# Reaction diffusion, combustion and multiphase flows

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June 20, 2011

# Applications of conservation laws

General form of the conservation law

$$q_t + \nabla \cdot f(q) = 0$$

where $f(q), q \in \mathcal{R}^m$.

With source term

$$q_t + \nabla \cdot f(q) = \Psi(q, \ldots)$$

Source term models some kind of chemical reaction, change of state, diffusion and so on.

# Applications

- Euler equations of gas dynamics
- Combustion and detonation
- Multiphase flow of air-steam-water mixtures
- Biological pattern formation
- Shallow water wave equations on the sphere

# Gas dynamics - the Euler equations

Compressible flow equations of gas dynamics :

$$\begin{aligned} \rho_t + (u\rho)_x &= 0 \\ (\rho u)_t + (\rho u^2 + p)_x &= 0 \\ E_t + (u\,(E+p))_x &= 0 \end{aligned}$$

The equation of state is given by :

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho u^2$$

where p is the pressure.

Conserved quantities are $\rho$, momentum $\rho u$, and energy $E$.

# Euler equations for compressible flow

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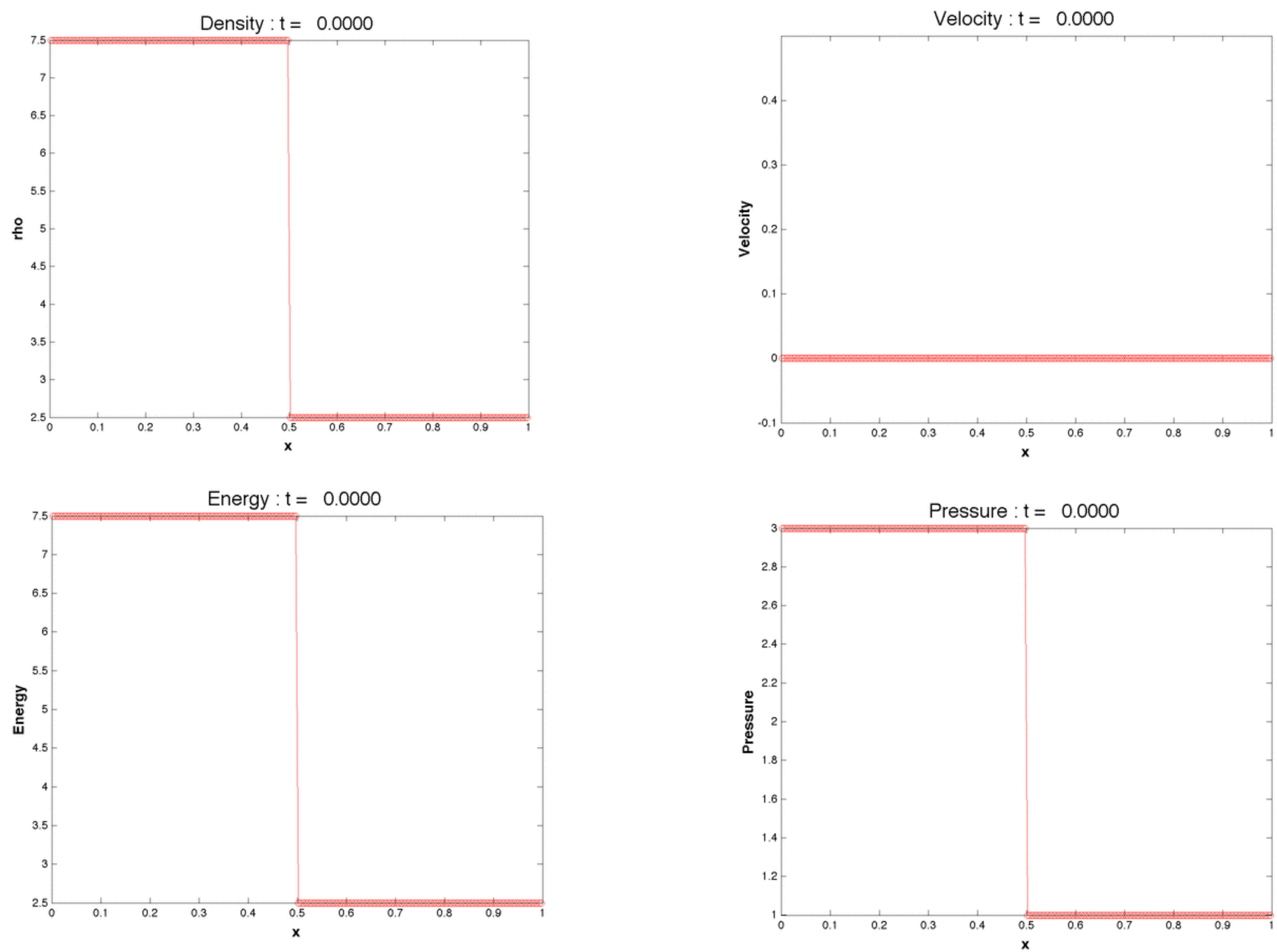

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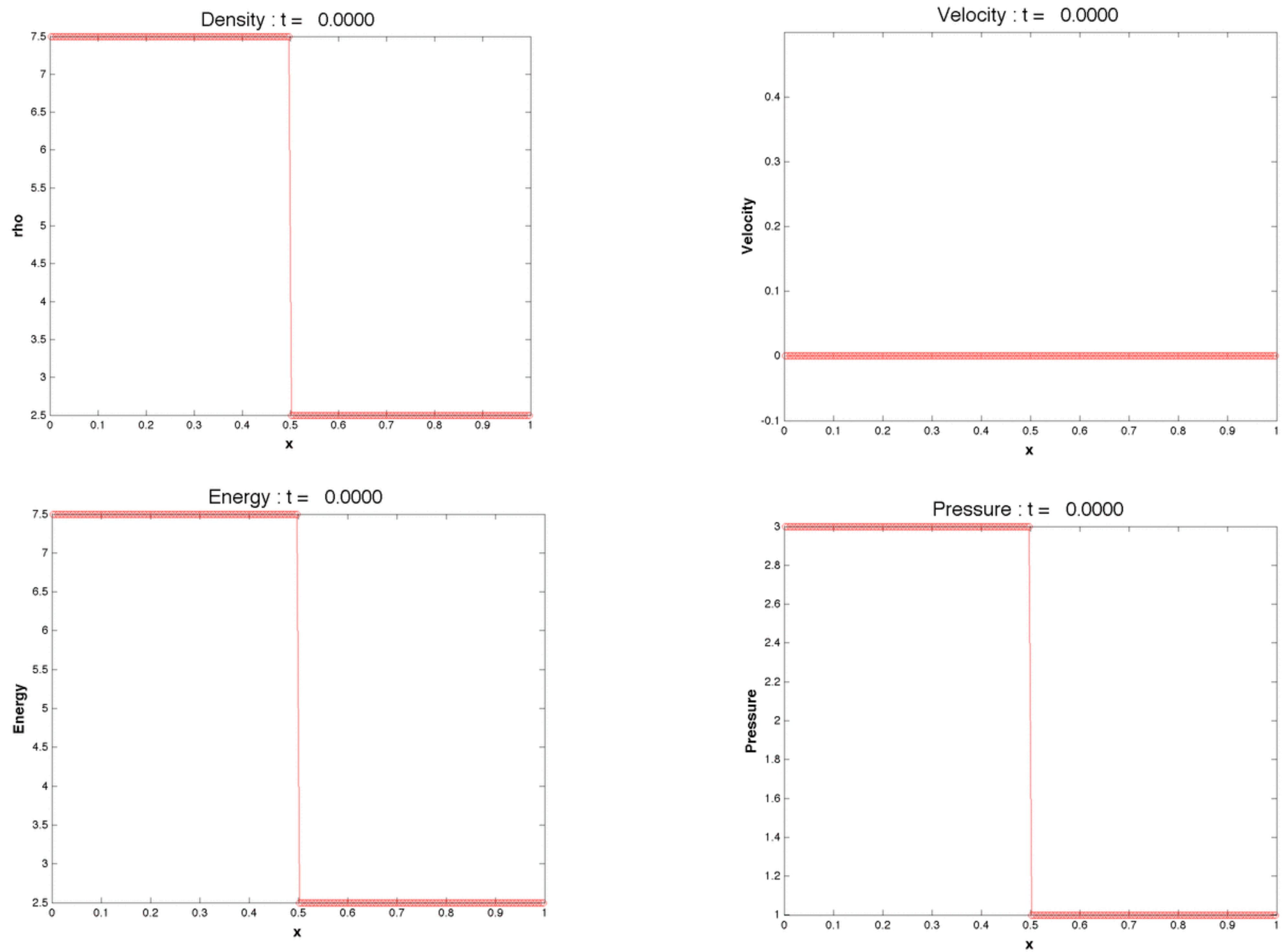

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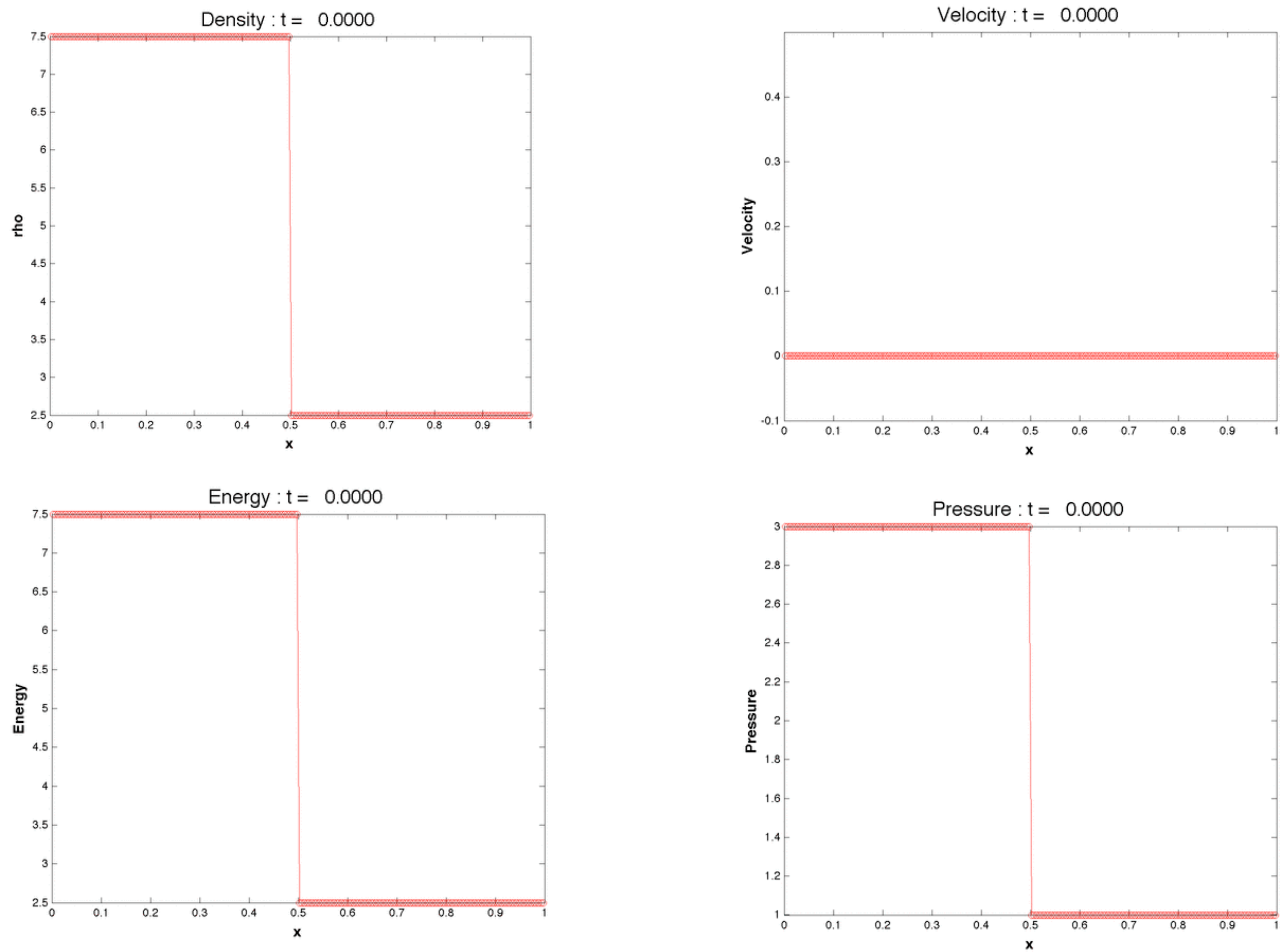

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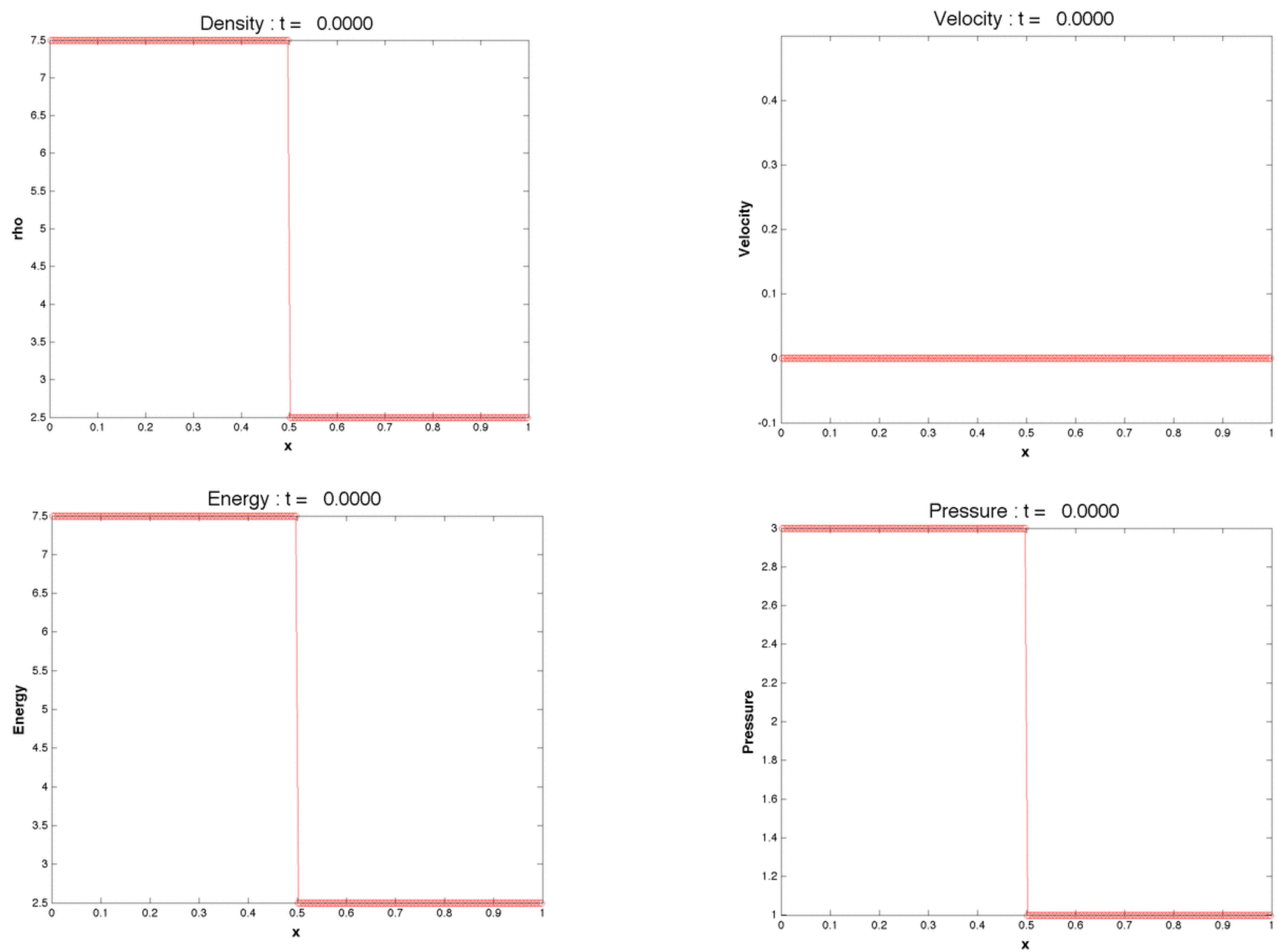
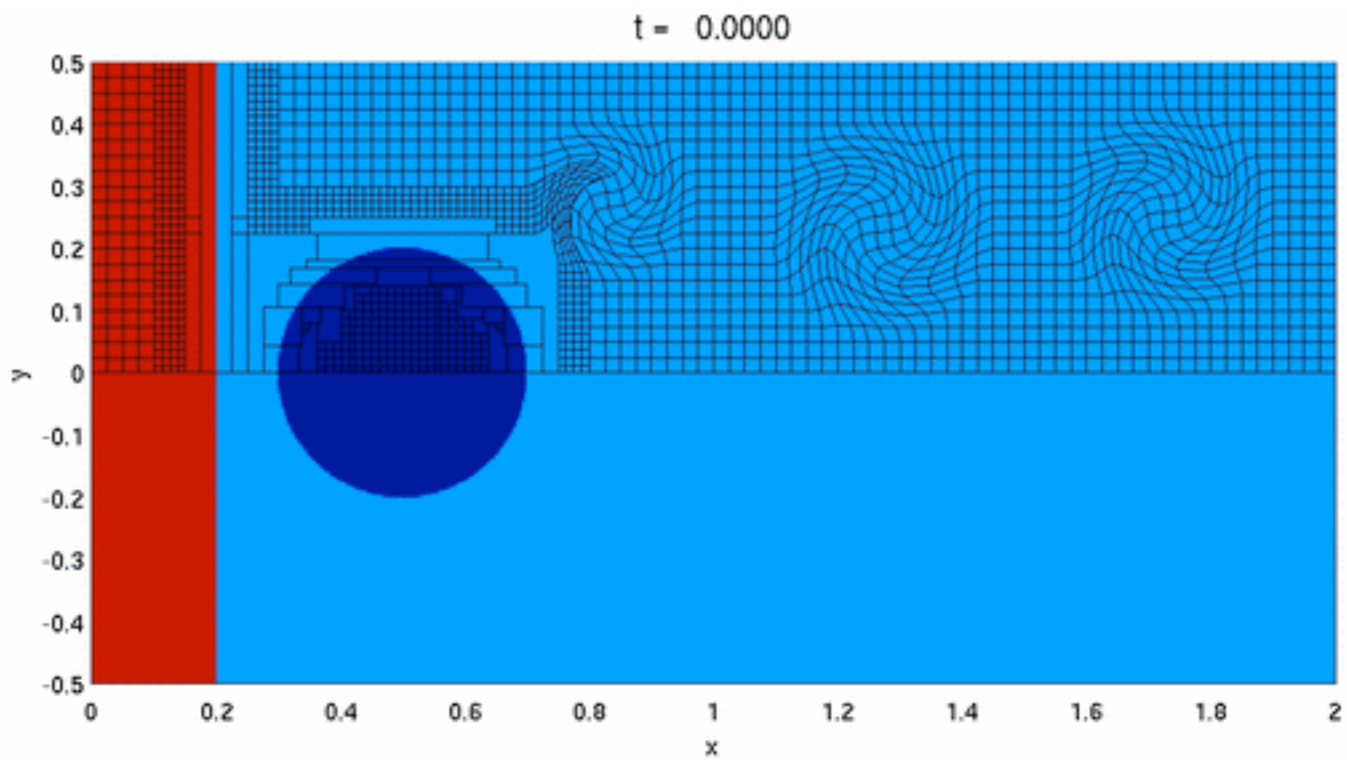


# Shockbubble interaction




Shock wave coming from the left interacts with a low density bubble. Solution is computed on an adaptively refined mapped grid (upper half) and a uniform Cartesian grid (lower half).

# Combustion - the detonation regime

Euler equations plus a reacting tracer :

$$\begin{aligned}
\rho_t + (u\rho)_x &= 0 \\
(\rho u)_t + (\rho u^2 + p)_x &= 0 \\
E_t + (u(E+p))_x &= 0 \\
(\rho Z)_t + (u\rho Z)_x &= K(Z, E, \rho, \ldots)
\end{aligned}$$

where $Z$ is fraction of unburned gas.

An equation of state is given by

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho u^2 + \rho Q Z$$

# Single step irreversible chemistry

Simplified Arrhenius law :

$$K(T) = \begin{cases} -\frac{1}{\tau} & T \geq T_{ign} \\ 0 & \text{otherwise} \end{cases}$$

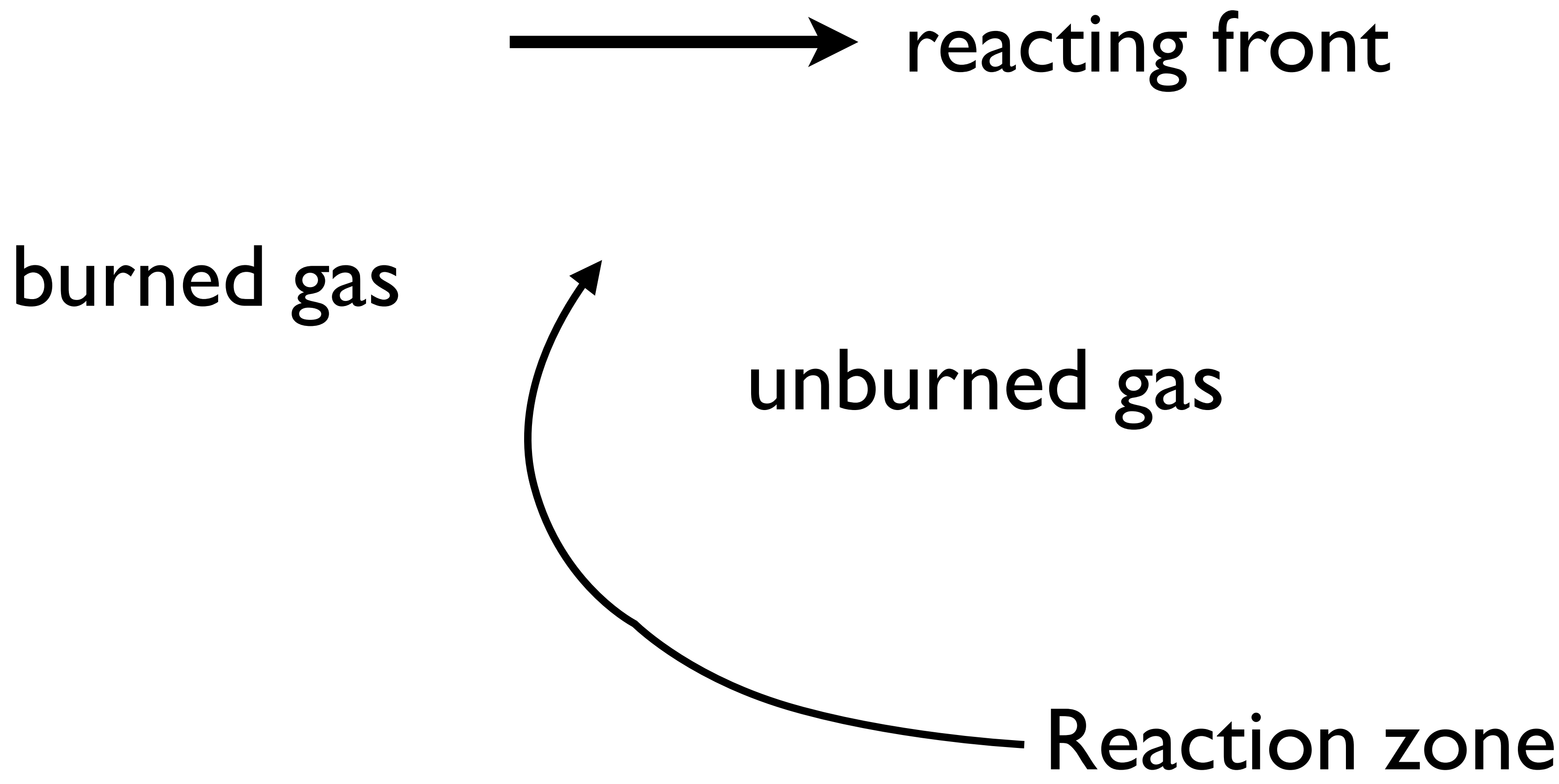
where $T$ is the temperature and $\tau$ is the reaction rate

The full Arrhenius law

$$K(T) = -Ae^{-T_{ign}/T}$$

An ideal gas law $P = \rho RT$ is used to obtain the temperature.

# Combustion - ZND solution



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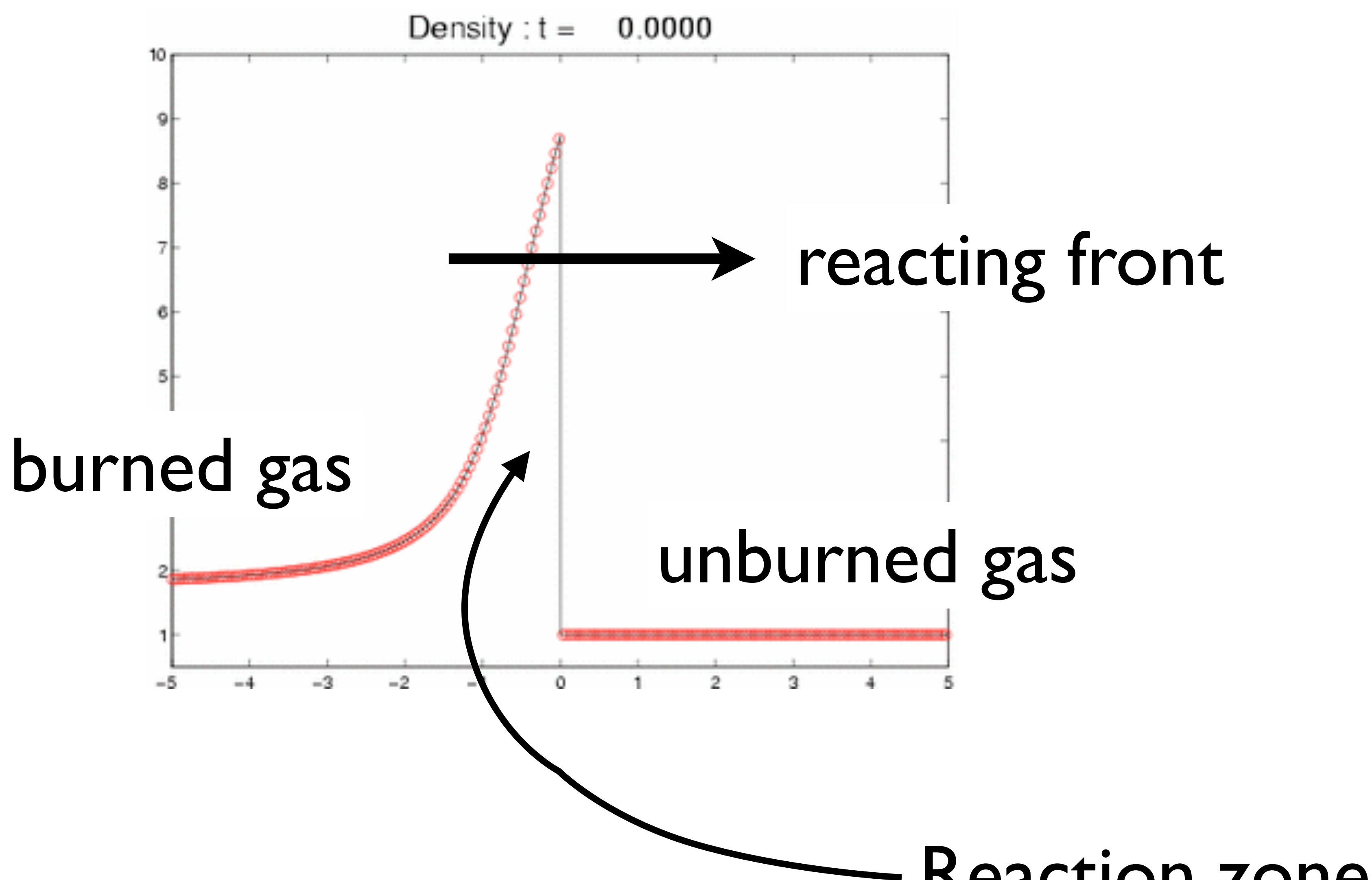
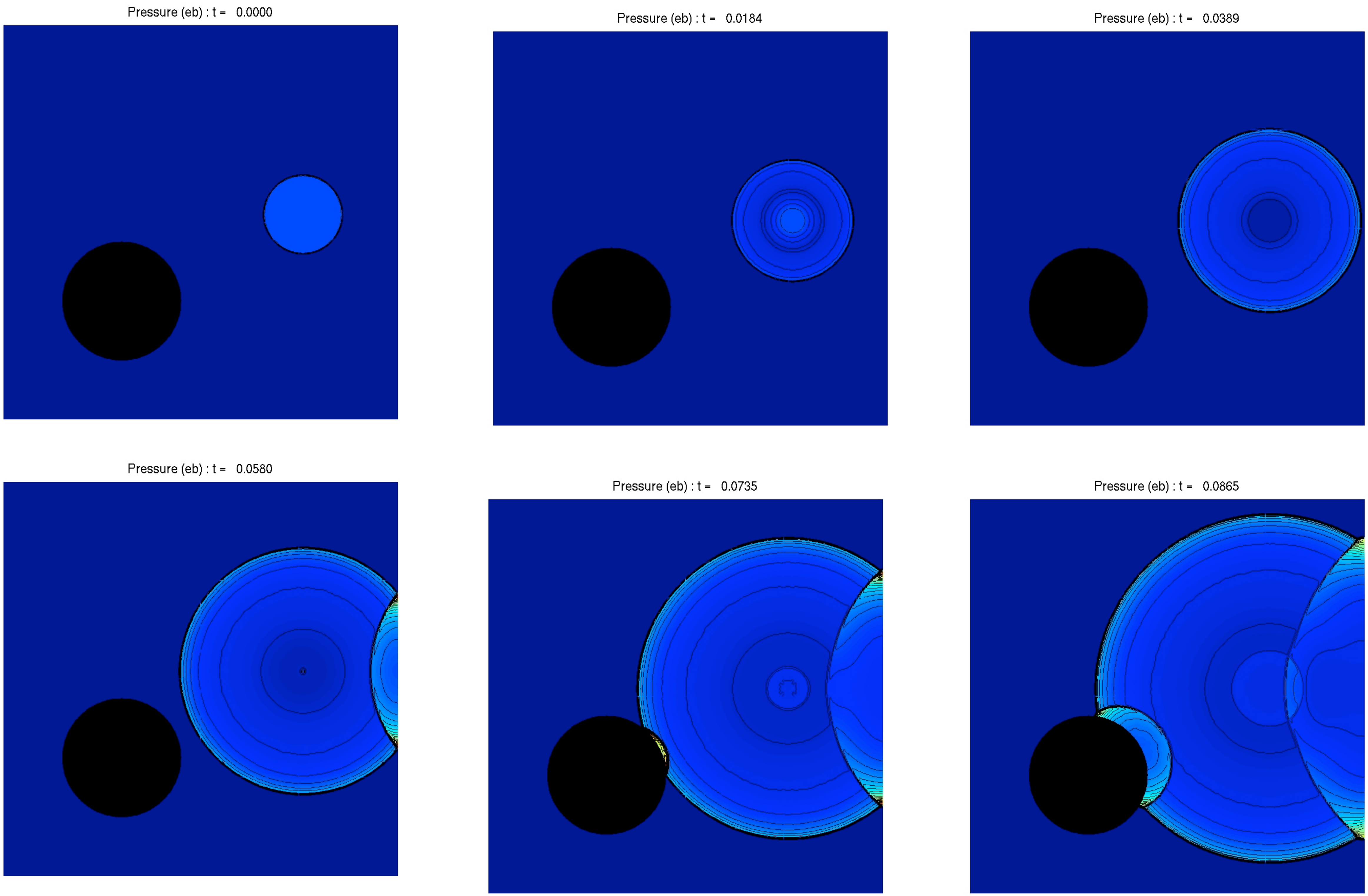


# Detonation with obstacles



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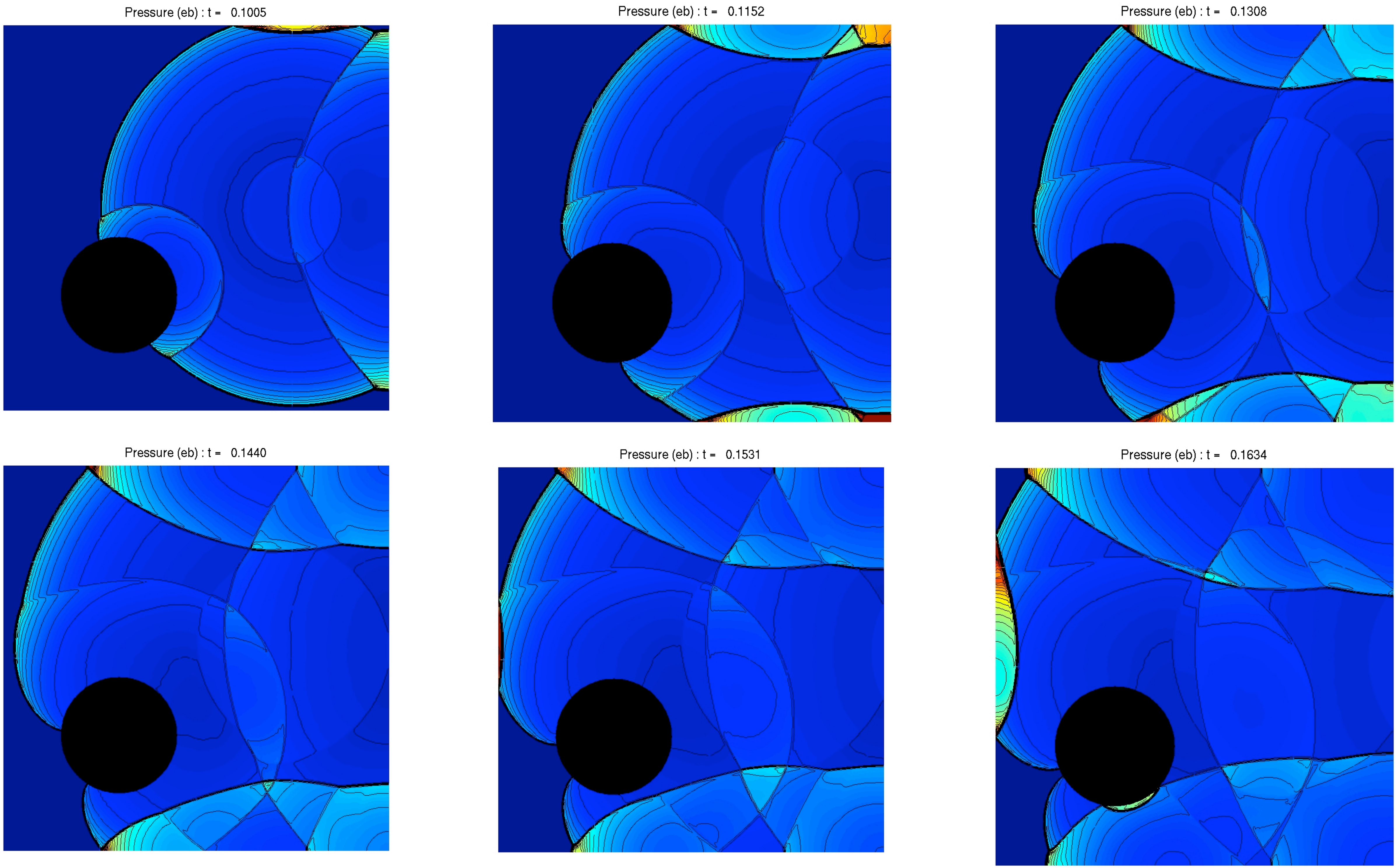

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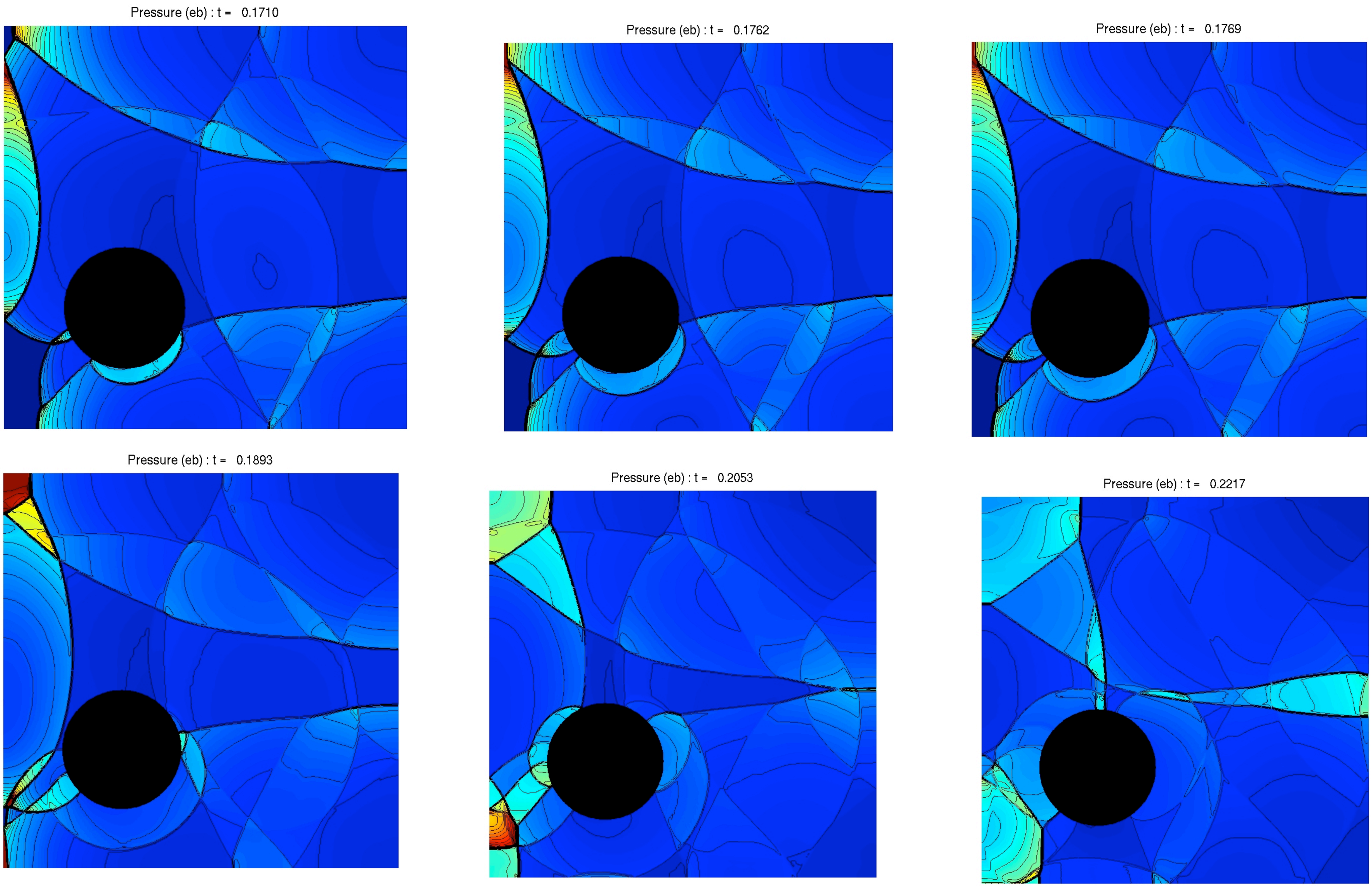
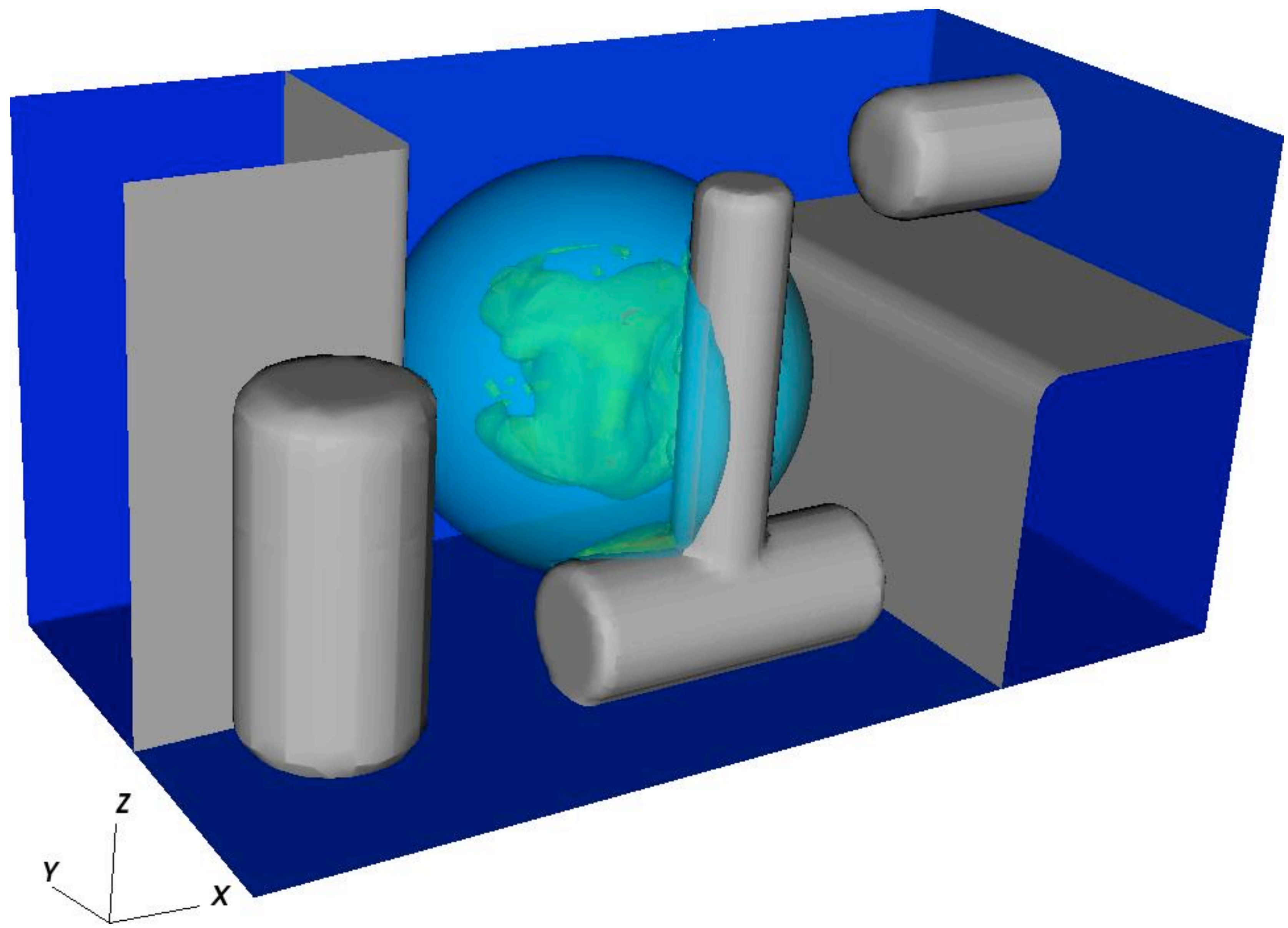


# Hydrogen combustion in industrial settings






Monday, June 20, 2011

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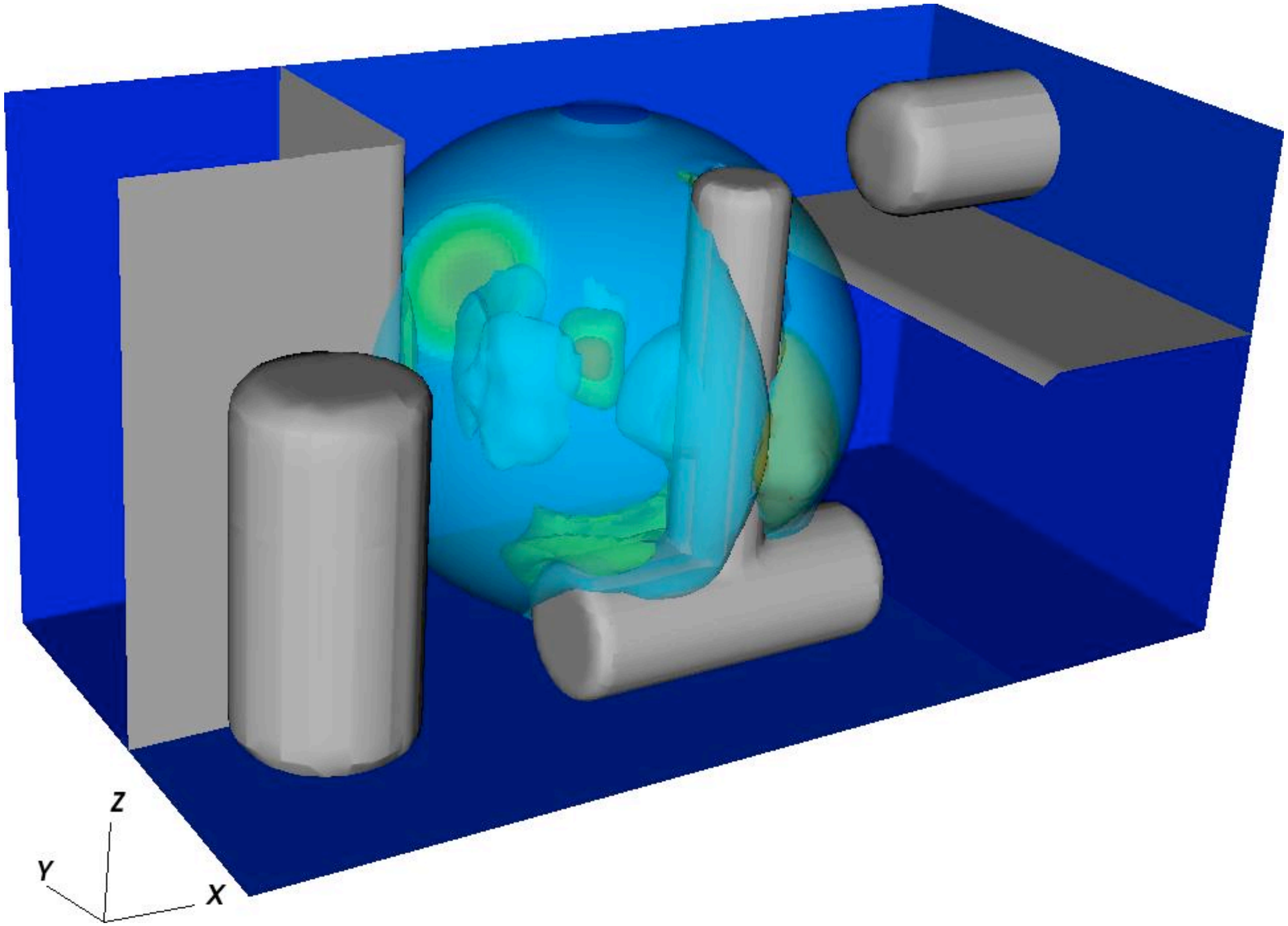

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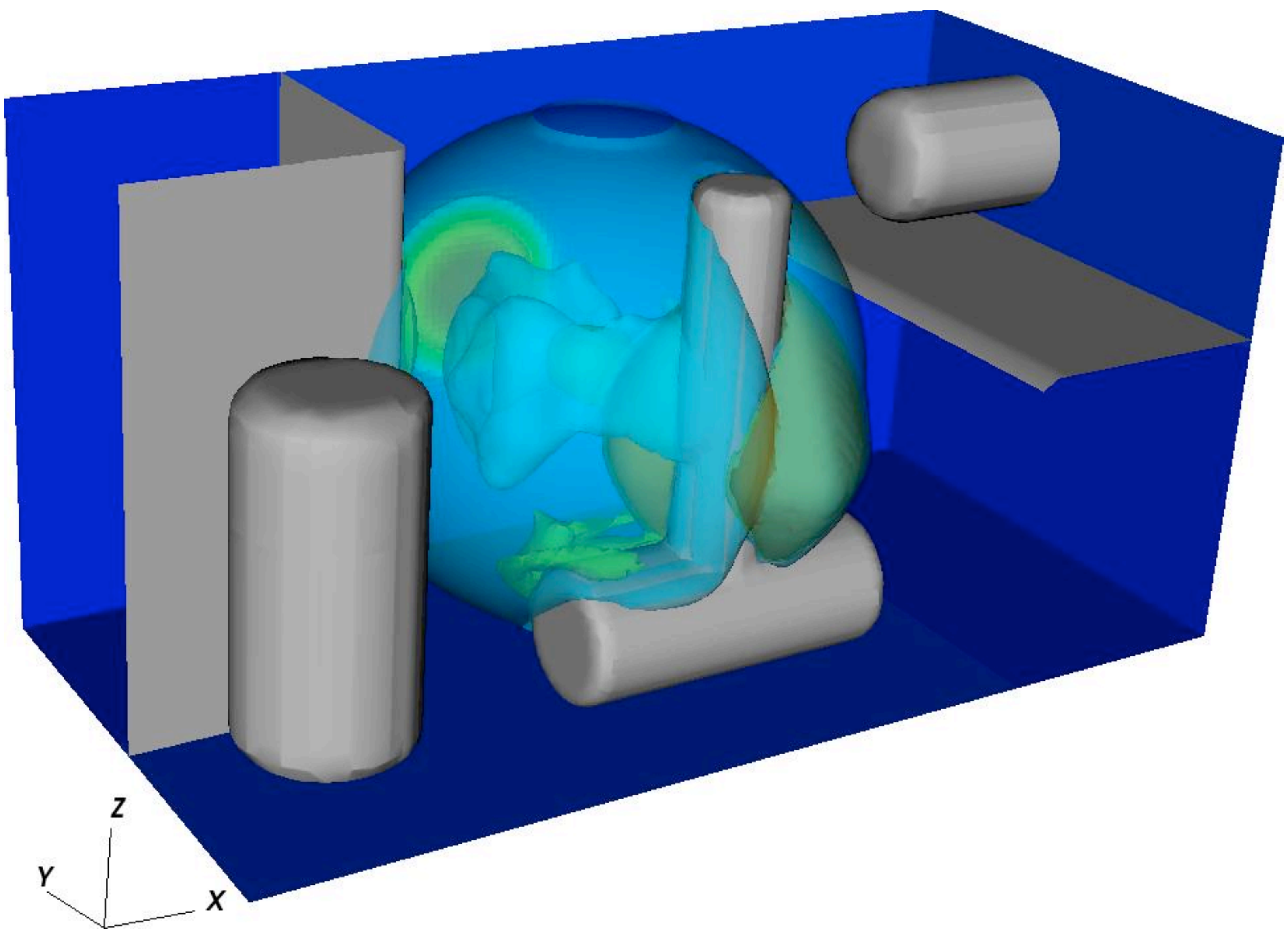

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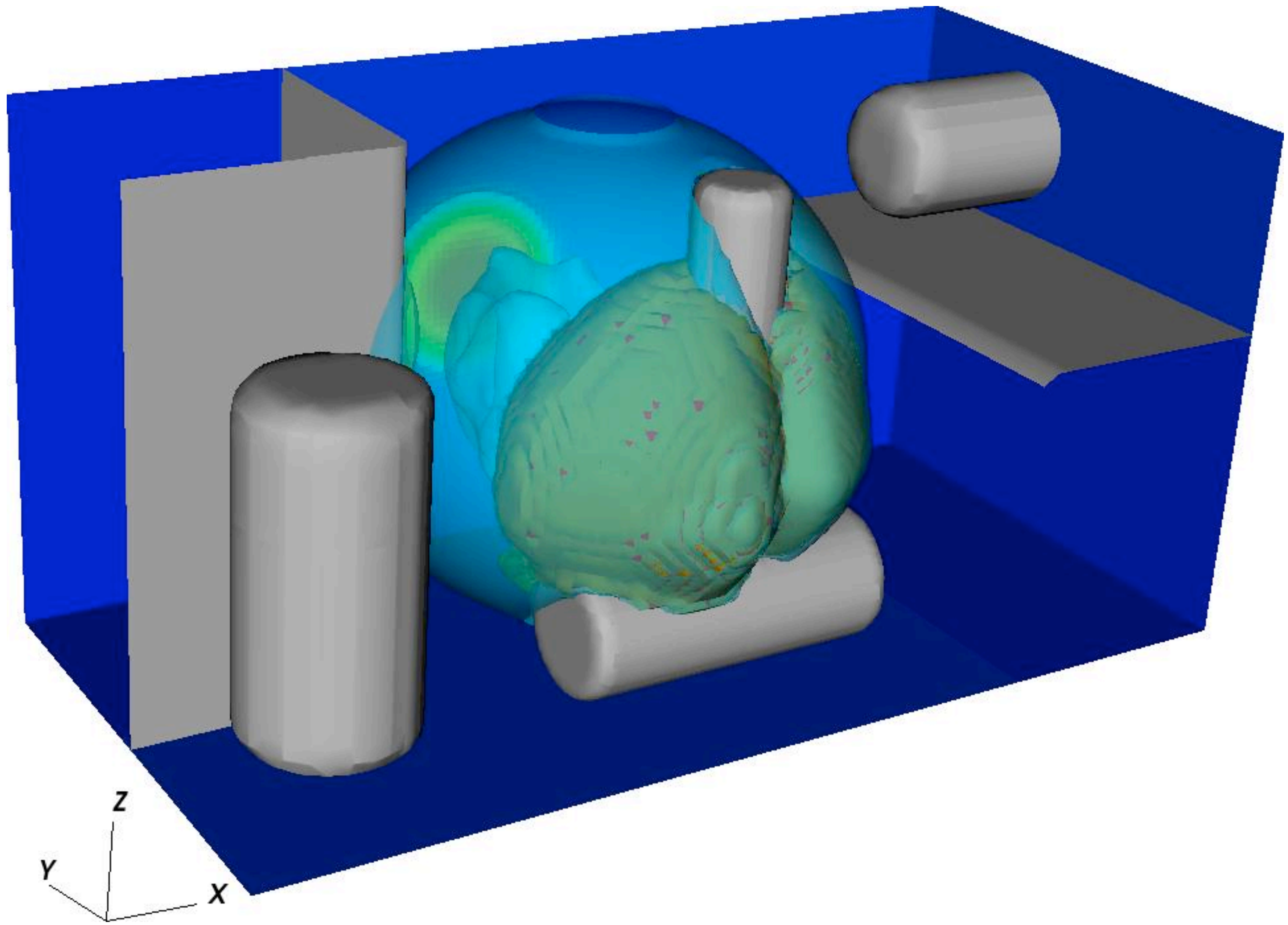
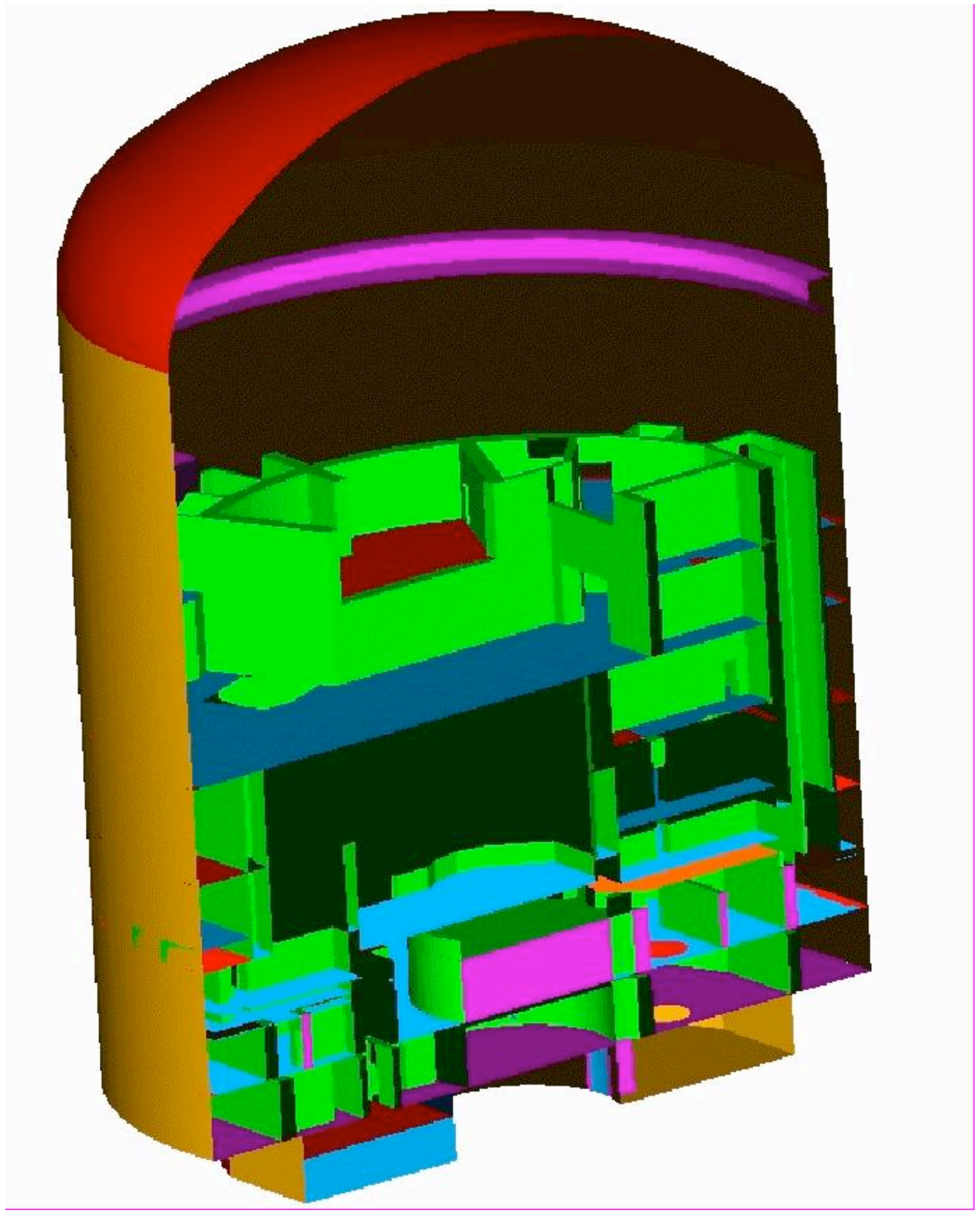



Results computed using EBChombo (Lawrence Berkeley Labs)

# Hydrogen risk in containment buildings



Nuclear reactor containment building

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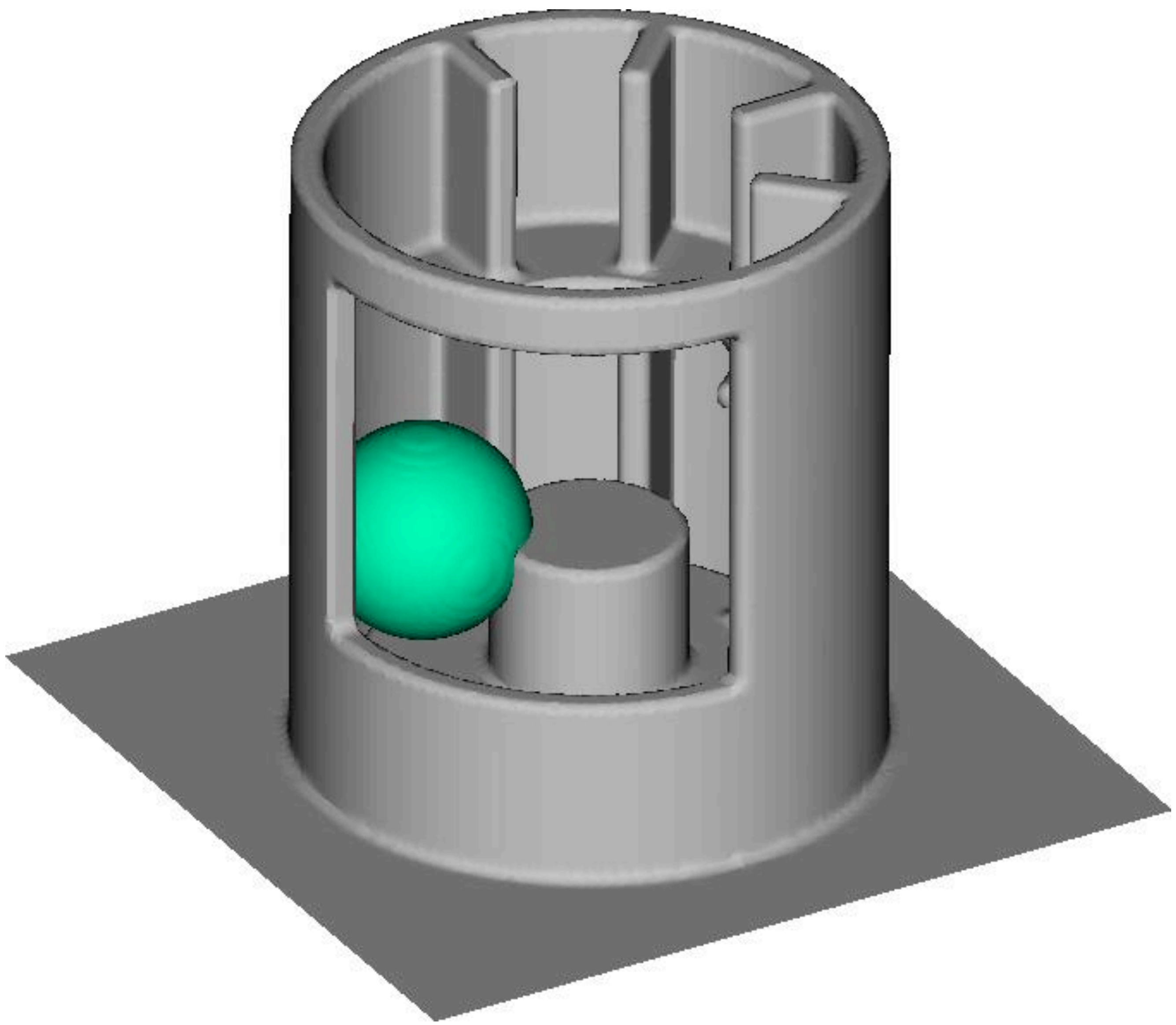

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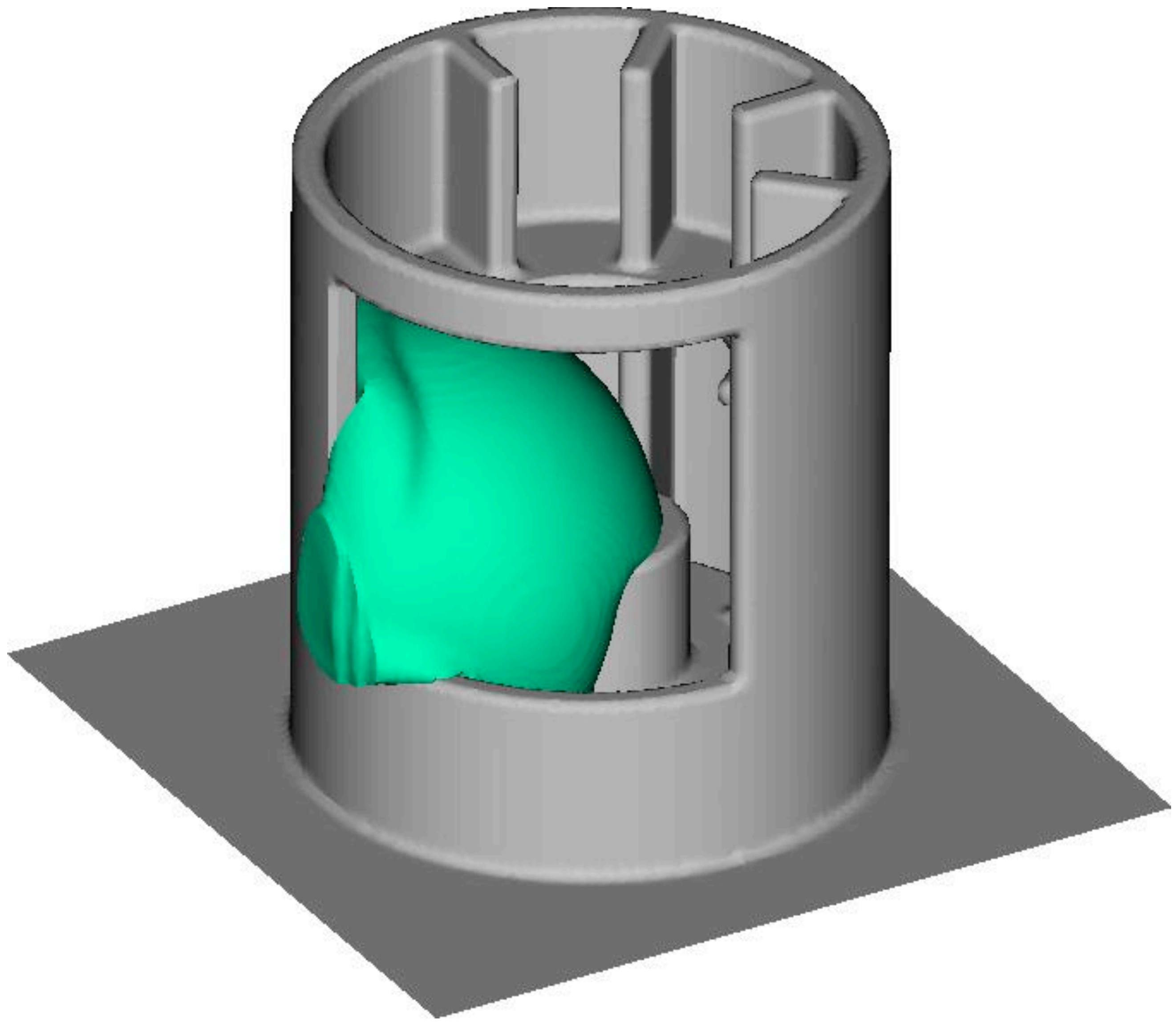

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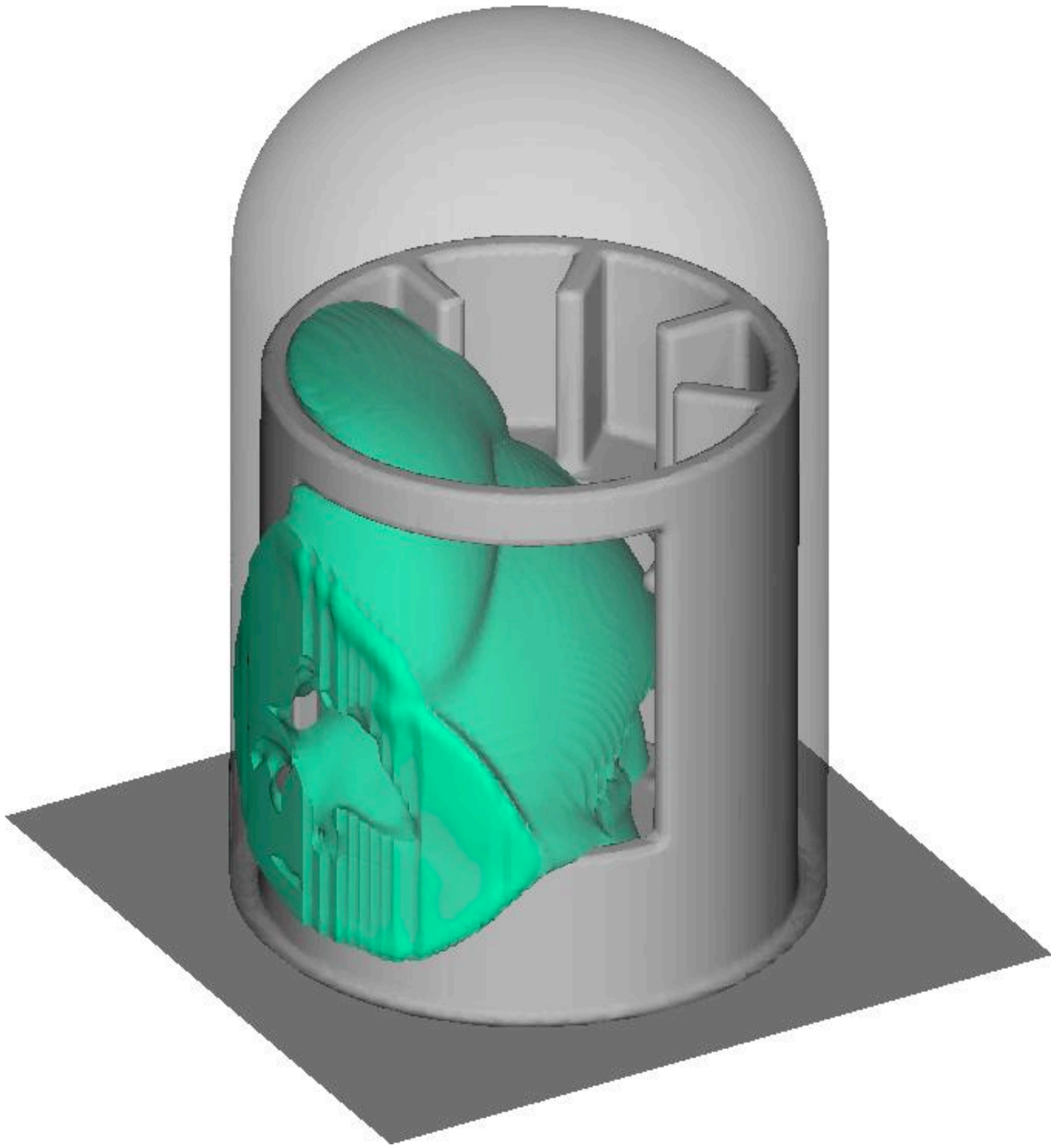

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# Unstable pattern formation in detonations

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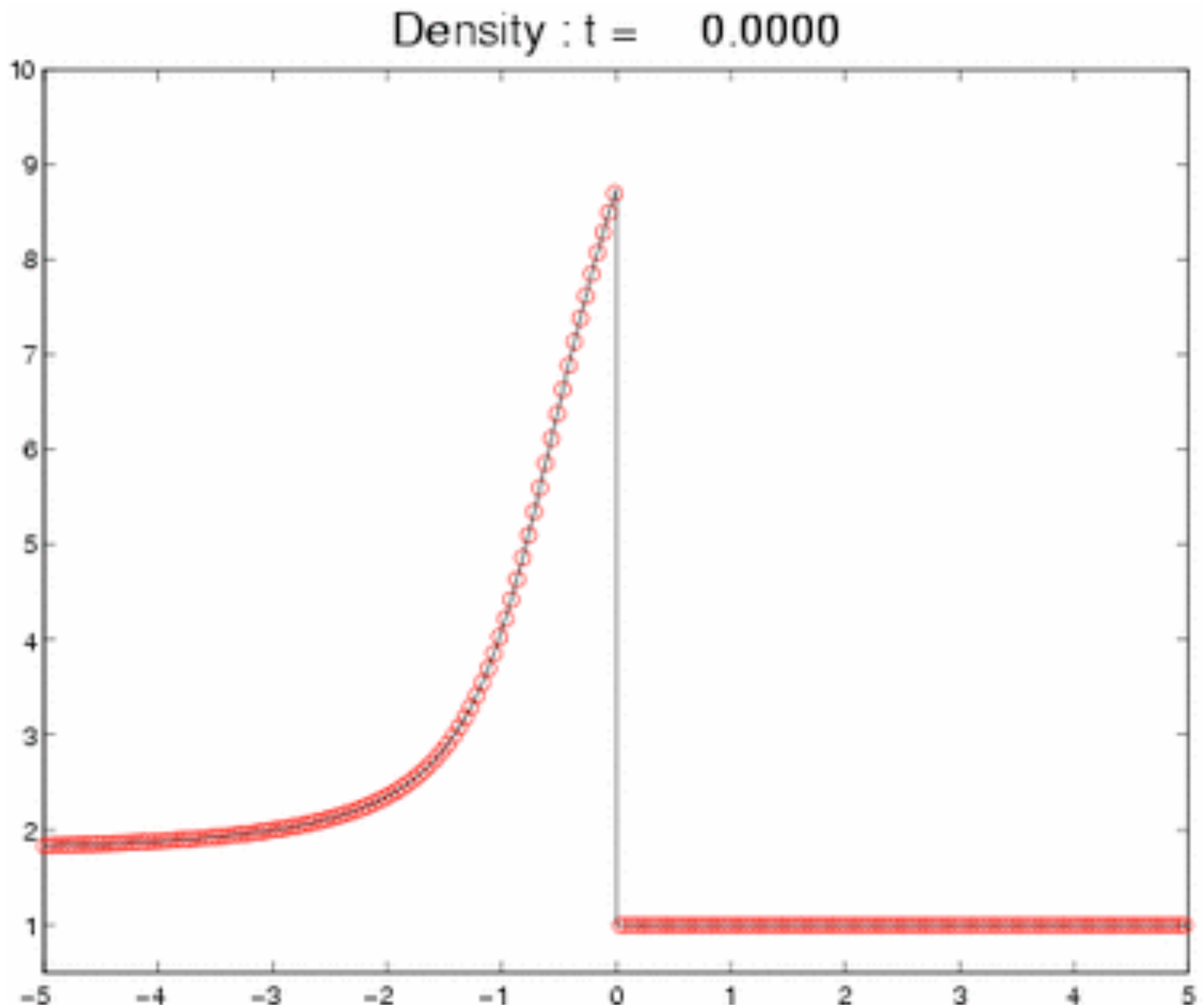
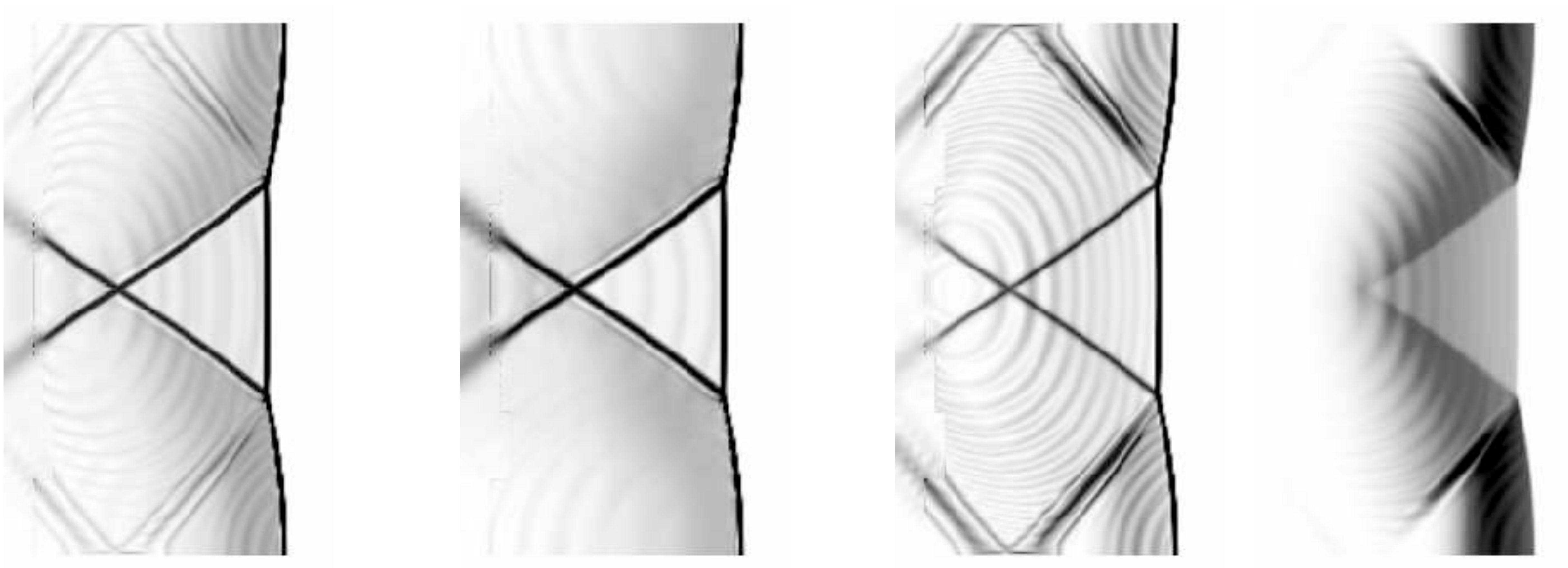


# Cellular structure in detonation fronts

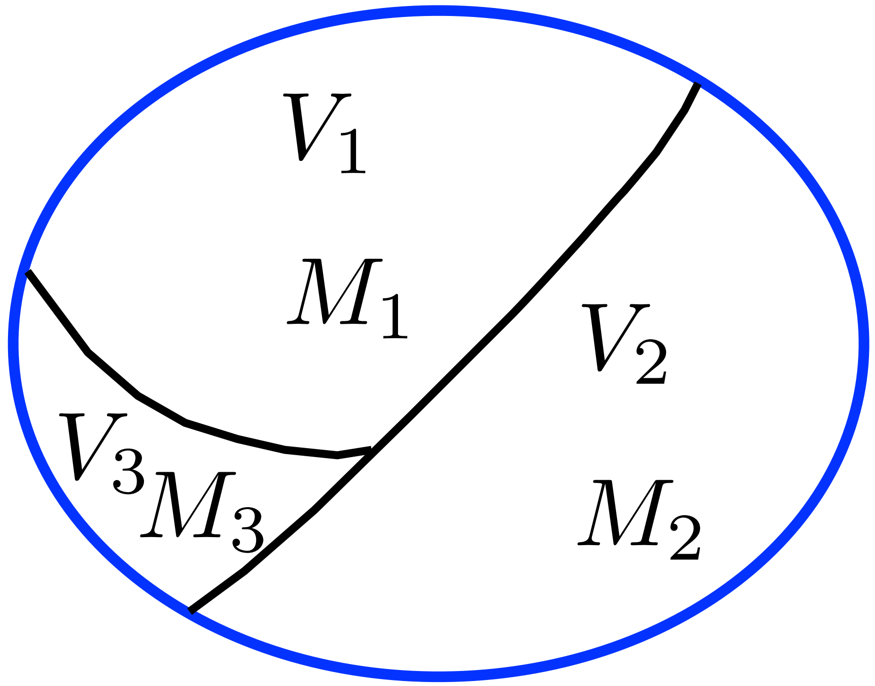


density pressure temperature Z

Ralf Deiterding, Oakridge National Laboratories (AMROC)

# Multiphase mixtures

Volume $V_k$, Temperature $T$, Pressure $P$, Mass $M_k$




$$\alpha_k = \frac{V_k}{V}$$

$$Y_k = \frac{M_k}{(\sum_k M_k)} = \frac{\alpha_k \rho_k}{\rho}$$

$$\begin{aligned}(\cdot)_1 &= \text{air}\\ (\cdot)_2 &= \text{vapor}\\ (\cdot)_3 &= \text{liquid water}\end{aligned}$$

* Density $\rho_3$ is constant and set to 1000 kg/m3

# Multiphase flow

Flow of air-steam-water mixtures can be modeled using the reduced model given by

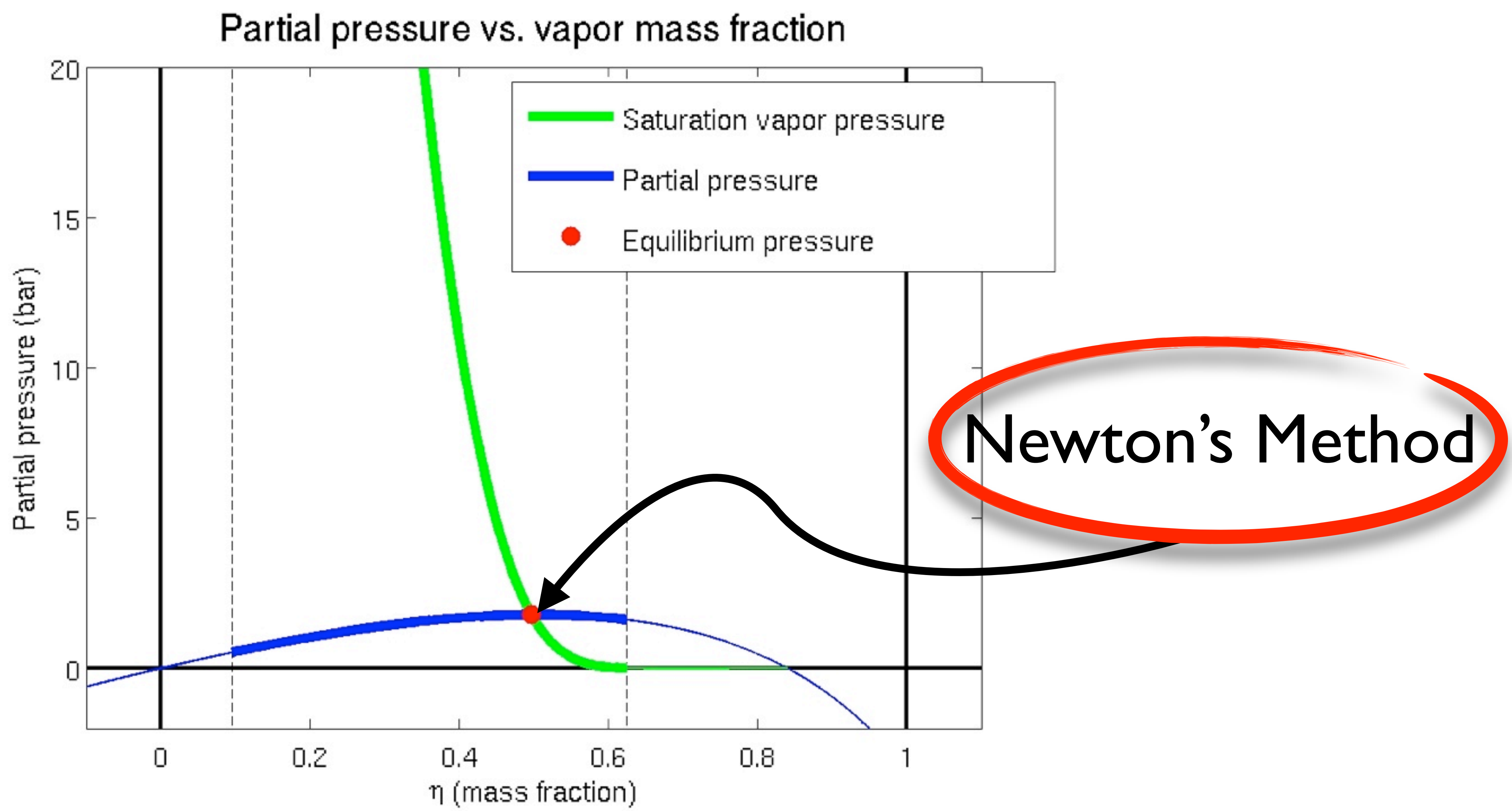
$$
\begin{aligned}
\rho_t + (u\rho)_x &= 0 \\
(\rho u)_t + (\rho u^2 + p)_x &= 0 \\
E_t + (u(E+p))_x &= 0 \\
(\rho Y_1)_t + (u\rho Y_1)_x &= 0 \\
(\rho Y_2)_t + (u\rho Y_2)_x &= \mu(\rho Y_2 - (\rho Y_2)_{eq})
\end{aligned}
$$

Equation of state :

$$
\begin{aligned}
E &= \frac{P}{\gamma - 1} + \frac{1}{2}\rho u^2 + \rho \Delta h^f \\
&= \rho e + \frac{1}{2}\rho u^2
\end{aligned}
$$

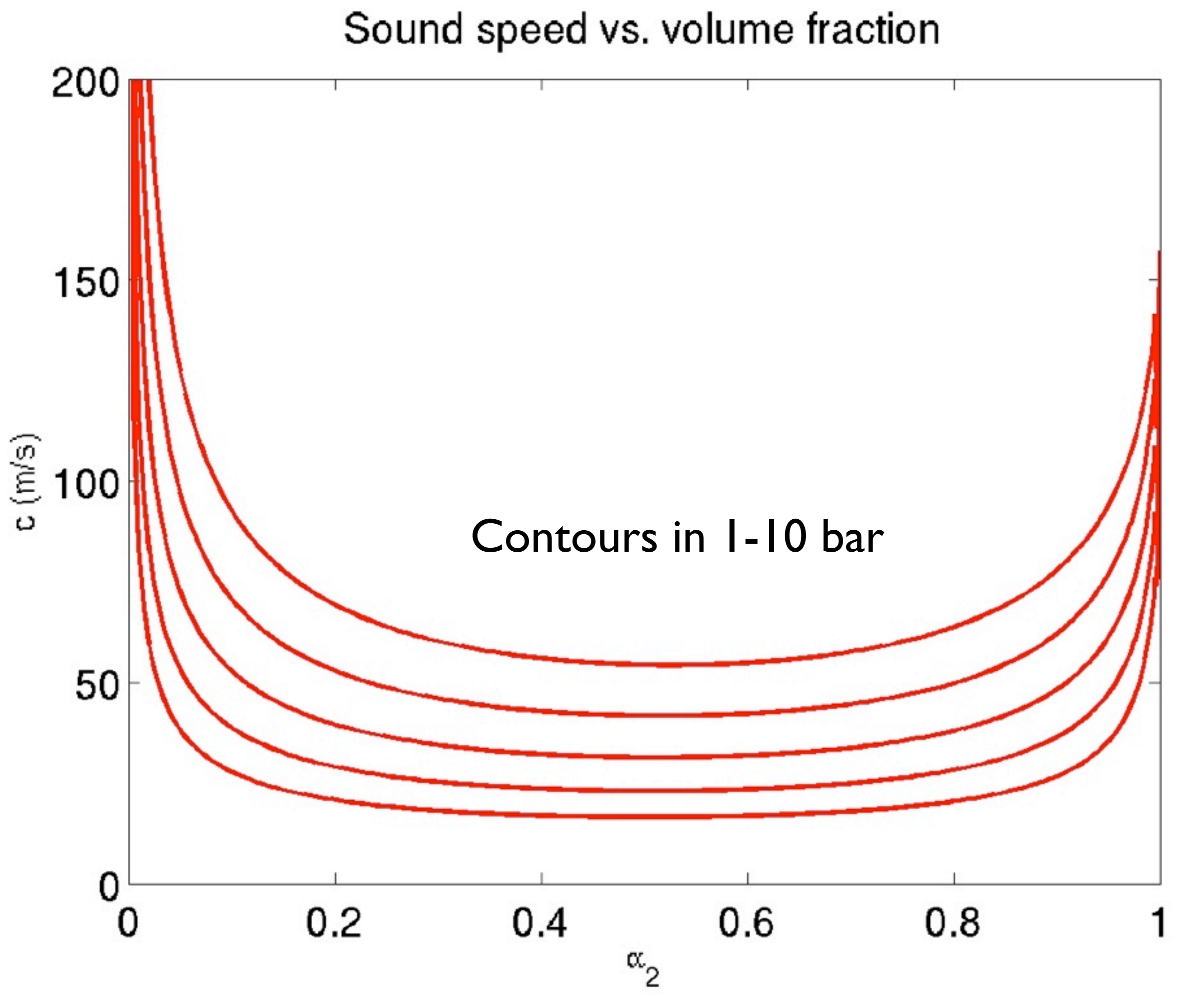
# Modeling equilibrium conditions

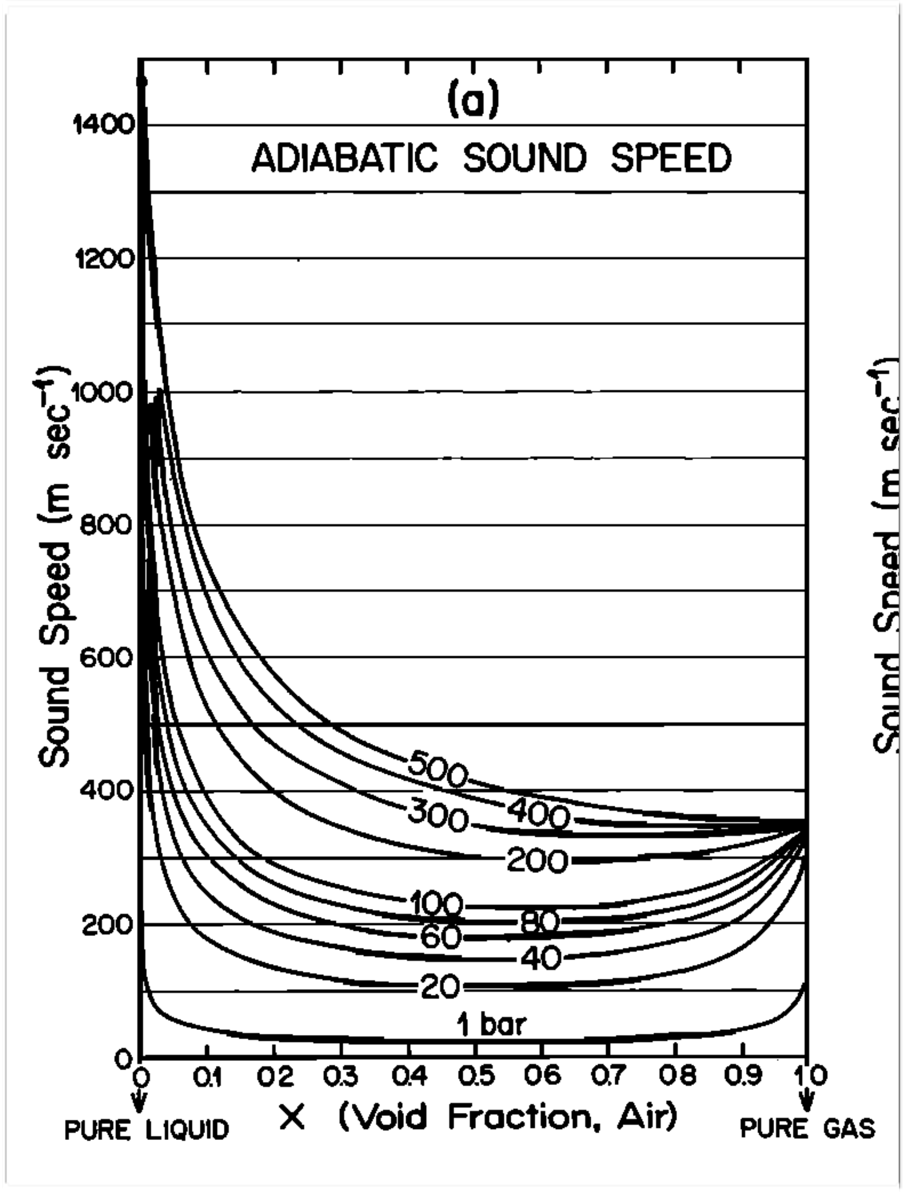
For fixed density and pressure, the equilibrium condition allows us to solve numerically for the mass fraction of vapor.




Condensation and vaporization are treated in the source term

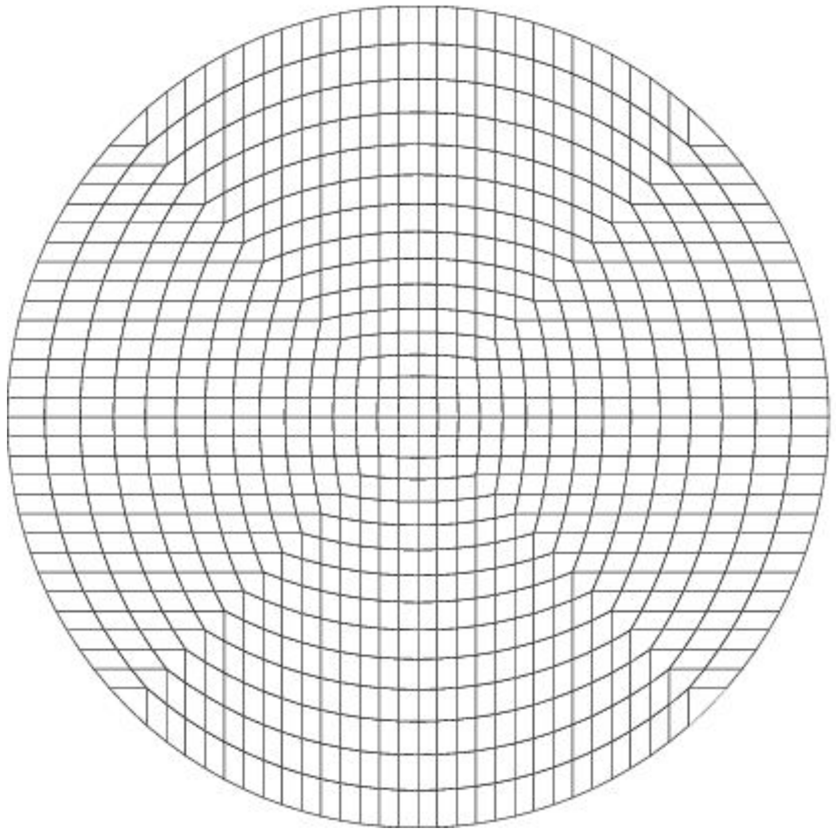
# Sound speed in mixtures




Good qualitative agreement with sound speed calculations from Kiefer, (JGR, 1977) for water-air mixtures.

# Solving on mapped grids

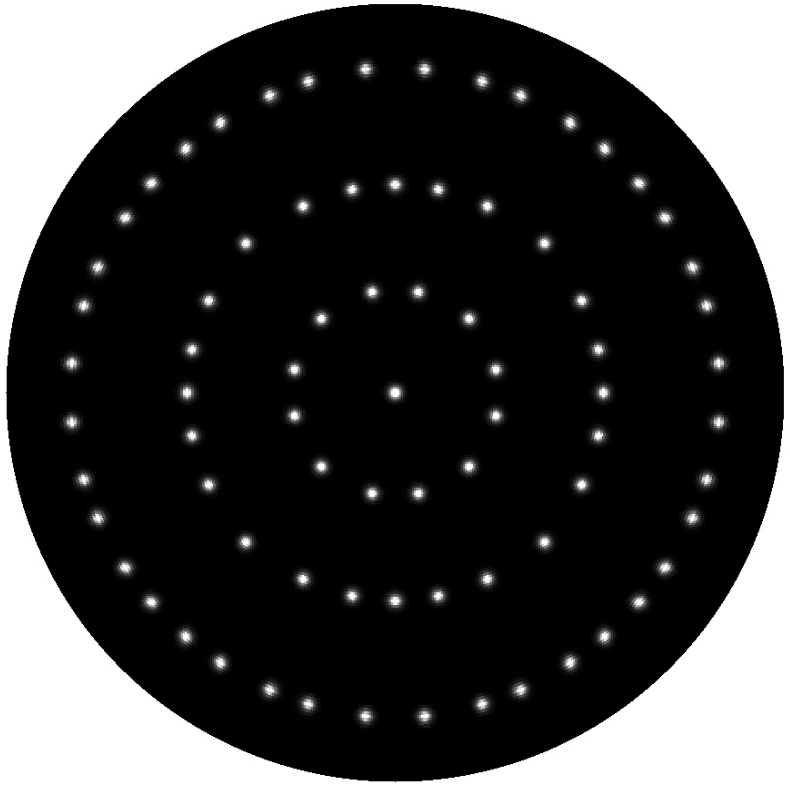
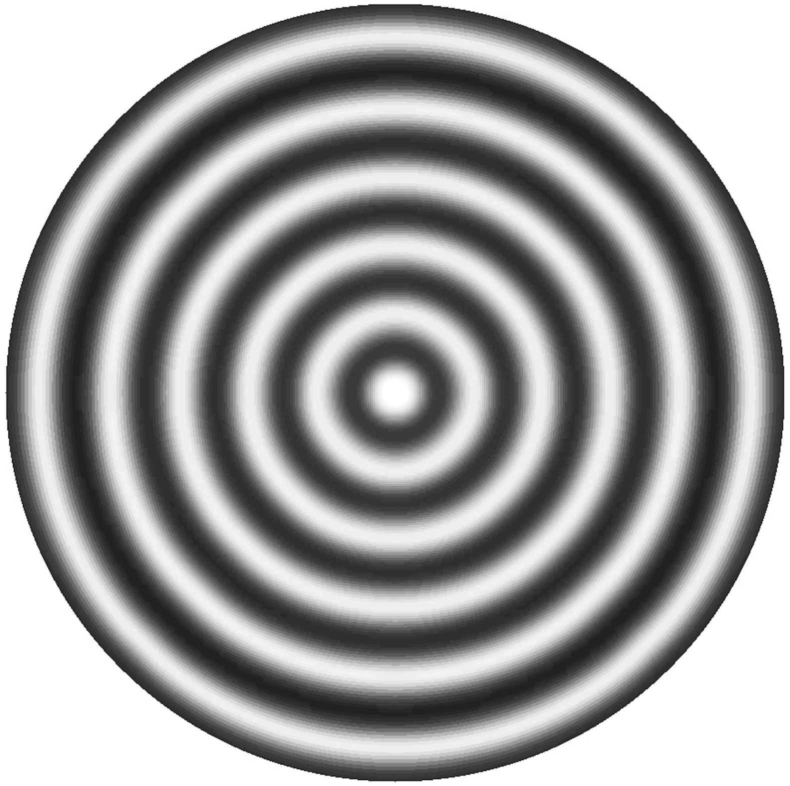


Mappings for the disk :

- Nearly uniform cell sizes
- Mapping generate from a simple analytic expression

D. Calhoun, C. Helzel, R. J. LeVeque, SIAM Review, 2008

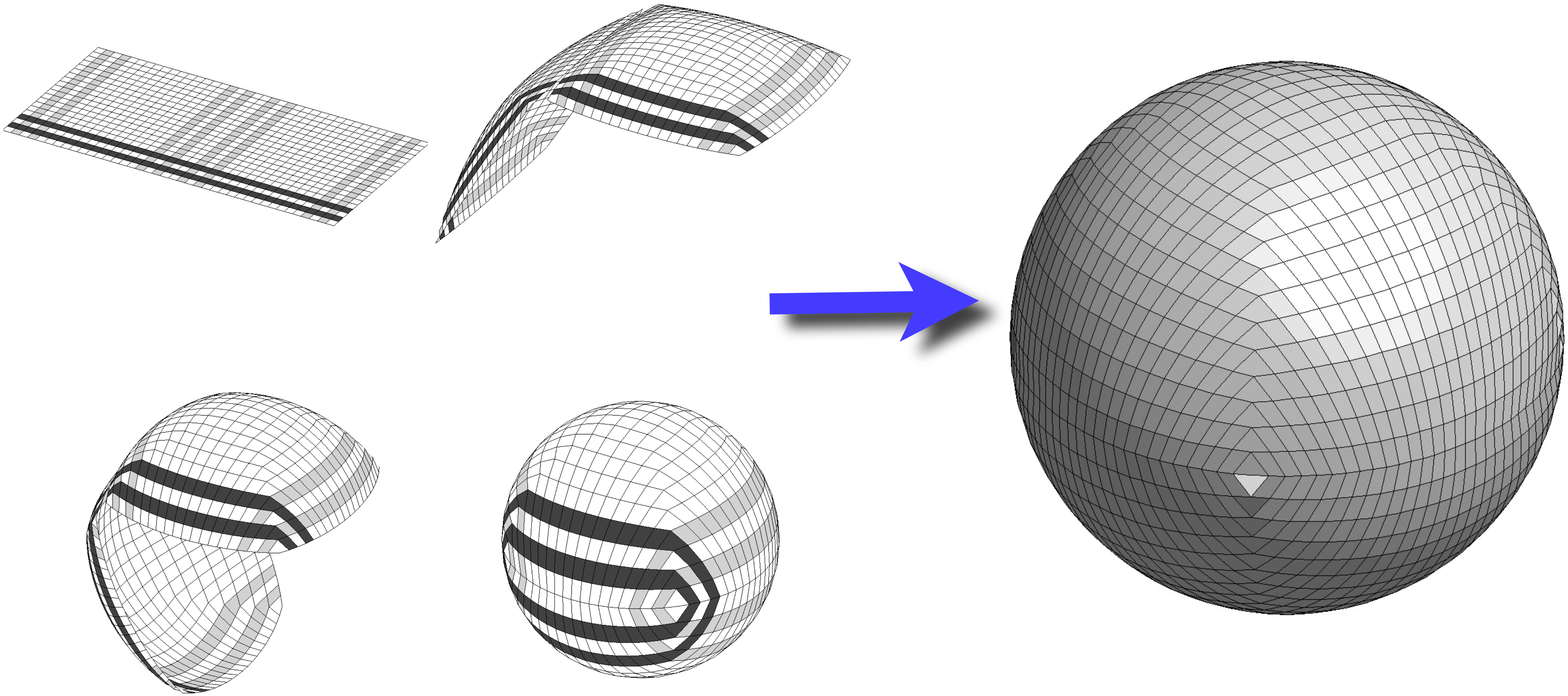
# Biological pattern formation - chemotaxis

$$\frac{\partial u}{\partial t} = d_u \nabla^2 u - \alpha \nabla \cdot \left( \left( \frac{\nabla v}{(1+v)^2} \right) u \right) + \rho u(\delta - u)$$

$$\frac{\partial v}{\partial t} = \nabla^2 v + \beta u^2 - uv.$$

# Sphere grids



D. Calhoun, C. Helzel, and R. LeVeque, SIAM Review, 50 (2008)

# Shallow water equations on the sphere

Initial disturbance

Underwater ridge

- M. Berger, D. Calhoun, C. Helzel, R. J. LeVeque, Phil. Trans. Proc. R. Soc. A, (367) 2009
- GeoCLAW, R. J. LeVeque, www.clawpack.org (code available)

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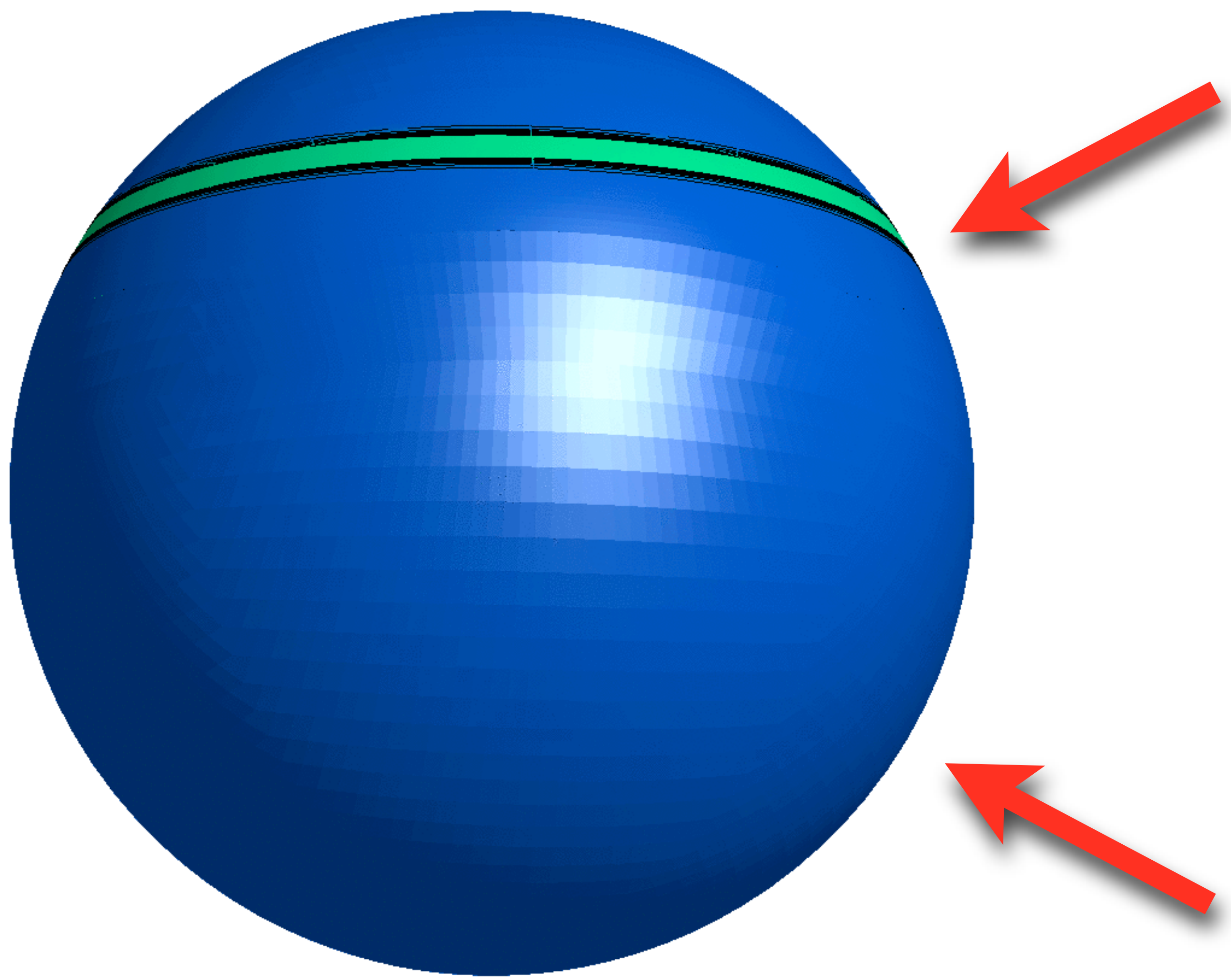


- M. Berger, D. Calhoun, C. Helzel, R. J. LeVeque, Phil. Trans. Proc. R. Soc. A, (367) 2009
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