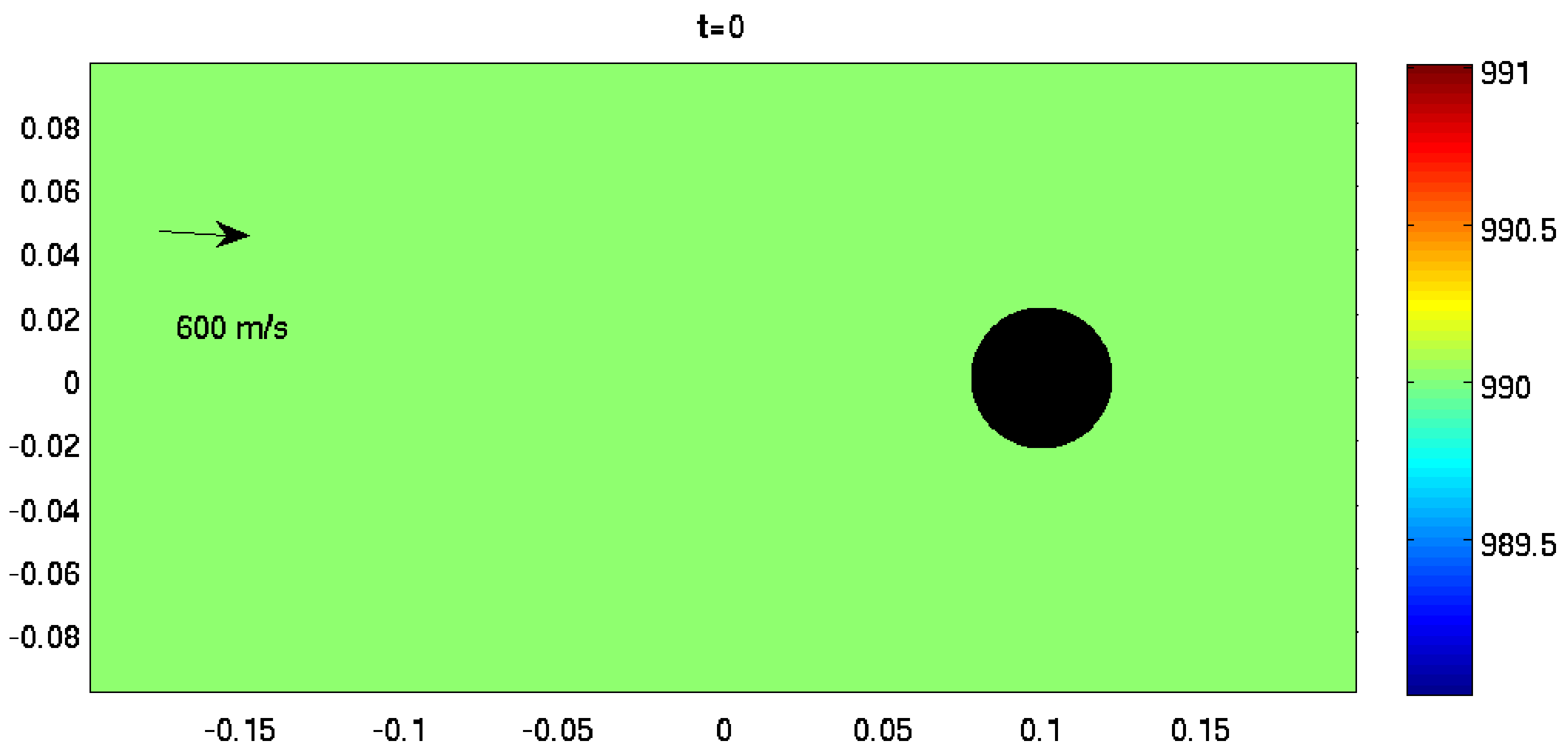
Shock waves over circular array

- Contours for density



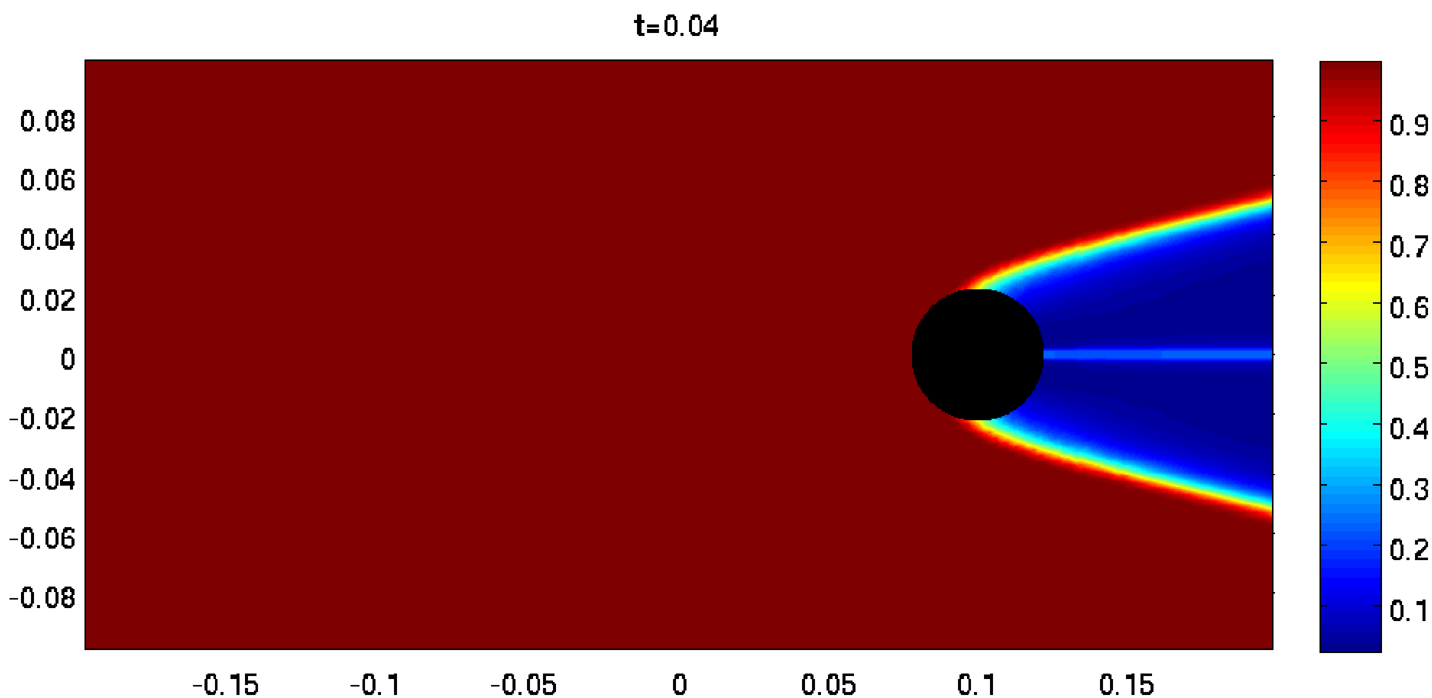
Cavitation test: 2D steady state

- Uniform gas-liquid mixture with speed 600m /s over a circular region



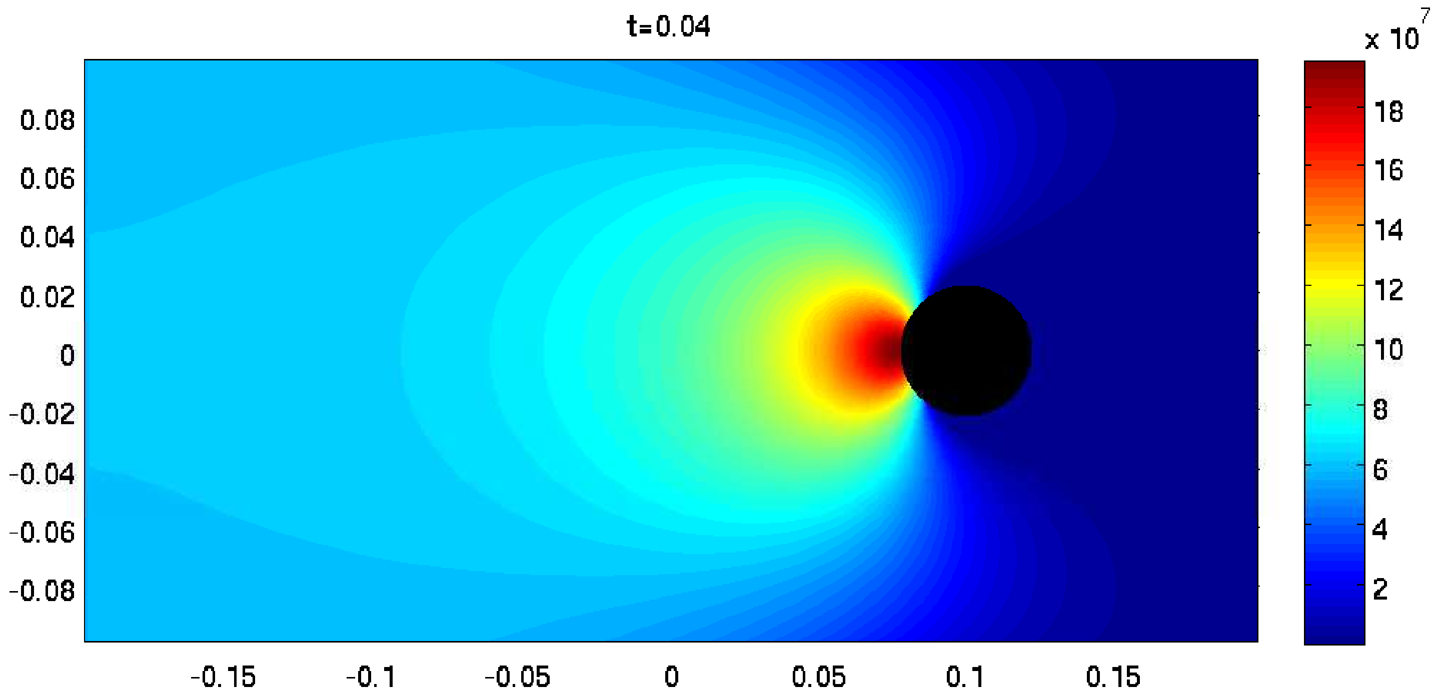
Cavitation test: 2D steady state

- Pseudo colors of volume fraction
  - Formation of cavitation zone (Onset–shock induced, diffusion, . . . ?)



Cavitation test: 2D steady state

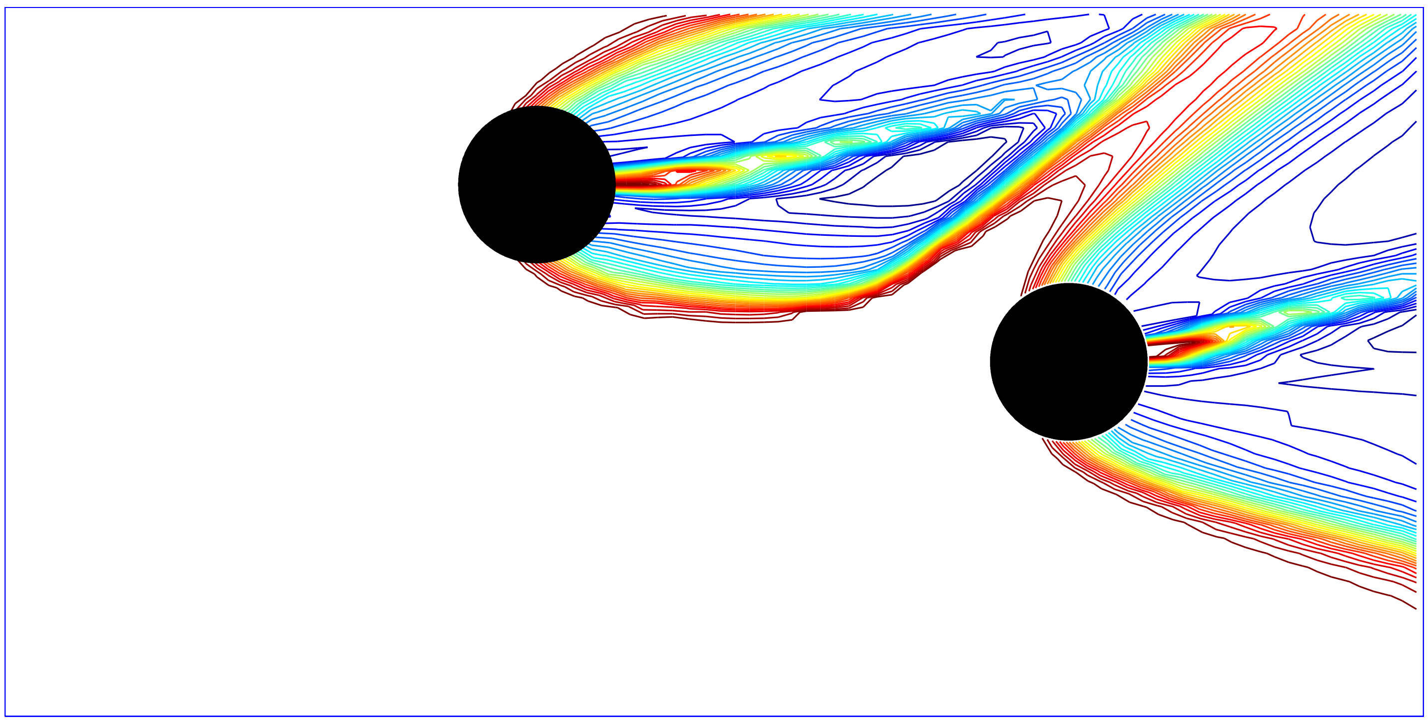
- Pseudo colors of pressure
  - Smooth transition across liquid-gas phase boundary



Cavitation test: 2D steady state

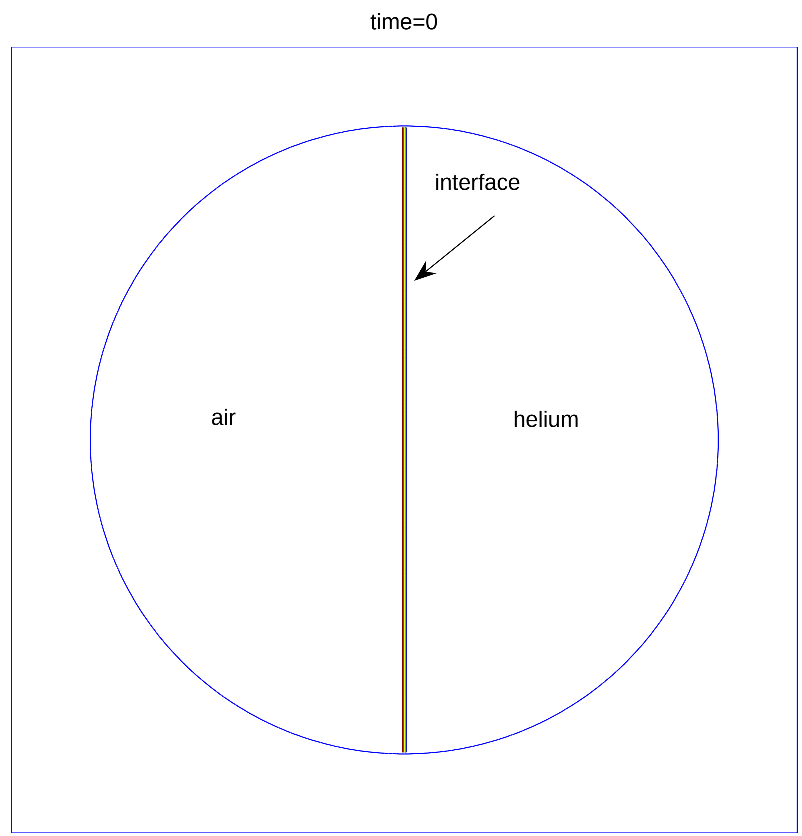
- Pseudo colors of volume fraction: 2 circular case
  - Convergence of solution as the mesh is refined ?

t=0.05



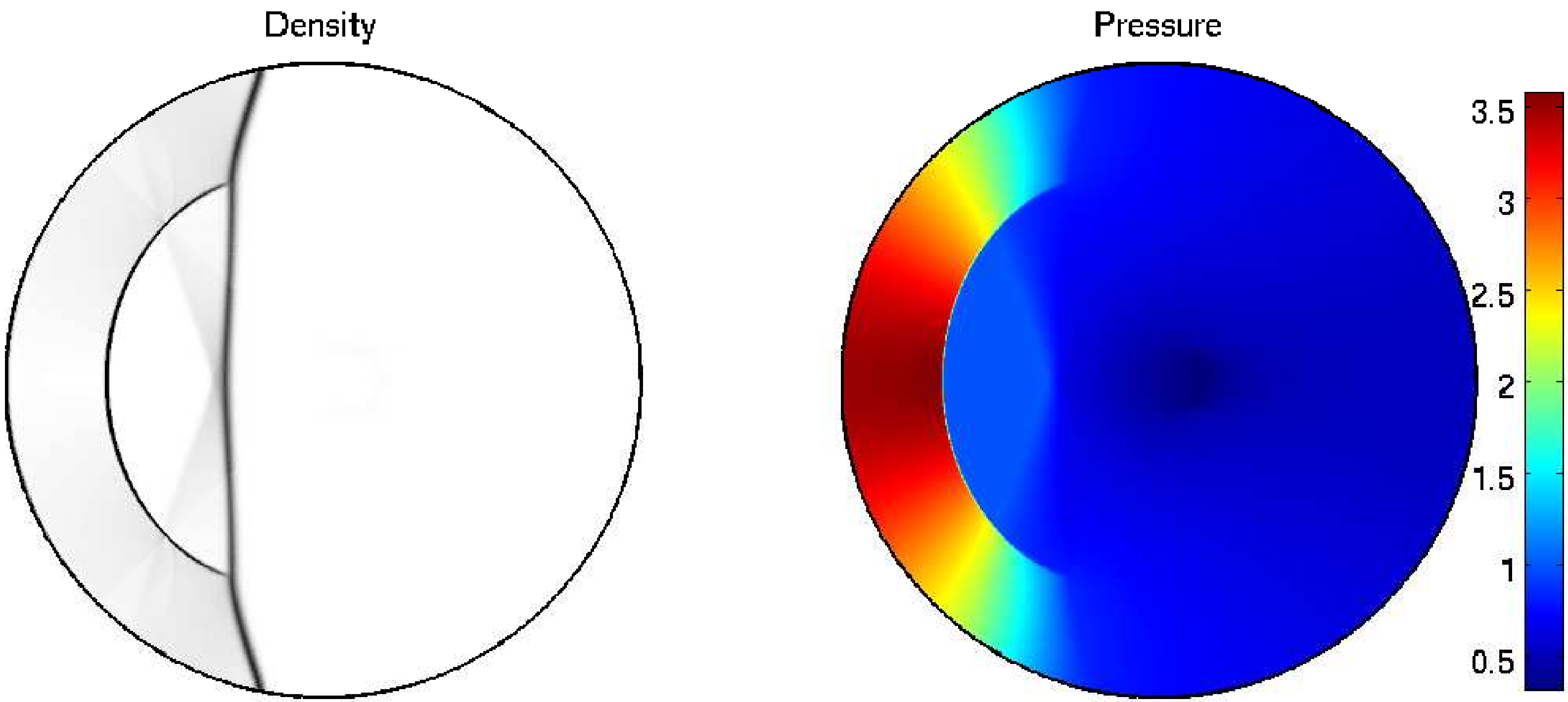
Moving cylindrical vessel

- Initial setup



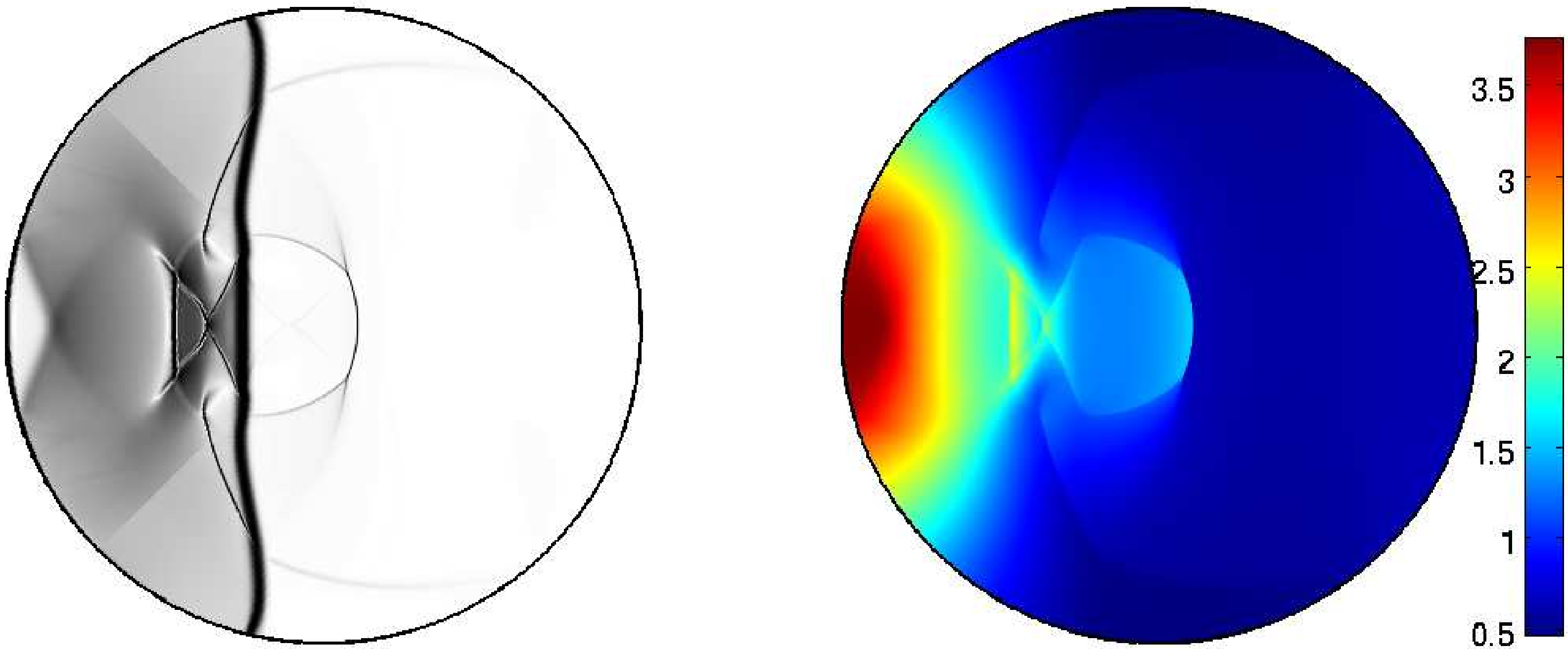
Moving cylindrical vessel

- Solution at time $t = 0.25$



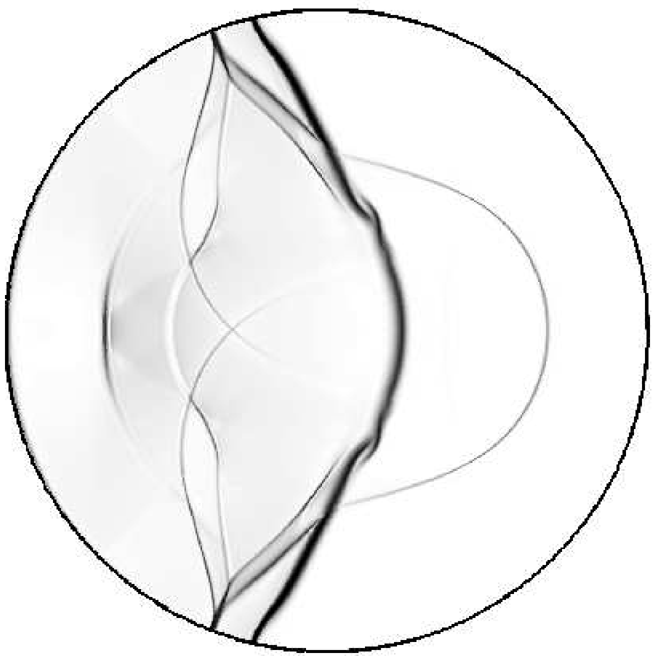
Moving cylindrical vessel

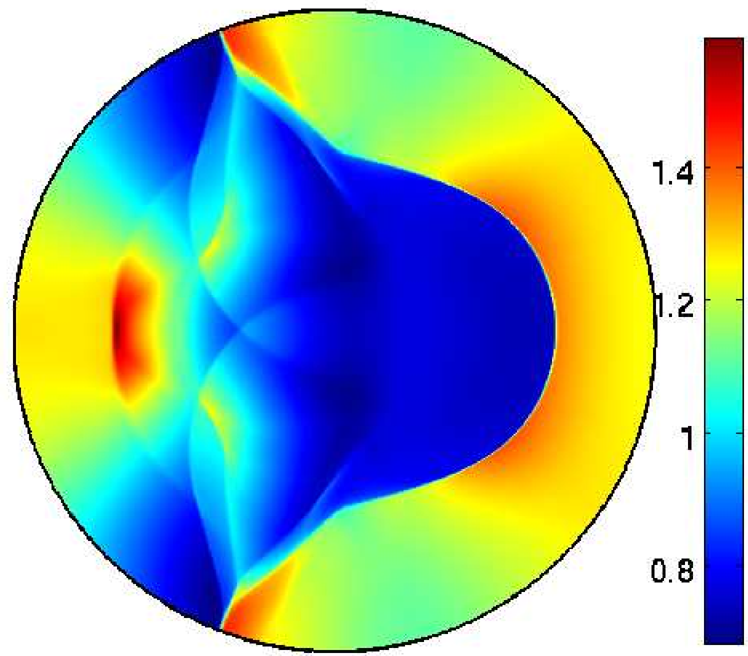
- Solution at time $t = 0.5$



Moving cylindrical vessel

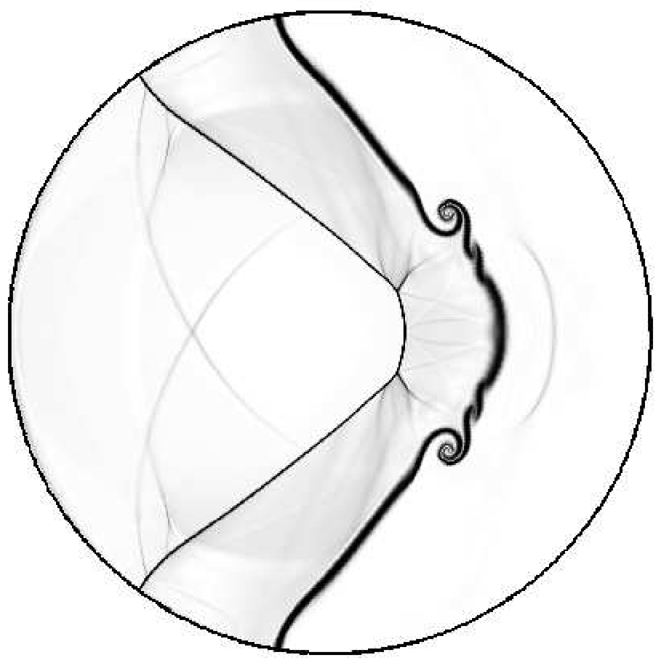
- Solution at time $t = 0.75$

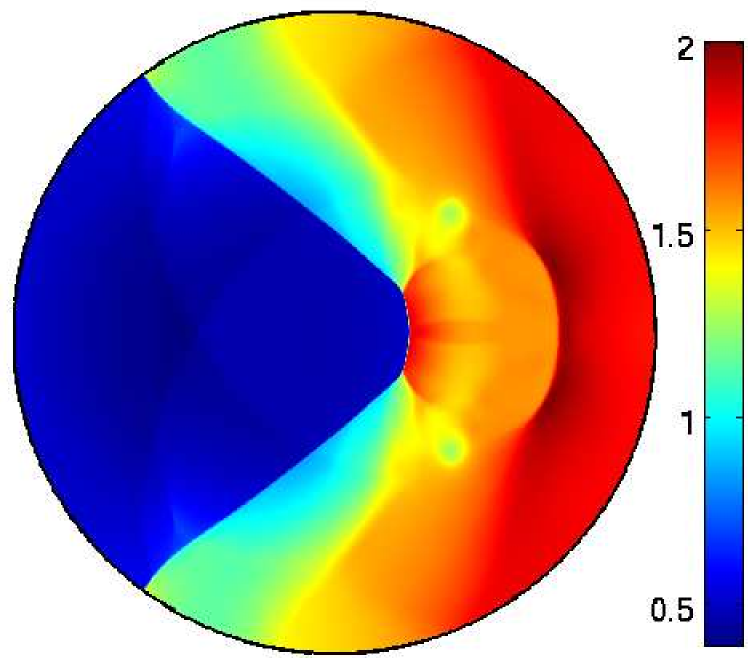




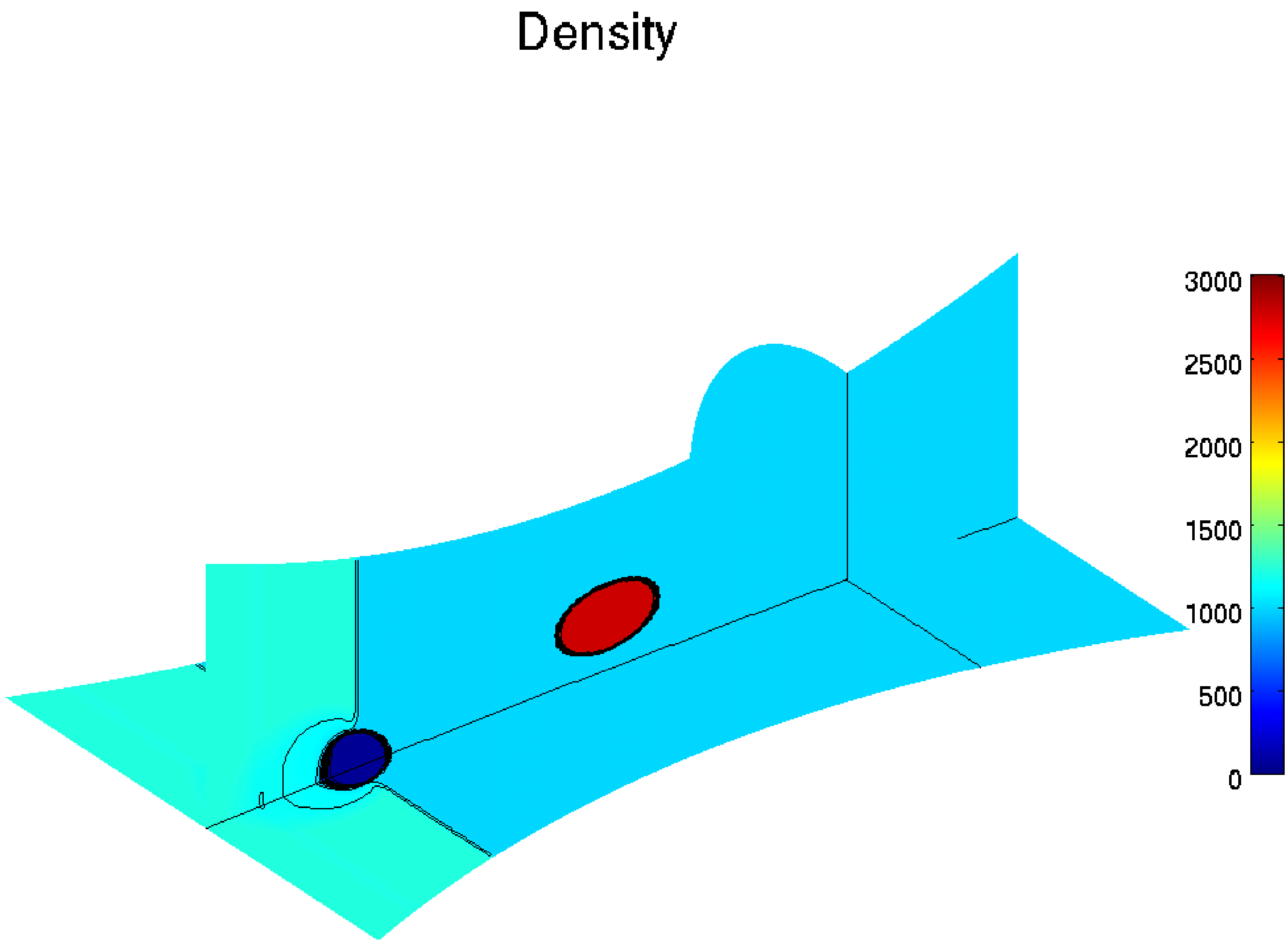
Moving cylindrical vessel

- Solution at time $t = 1$

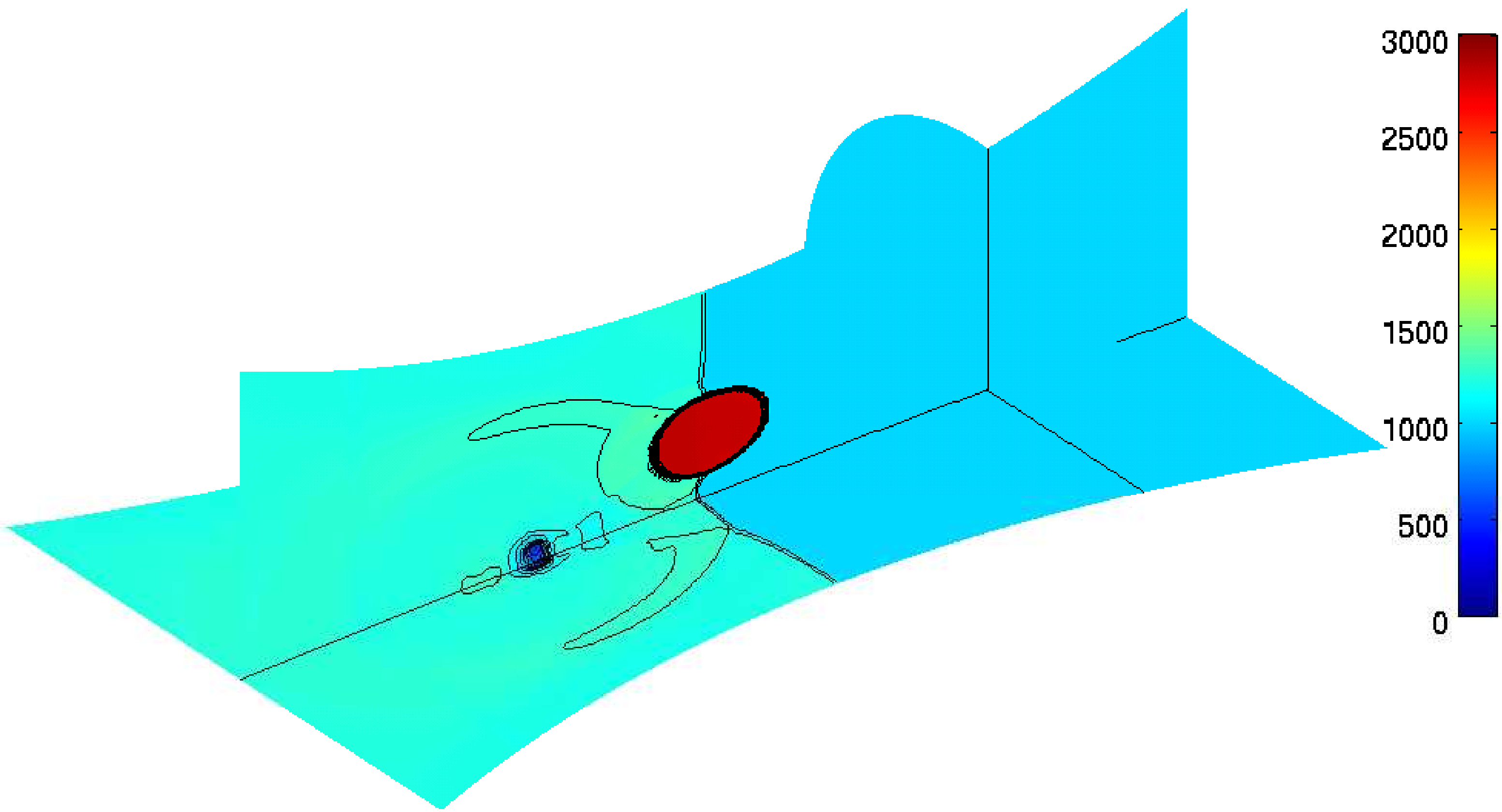




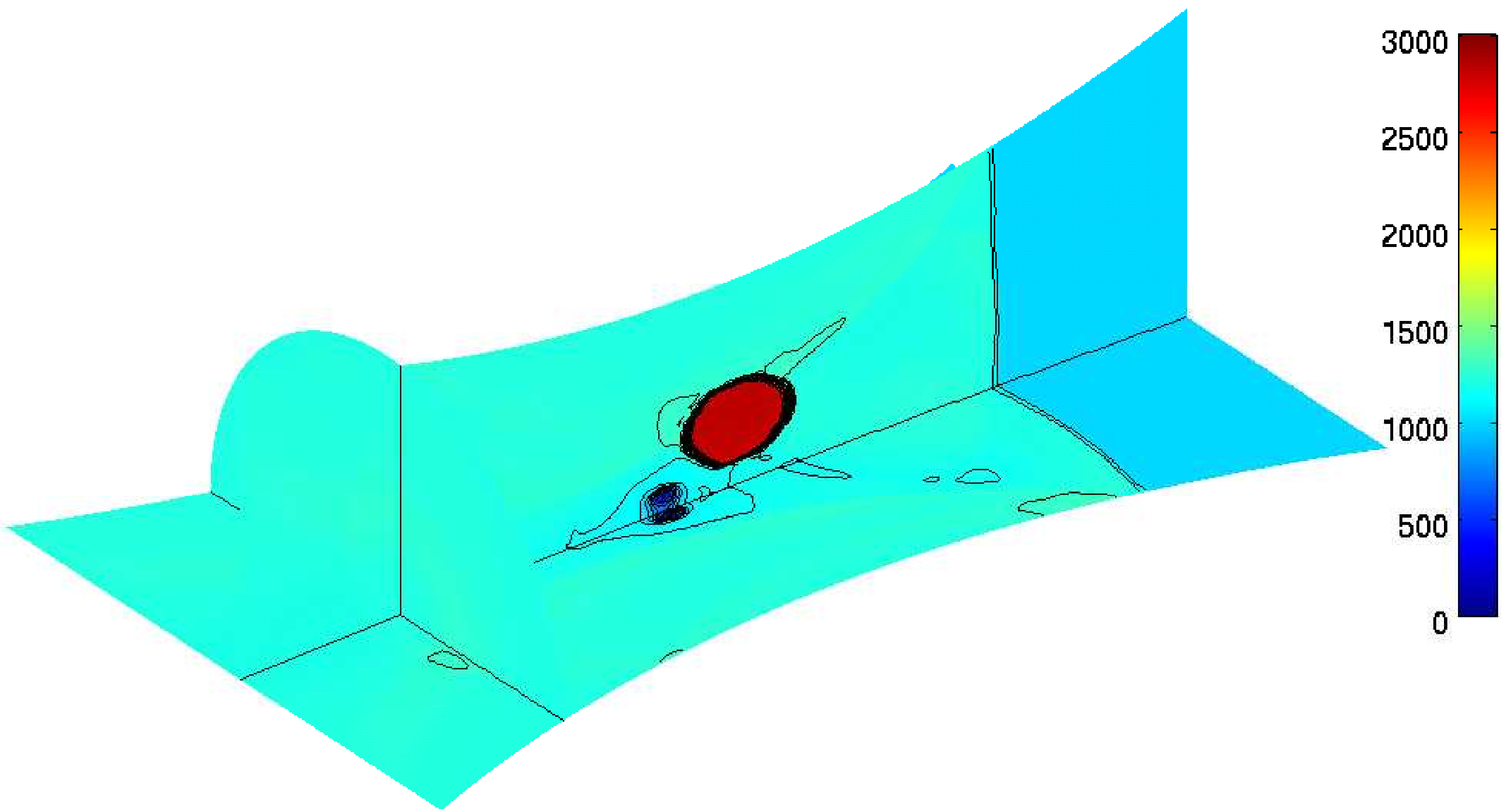
Shock wave & Disperse phases



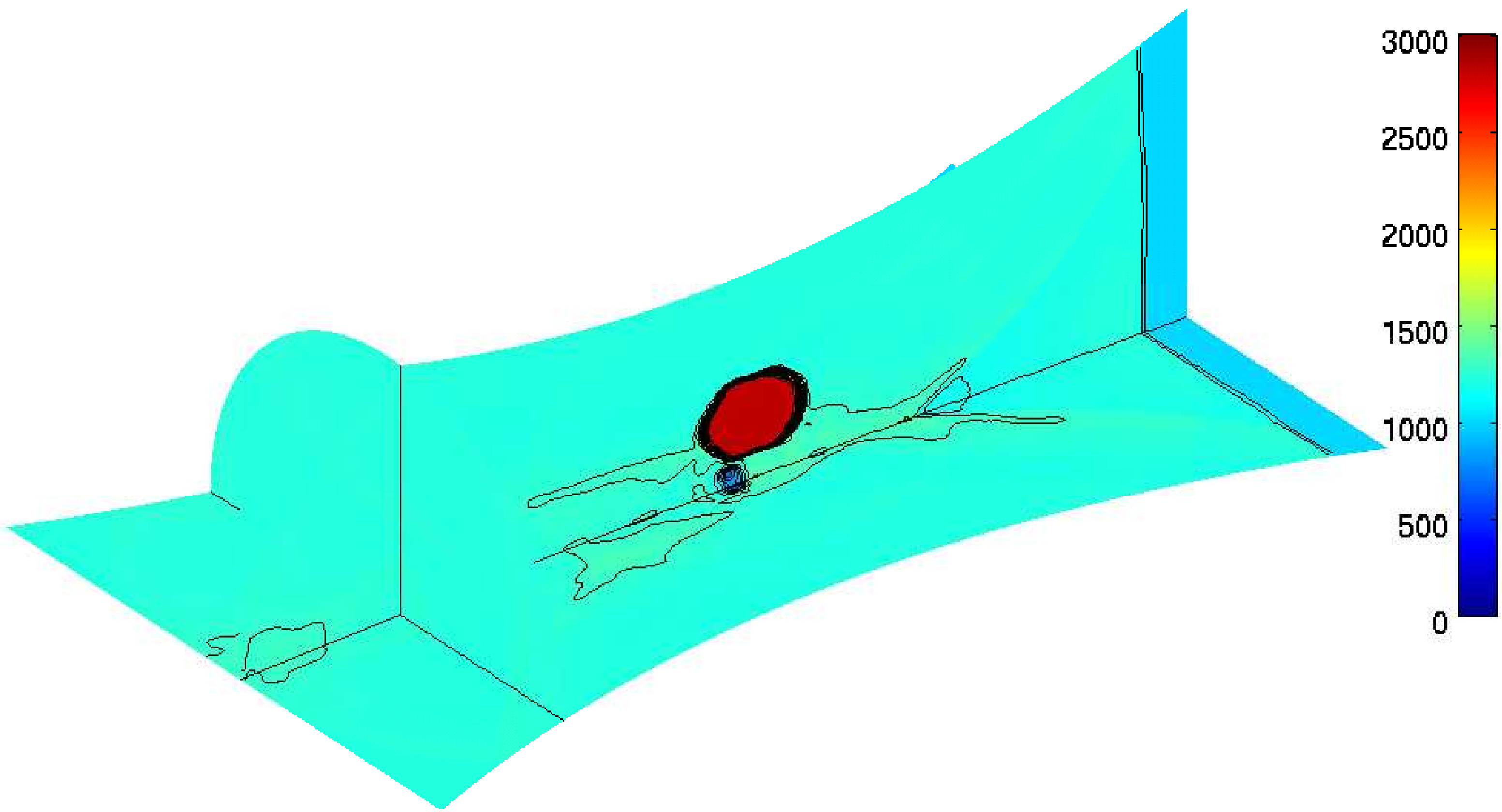
Shock wave & Disperse phases



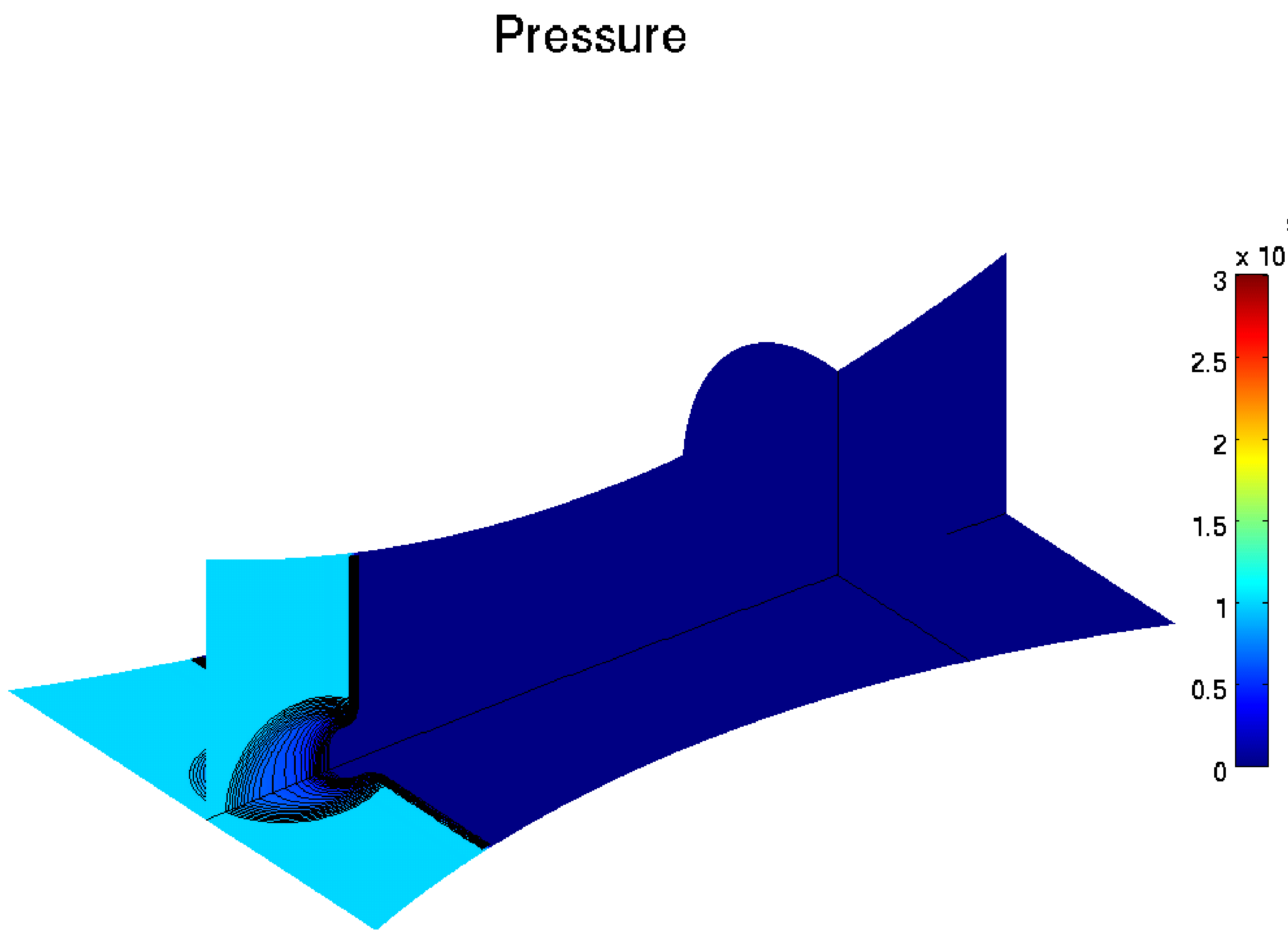
Shock wave & Disperse phases



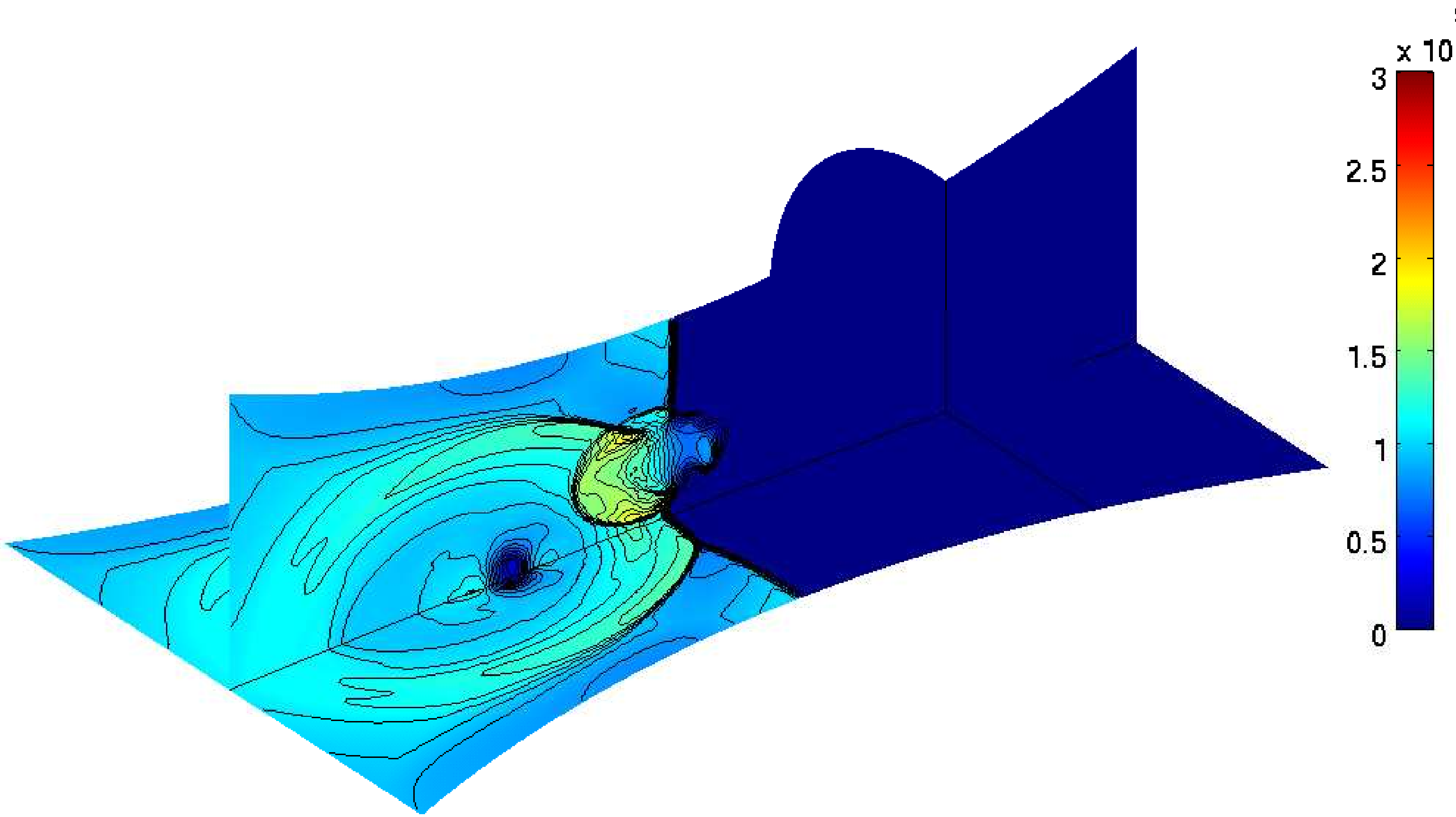
Shock wave & Disperse phases



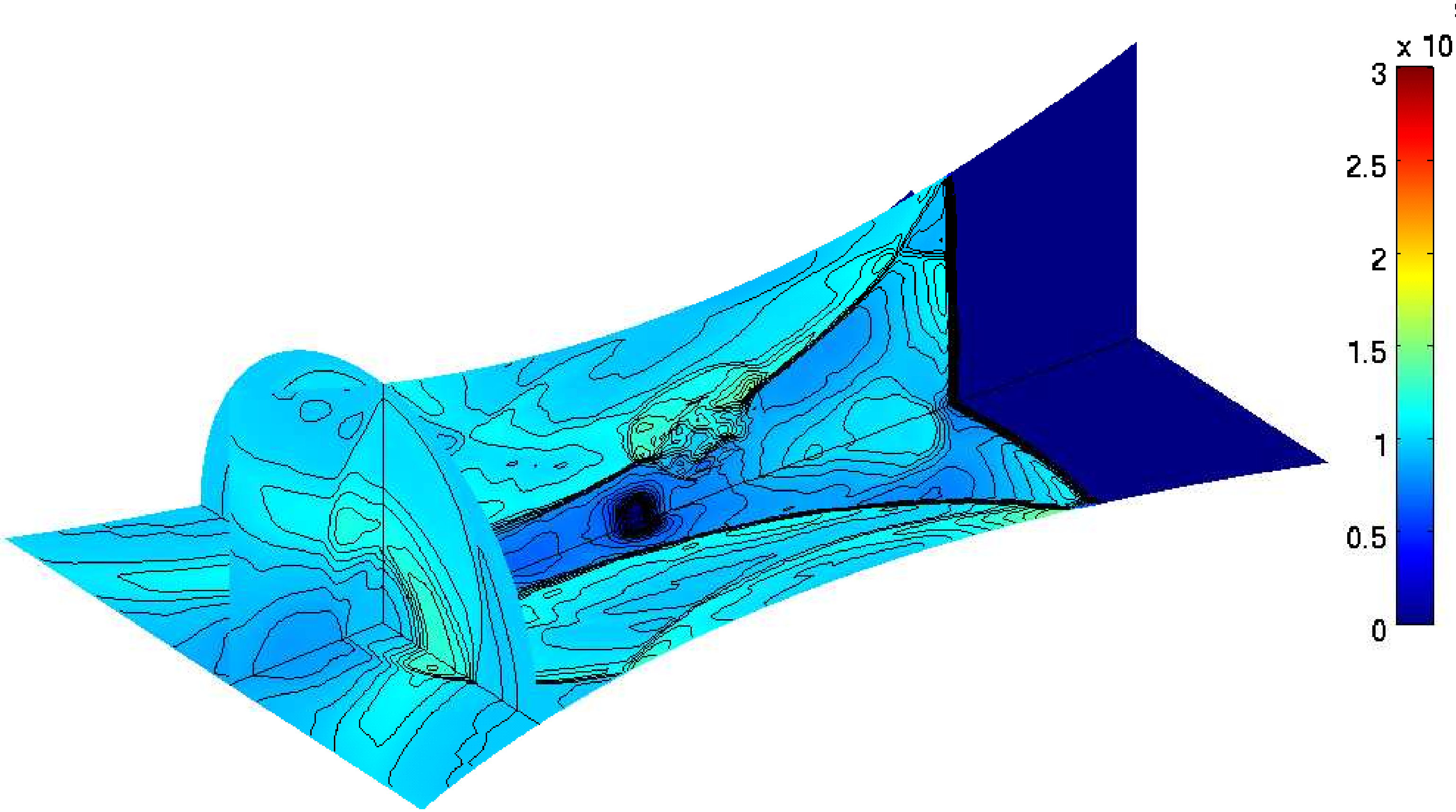
Shock wave & Disperse phases



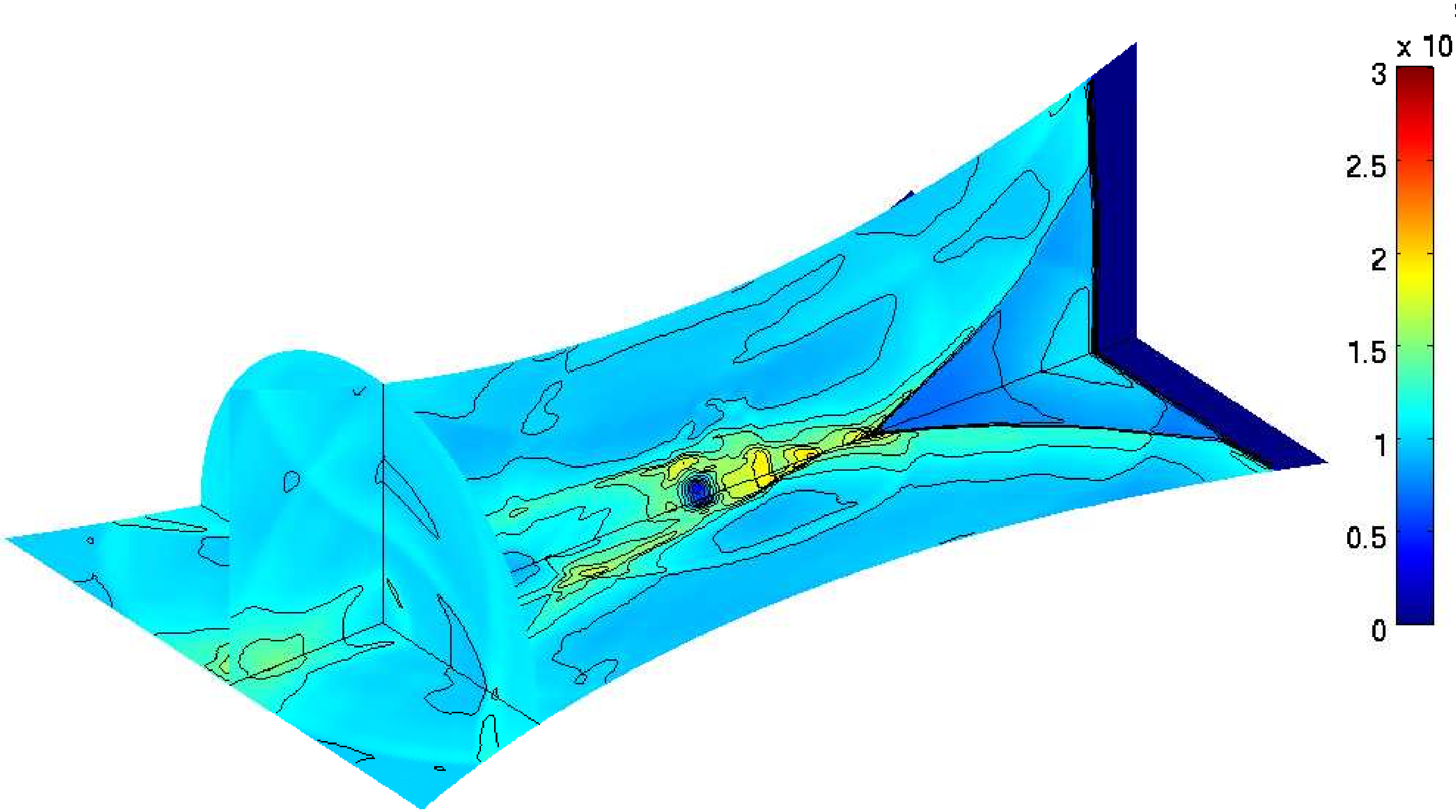
Shock wave & Disperse phases



Shock wave & Disperse phases



Shock wave & Disperse phases



Compressible Multiphase Flow

- Homogeneous equilibrium pressure & velocity across material interfaces
- Volume-fraction based model equations (Shyue JCP '98, Allaire *et al.* JCP '02)

$$\frac{\partial}{\partial t}(\alpha_i\rho_i) + \frac{1}{J}\sum_{j=1}^{N_d}\frac{\partial}{\partial \xi_j}(\alpha_i\rho_i U_j) = 0, \quad i = 1,2,\ldots,m_f$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{1}{J}\sum_{j=1}^{N_d}\frac{\partial}{\partial \xi_j}(\rho u_i U_j + pJ_{ji}) = 0, \quad i = 1,2,\ldots,N_d,$$

$$\frac{\partial E}{\partial t} + \frac{1}{J}\sum_{j=1}^{N_d}\frac{\partial}{\partial \xi_j}(EU_j + pU_j) = 0,$$

$$\frac{\partial \alpha_i}{\partial t} + \frac{1}{J}\sum_{j=1}^{N_d}U_j\frac{\partial \alpha_i}{\partial \xi_j} = 0, \quad i = 1,2,\ldots,m_f - 1;$$

Thank You