

MODELLING AND SIMULATION OF LIQUID-VAPOR PHASE TRANSITION

A Boiling Crisis Study Contribution

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BOILING CRISIS

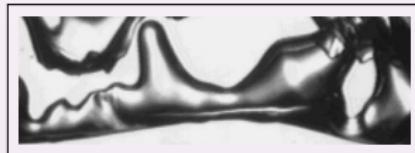
PHENOMENON

Liquid phase heated by a wall at a fixed temperature T^{wall} (pool boiling). When T^{wall} increases, we switch from a **nucleate boiling** to a **film boiling**.

Nucleate Boiling



Film Boiling



source: http://www.spaceflight.esa.int/users/fluids/TT_boiling.htm

OUTLINE

- 1 Model
- 2 Numerical Method
- 3 Numerical Tests
- 4 Conclusion

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EULER SYSTEM

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0, \\ \partial_t (\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P \mathbb{I}) = \mathfrak{V}_{\text{vf}} - \mathfrak{S}_{\text{sf}}, \\ \partial_t \left(\rho \left(\frac{|\mathbf{u}|^2}{2} + \varepsilon \right) \right) + \operatorname{div} \left(\rho \left(\frac{|\mathbf{u}|^2}{2} + \varepsilon \right) \mathbf{u} + P \mathbf{u} \right) = (\mathfrak{V}_{\text{vf}} - \mathfrak{S}_{\text{sf}}) \cdot \mathbf{u} - \operatorname{div}(q). \end{cases}$$

- $(\mathbf{x}, t) \mapsto \rho$ specific density,
- $(\mathbf{x}, t) \mapsto \varepsilon$ specific internal energy,
- $(\mathbf{x}, t) \mapsto \mathbf{u}$ velocity;
- $(\rho, \varepsilon) \mapsto \mathfrak{V}_{\text{vf}}$ volumic forces,
- $(\rho, \varepsilon) \mapsto \mathfrak{S}_{\text{sf}}$ surface forces,
- $(\rho, \varepsilon) \mapsto \operatorname{div}(q)$ heat transfert.

$(\rho, \varepsilon) \mapsto P$ pressure law.

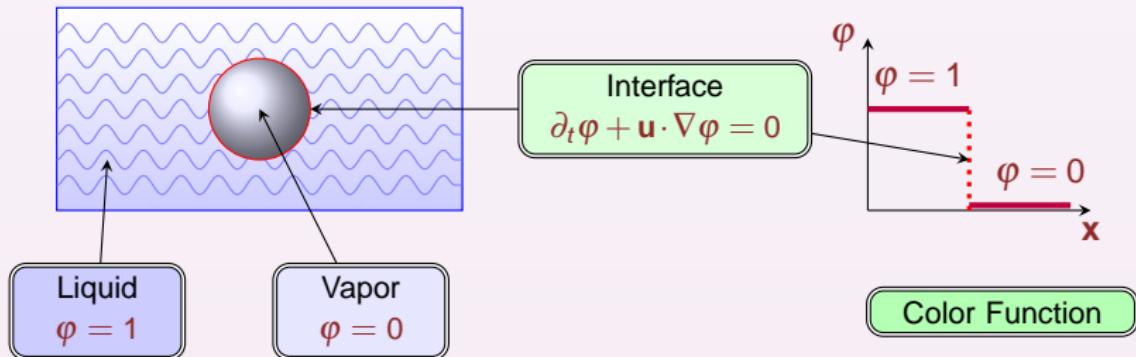
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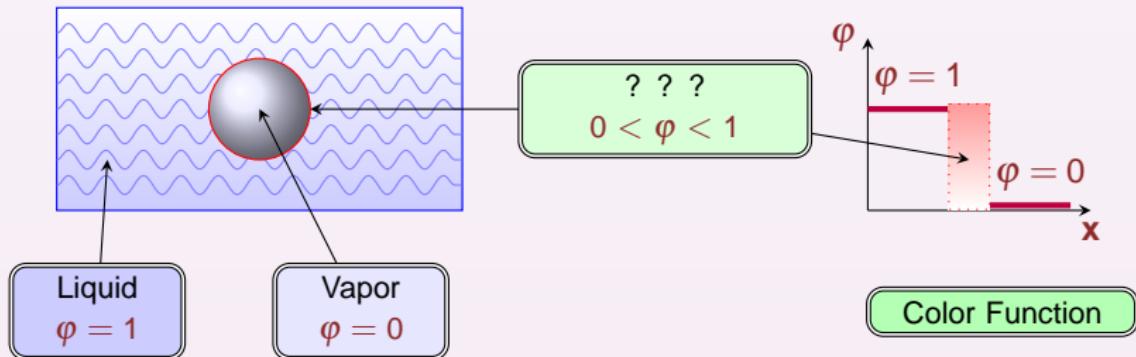
$\boxed{(\rho, \varepsilon) \mapsto P}$ pressure law.

LIQUID-VAPOR INTERFACE



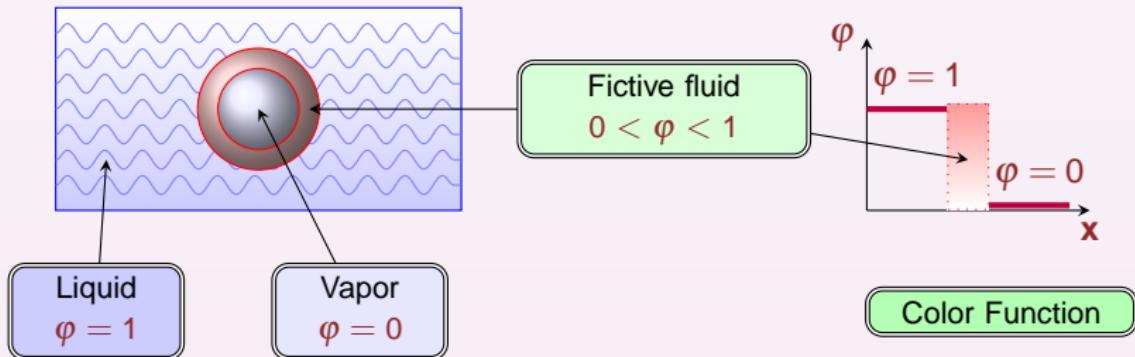
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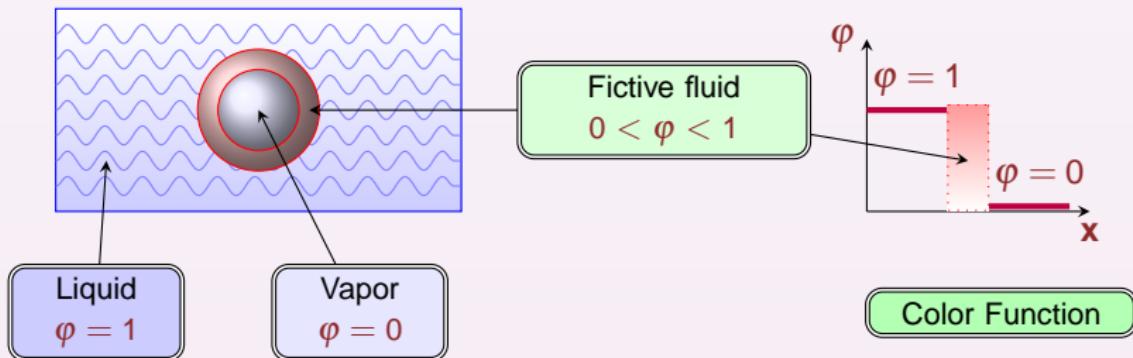
$$(\rho, \varepsilon) \mapsto P = \begin{cases} P^{\text{liq}} & \text{if } \varphi = 1; \\ ??? & \text{if } 0 < \varphi < 1; \\ P^{\text{vap}} & \text{if } \varphi = 0. \end{cases}$$

LIQUID-VAPOR INTERFACE



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LIQUID-VAPOR INTERFACE



→ Goal: define a global pressure law such that

- $(\rho, \varepsilon, \mathbf{u}, P)$ are continuous (3 zones)
- the interface position and the phase change are implicit ($\leadsto \text{RK}$)
- coherence with classical thermodynamics [H. Callen]

EOS OF EACH PHASE $\alpha = 1, 2$

$$\left. \begin{array}{l} \tau_\alpha \text{ specific volume} \\ \varepsilon_\alpha \text{ specific internal energy} \end{array} \right\} \Rightarrow \mathbf{w}_\alpha \stackrel{\text{def}}{=} (\tau_\alpha, \varepsilon_\alpha);$$

$\mathbf{w}_\alpha \mapsto s_\alpha$ specific entropy (Hessian matrix neg. def.);



$$\left\{ \begin{array}{ll} T_\alpha \stackrel{\text{def}}{=} \left(\frac{\partial s_\alpha}{\partial \varepsilon_\alpha} \Big|_{\tau_\alpha} \right)^{-1} > 0 & \text{temperature,} \\ P_\alpha \stackrel{\text{def}}{=} T_\alpha \frac{\partial s_\alpha}{\partial \tau_\alpha} \Big|_{\varepsilon_\alpha} > 0 & \text{pressure,} \\ g_\alpha \stackrel{\text{def}}{=} \varepsilon_\alpha + P_\alpha \tau_\alpha - T_\alpha s_\alpha & \text{free enthalpy (Gibbs potential).} \end{array} \right.$$

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EOS WITHOUT PHASE CHANGE

- $\mathbf{w} \stackrel{\text{def}}{=} y\mathbf{w}_1 + (1-y)\mathbf{w}_2;$
- y mass fraction;
- z volume fraction s.t. $y\tau_1 = z\tau$;
- ψ energy fraction s.t. $y\varepsilon_1 = \psi\varepsilon$.

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ENTROPY WITHOUT PHASE CHANGE

$$\sigma \stackrel{\text{def}}{=} ys_1(\mathbf{w}_1) + (1-y)s_2(\mathbf{w}_2) = ys_1\left(\frac{z}{y}\tau, \frac{\psi}{y}\varepsilon\right) + (1-y)s_2\left(\frac{1-z}{1-y}\tau, \frac{1-\psi}{1-y}\varepsilon\right)$$

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EOS WITH PHASE CHANGE

ENTROPY WITHOUT PH.CH.

$$(w, z, y, \psi) \mapsto \sigma$$



ENTROPY AT EQUILIBRIUM

$$w \mapsto s^{\text{eq}}$$

DEFINITION [H. CALLEN, PH. HELLUY ...]

Optimization Problem:

$$s^{\text{eq}}(w) \stackrel{\text{def}}{=} \max_{z, y, \psi \in [0, 1]^3} \sigma(w, z, y, \psi)$$

Optimality Condition: $\begin{cases} T_1(z, y, \psi) = T_2(z, y, \psi) \\ P_1(z, y, \psi) = P_2(z, y, \psi) \\ g_1(z, y, \psi) = g_2(z, y, \psi) \\ z, y, \psi \in [0, 1]^3 \end{cases}$

Solution: (z^*, y^*, ψ^*)

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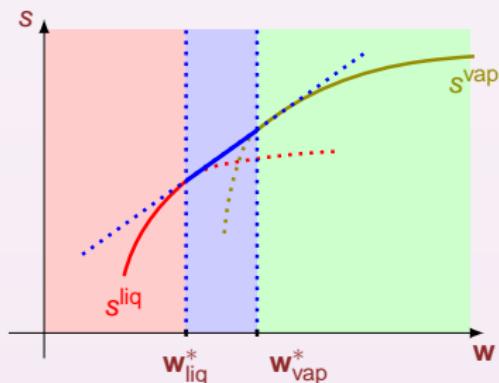
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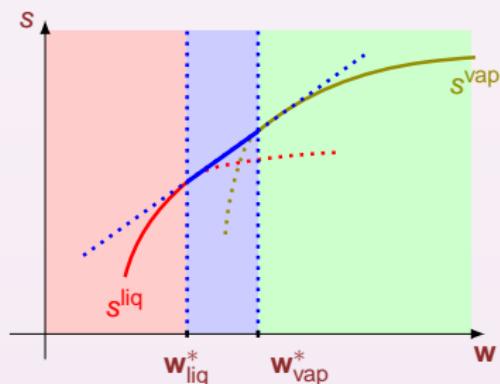
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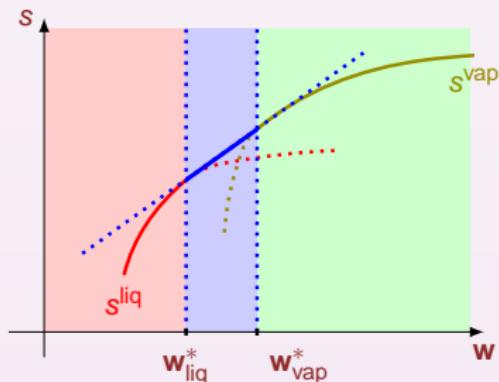
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DYNAMIC LIQUID-VAPOR PHASE CHANGE

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PROPERTIES [G. ALLAIRE, G. FACCANONI, S. KOKH]

If $\tau_1^* \neq \tau_2^*$ and $\varepsilon_1^* \neq \varepsilon_2^*$ (first order phase transition) then

$$\textcircled{1} \ c(w) > 0, \quad \textcircled{2} \ s_{TE}^{\text{eq}}(w) > 0$$

- ① Euler system: strict hyperbolicity ($\neq p$ -system),
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HOW TO SIMULATE THE LIU SOLUTION

- Exact Riemann Solver [A. Voß]
- Viscous Solver (the Liu solution is the only solution that has a viscous profile) [S. Jaouen]
- Solver(s) based on **Relaxation Approach** [F. Coquel, B. Perthame],
[Th. Barberon, Ph. Helluy], [Ph. Helluy, N. Seguin], [F. Coquel, F. Caro, D. Jamet, S. Kokh],
...

RELAXATION APPROACH

$$\partial_t \mathbf{U} + \operatorname{div} \mathbf{F}(\mathbf{U}) = \mathbf{0}$$

RELAXATION APPROACH

$$\partial_t \mathbf{V} + \operatorname{div} \mathbf{G}(\mathbf{V}) = \frac{1}{\mu} \mathbf{R}(\mathbf{V}) \quad \xrightarrow[\mu \rightarrow 0]{\text{Formally}} \quad \partial_t \mathbf{U} + \operatorname{div} \mathbf{F}(\mathbf{U}) = \mathbf{0}$$

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$$P^{\text{eq}}(\rho, \varepsilon) = \frac{s_{\tau}^{\text{eq}}}{s_{\varepsilon}^{\text{eq}}}, \quad e \stackrel{\text{def}}{=} \frac{|\mathbf{u}|^2}{2} + \varepsilon$$

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AUGMENTED SYSTEM

In the interface

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P \mathbb{I}) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + P)\mathbf{u}) = 0 \\ \left\{ \begin{array}{l} \partial_t z + \mathbf{u} \cdot \operatorname{grad} z = \frac{1}{\mu_z} \left(\frac{P_2}{T_2} - \frac{P_1}{T_1} \right) \\ \partial_t y + \mathbf{u} \cdot \operatorname{grad} y = \frac{1}{\mu_y} \left(\frac{g_1}{T_1} - \frac{g_2}{T_2} \right) \frac{1}{\rho} \\ \partial_t \psi + \mathbf{u} \cdot \operatorname{grad} \psi = \frac{1}{\mu_\psi} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \varepsilon \end{array} \right. \\ P(\rho, \varepsilon, z, y, \psi) = \frac{\sigma_\tau}{\sigma_\varepsilon} \end{cases}$$

REMARK: $\partial_t \psi + \mathbf{u} \cdot \operatorname{grad} \psi = 0 \rightsquigarrow T_1 = T_2$.

EQUILIBRIUM SYSTEM

$$\xrightarrow[\mu_j \rightarrow 0]{\text{Formally}}$$

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P^{\text{eq}} \mathbb{I}) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + P^{\text{eq}})\mathbf{u}) = 0 \\ P^{\text{eq}}(\rho, \varepsilon) = \frac{s_\tau^{\text{eq}}}{s_\varepsilon^{\text{eq}}}, \quad e \stackrel{\text{def}}{=} \frac{|\mathbf{u}|^2}{2} + \varepsilon \end{cases}$$

NUMERICAL SCHEME

$$\partial_t \mathbf{V} + \operatorname{div} \mathbf{G}(\mathbf{V}) = \mathbf{S}(\mathbf{V}) + \frac{1}{\mu} \mathbf{R}(\mathbf{V})$$



Aug. System: 5-eq. iso-T
Num. Scheme: op. splitting

Conv.: [G. Allaire and all.]

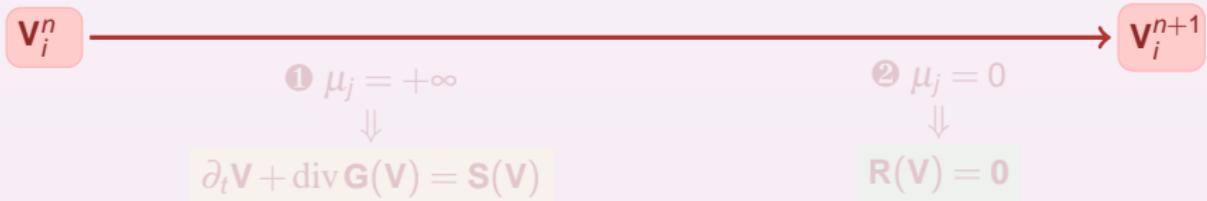
Surf. Tens.: [J. U. Brackbill and all.]

Heat: 2D Implicit

update fractions
 (y, z, ψ) by
projecting $\mathbf{v}_i^{n+1/2}$
onto the
 P, T, g equilibrium

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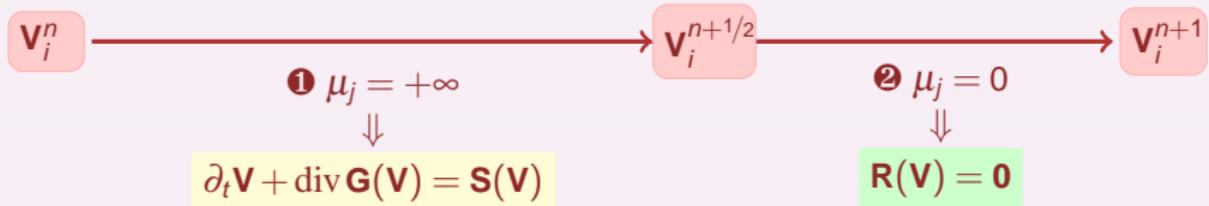


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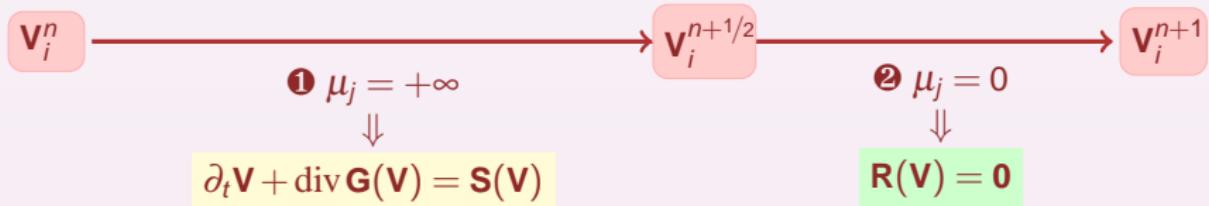
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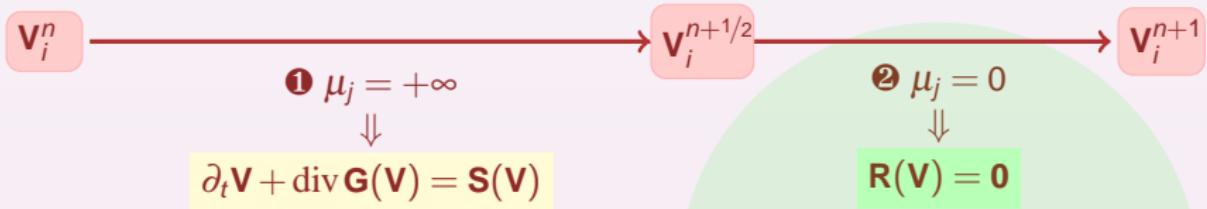
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ANALYTICAL EOS

▶ Water Example

(τ, ε) fixed

$(\tau_1, \varepsilon_1, \tau_2, \varepsilon_2, y)$ SOLUTION OF

$$\begin{cases} g_1(\tau_1, \varepsilon_1) = g_2(\tau_2, \varepsilon_2) \\ P_1(\tau_1, \varepsilon_1) = P_2(\tau_2, \varepsilon_2) \\ T_1(\tau_1, \varepsilon_1) = T_2(\tau_2, \varepsilon_2) \\ \tau = y\tau_1 + (1-y)\tau_2 \\ \varepsilon = y\varepsilon_1 + (1-y)\varepsilon_2 \end{cases}$$

(P, T) SOLUTION OF

$$\begin{cases} g_1(P, T) = g_2(P, T) \\ \frac{\tau - \tau_2(P, T)}{\tau_1(P, T) - \tau_2(P, T)} = \frac{\varepsilon - \varepsilon_2(P, T)}{\varepsilon_1(P, T) - \varepsilon_2(P, T)} \end{cases}$$

$$T \mapsto P = P^{\text{sat}}(T) \approx P^{\text{sat}}(T)$$

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$$\frac{\tau - \tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T) - \tau_2^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T) - \varepsilon_2^{\text{sat}}(T)} \quad \text{where } \left(\frac{\tau}{\varepsilon} \right)_\alpha^{\text{sat}}(T) \stackrel{\text{def}}{=} \left(\frac{\tau}{\varepsilon} \right)_\alpha(P^{\text{sat}}(T), T)$$

ANALYTICAL EOS

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least square approximation

$$T \mapsto P = \hat{P}^{\text{sat}}(T) \approx P^{\text{sat}}(T)$$

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$$\frac{\tau - \tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T) - \tau_2^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T) - \varepsilon_2^{\text{sat}}(T)} \quad \text{where } \left(\begin{matrix} \tau \\ \varepsilon \end{matrix} \right)_\alpha^{\text{sat}}(T) \stackrel{\text{def}}{=} \left(\begin{matrix} \tau \\ \varepsilon \end{matrix} \right)_\alpha(\hat{P}^{\text{sat}}(T), T)$$

TABULATED EOS

▶ Water Examples

(τ, ε) fixed

T SOLUTION OF

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||

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TABULATED EOS

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$$\left(\begin{matrix} \hat{\tau} \\ \hat{\varepsilon} \end{matrix}\right)_\alpha^{\text{sat}}(T)$$

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least square
approximations

TABULATED EOS

► Water Examples

(τ, ε) fixed

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↔

$$\left(\begin{matrix} \hat{\tau} \\ \hat{\varepsilon} \end{matrix}\right)_\alpha^{\text{sat}}(T)$$

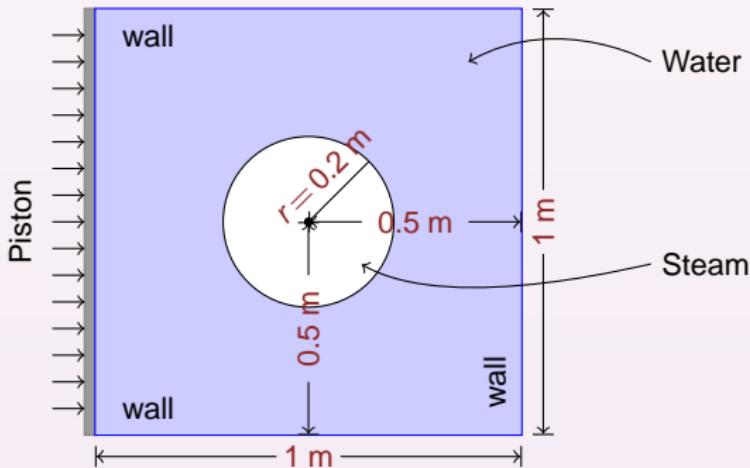
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least square
approximations

OUTLINE

- 1 Model
- 2 Numerical Method
- 3 Numerical Tests
- 4 Conclusion

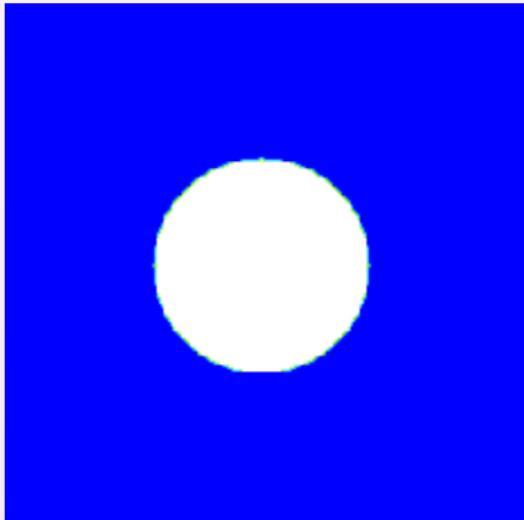
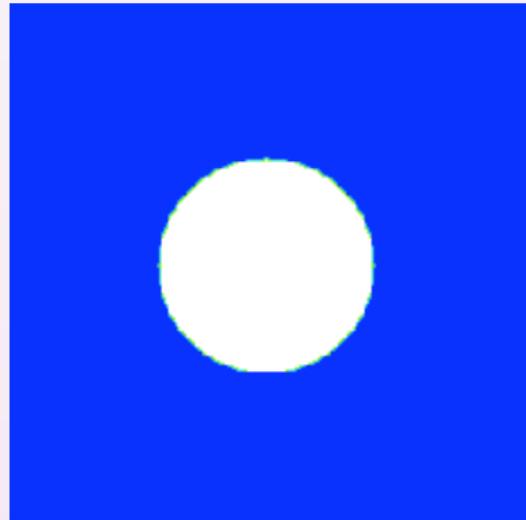
COMPRESSION OF A VAPOR BUBBLE



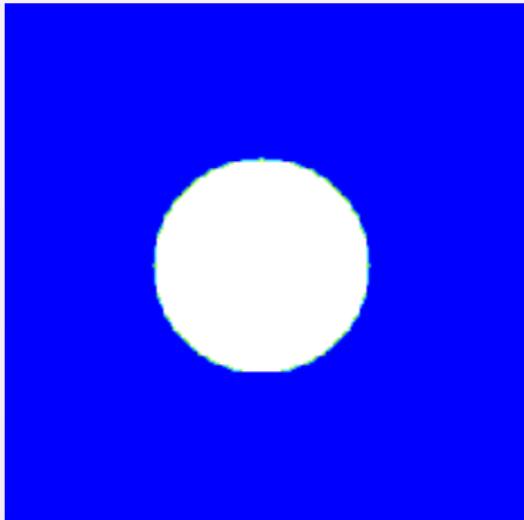
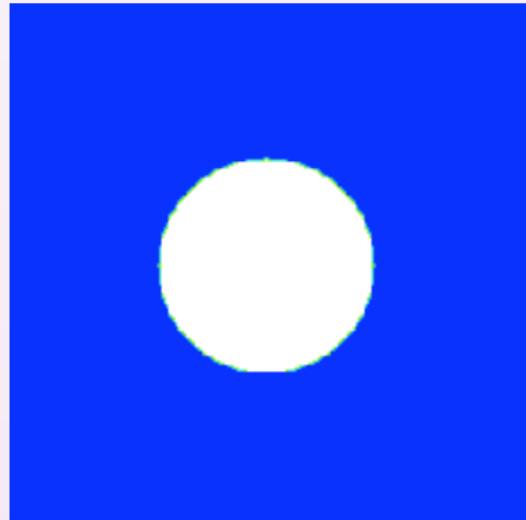
Compression of a 2D Vapor Bubble involving two Stiffened Gases for water and steam.

The piston moves towards right at constant speed $u_p = 30 \text{ m/s}$.

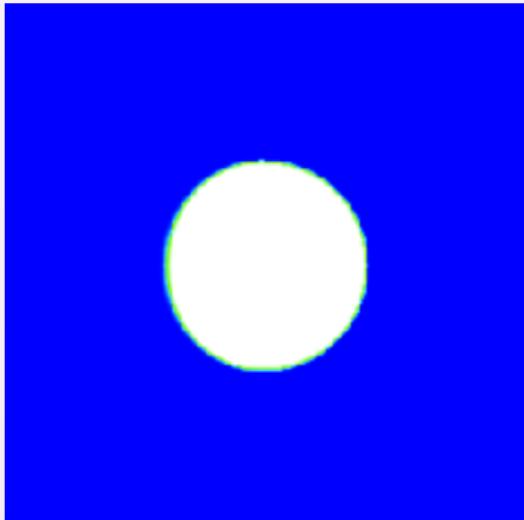
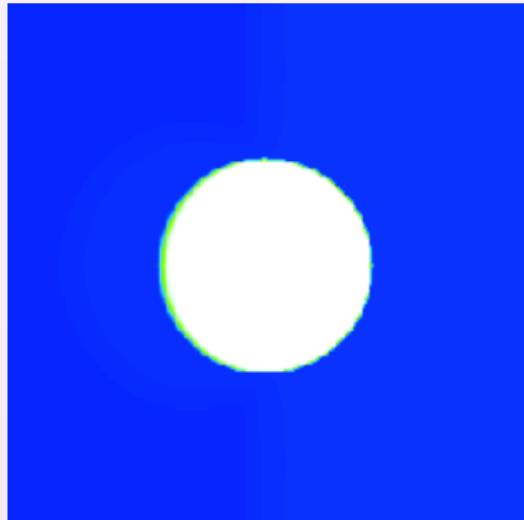
COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ  $t = 0.00 \text{ ms}$ [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

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Mass Fraction y Density ρ  $t = 0.00 \text{ ms}$ [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

COMPRESSION OF A VAPOR BUBBLE

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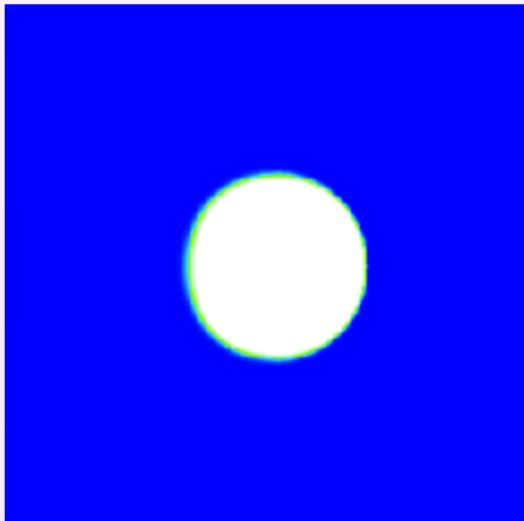
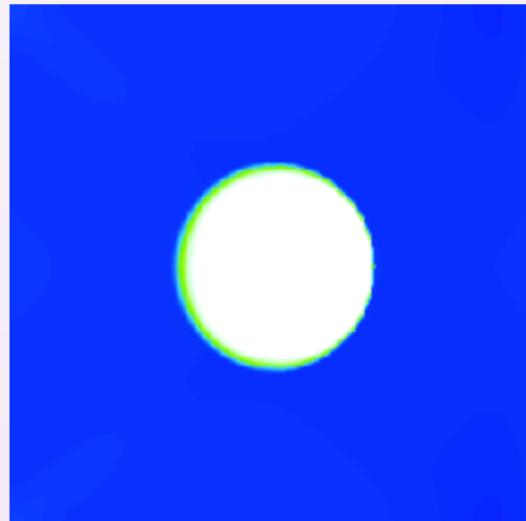
$t = 0.89 \text{ ms}$

◀ Geometry

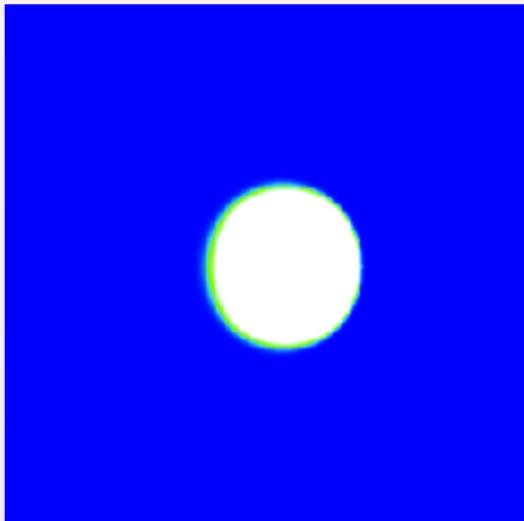
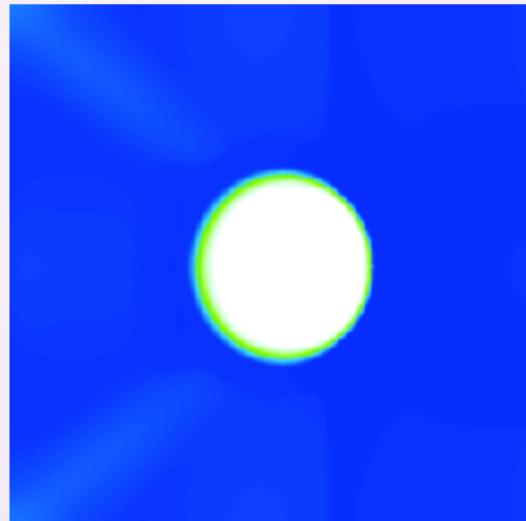
▶ Play

▶ Skip

COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ  $t = 1.49 \text{ ms}$ [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ 

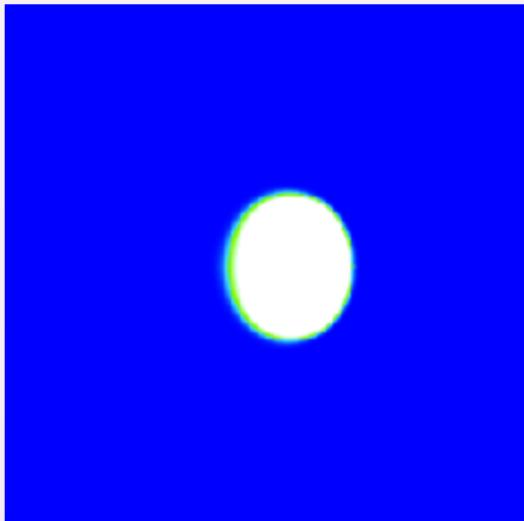
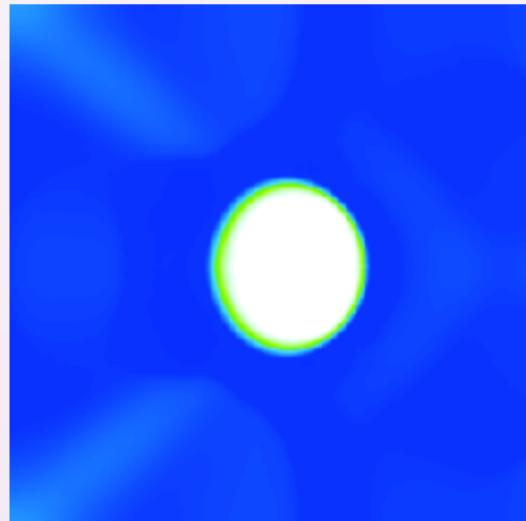
$t = 2.09 \text{ ms}$

◀ Geometry

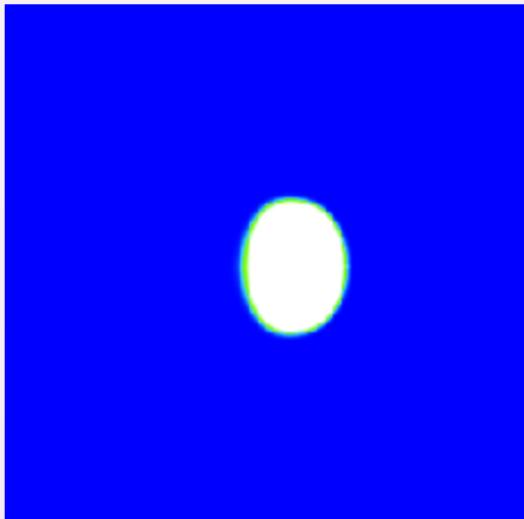
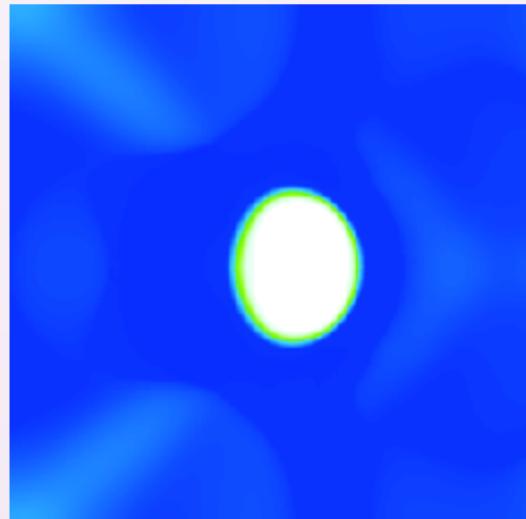
▶ Play

▶ Skip

COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ  $t = 2.69 \text{ ms}$ [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ 

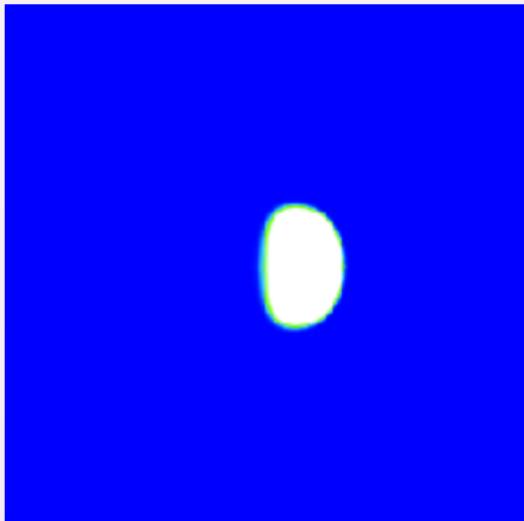
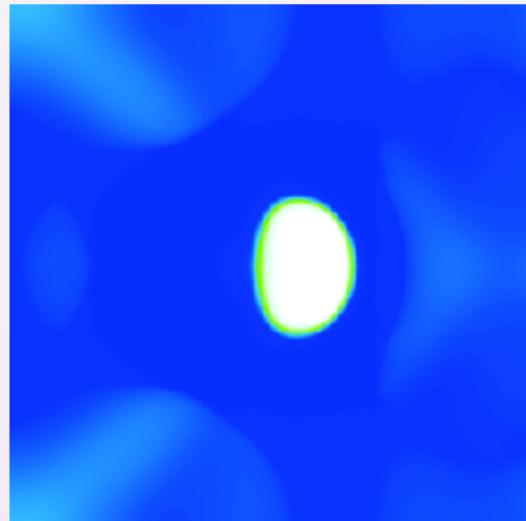
$t = 3.30 \text{ ms}$

◀ Geometry

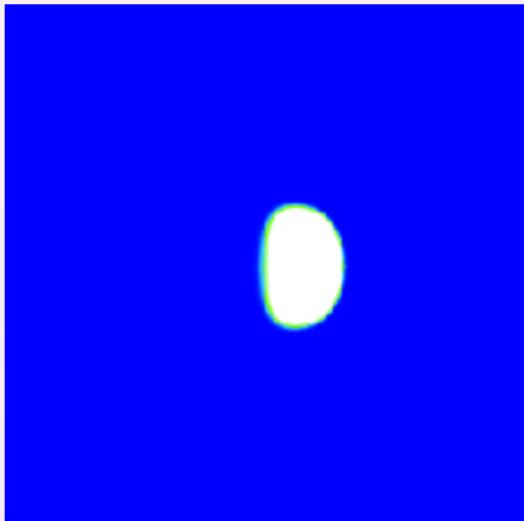
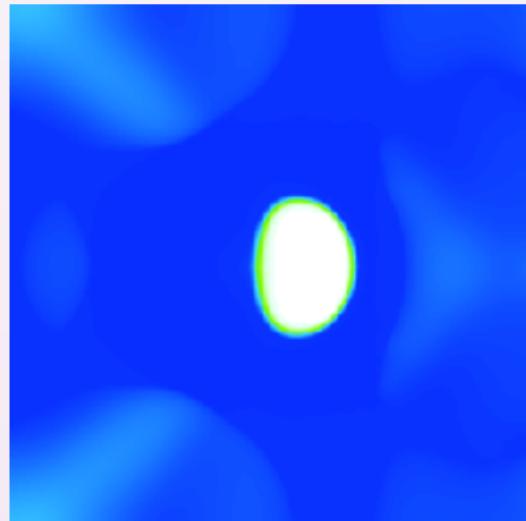
▶ Play

▶ Skip

COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ  $t = 3.60 \text{ ms}$ [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ 

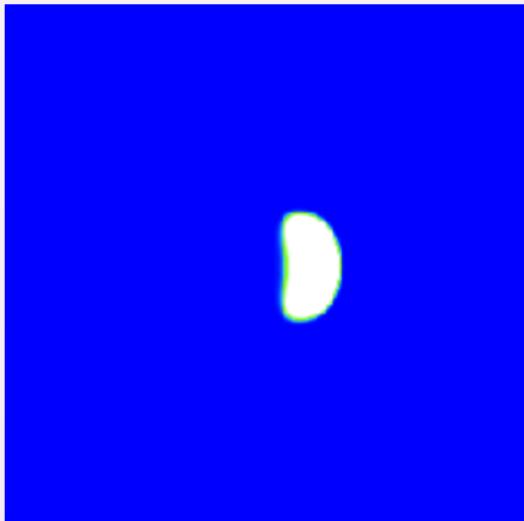
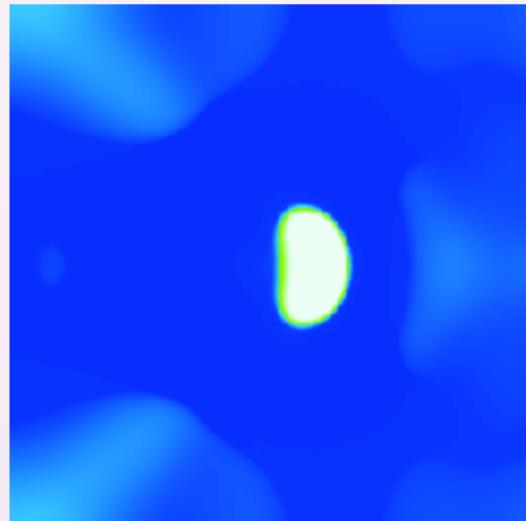
$t = 3.60 \text{ ms}$

◀ Geometry

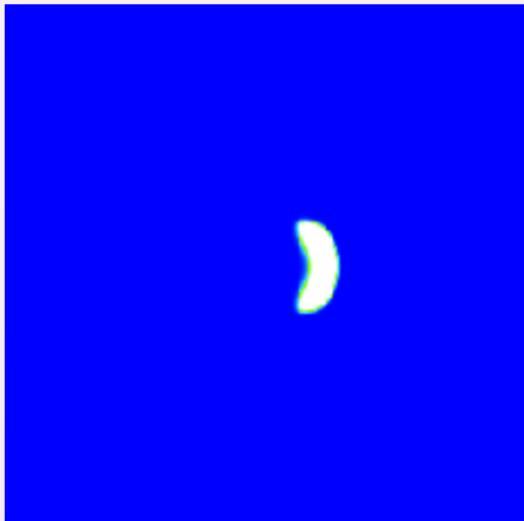
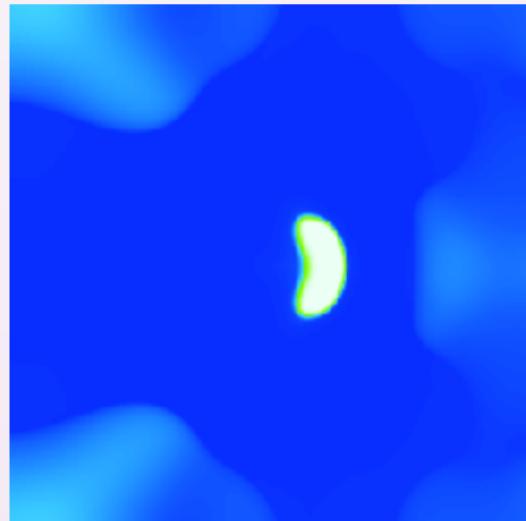
▶ Play

▶ Skip

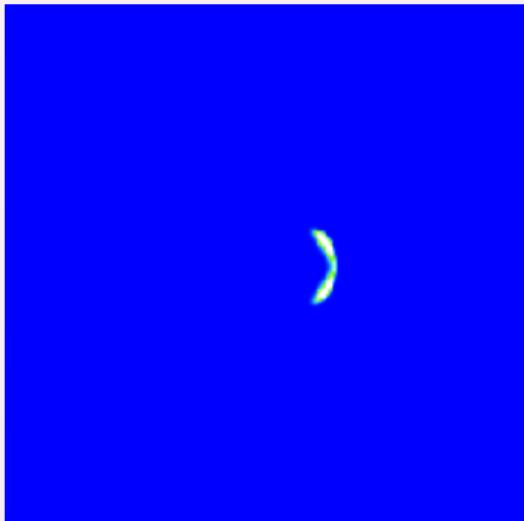
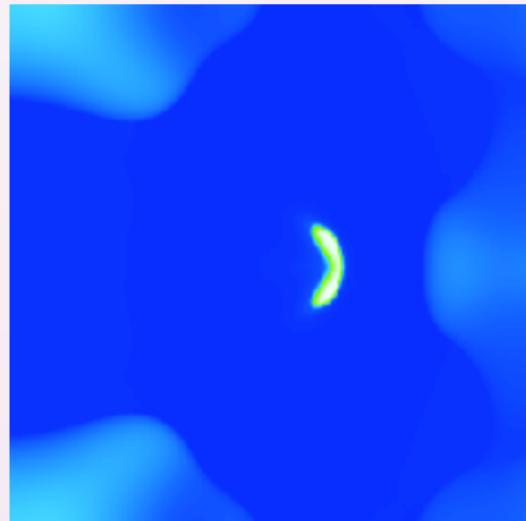
COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ  $t = ? \text{ ms}$ [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

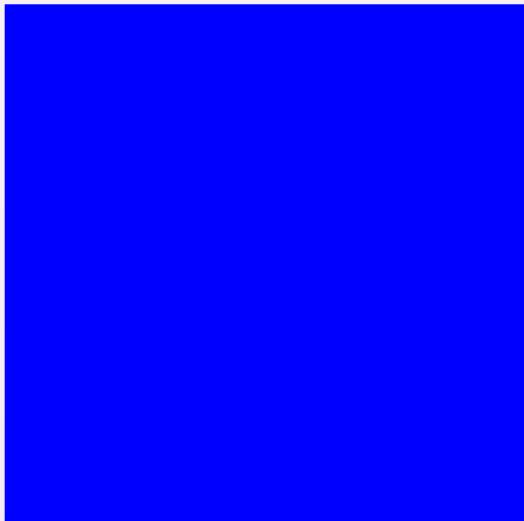
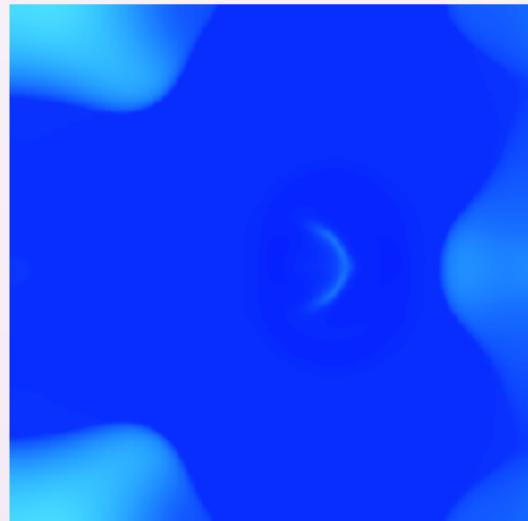
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Mass Fraction y Density ρ  $t = ? \text{ ms}$ [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

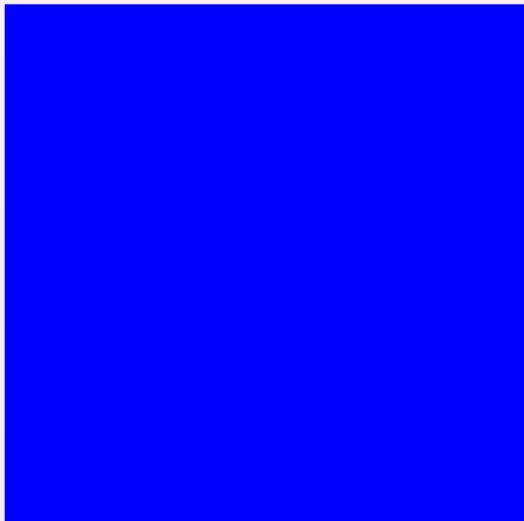
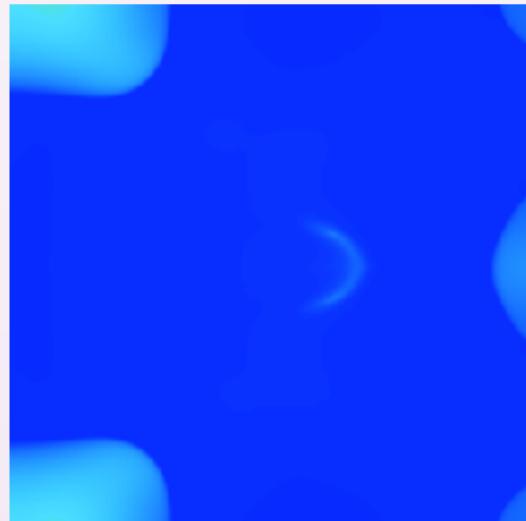
COMPRESSION OF A VAPOR BUBBLE

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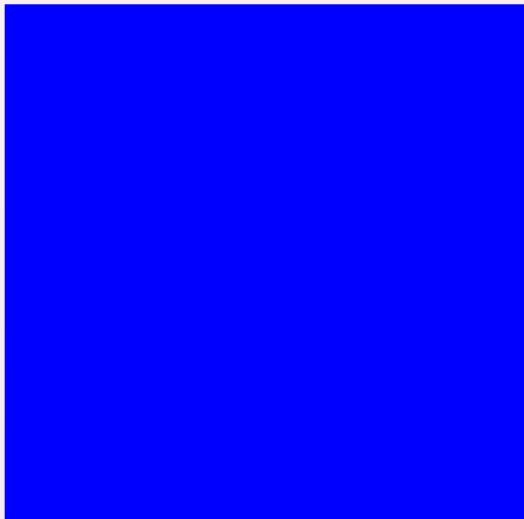
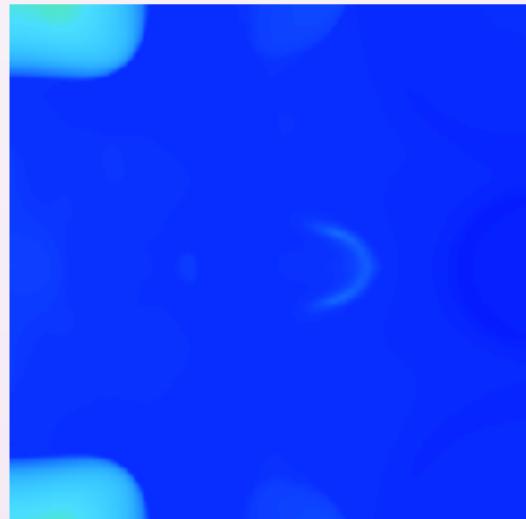
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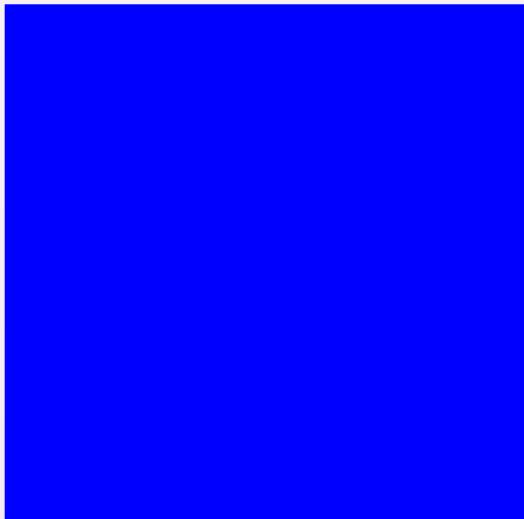
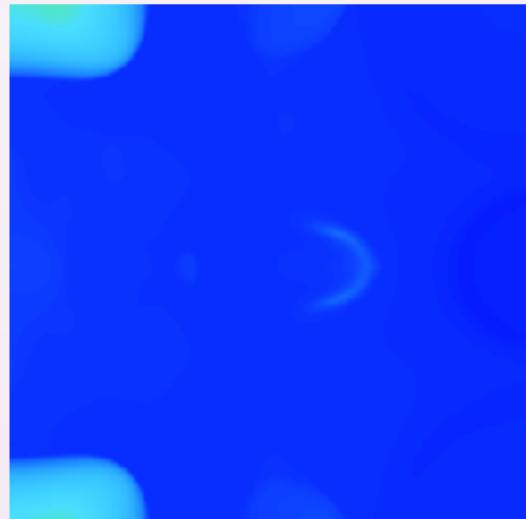
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OUTLINE

- 1 Model
- 2 Numerical Method
- 3 Numerical Tests
- 4 Conclusion

LIQUID-VAPOR PHASE TRANSITION

- Diffuse Interface Model
 - global EOS always at equilibrium (entropy maximization),
 - strict hyperbolicity of the Euler system,
 - uniqueness of Liu solution for the Riemann problem;
- Relaxation Approach
 - 6 (or 5) equation system with relaxation terms;
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 - operator splitting,
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STIFFENED GAS FOR WATER

$$(\tau_\alpha, \varepsilon_\alpha) \mapsto s_\alpha = c_{v_\alpha} \ln(\varepsilon_\alpha - q_\alpha - \pi_\alpha \tau_\alpha) + c_{v_\alpha} (\gamma_\alpha - 1) \ln \tau_\alpha + m_\alpha$$

Phase	c_v [J/(kg · K)]	γ	π [Pa]	q [J/kg]	m [J/(kg · K)]
Water	1816.2	2.35	10^9	-1167.056×10^3	-32765.55596
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TABLE: Parameters proposed by [Le Metayer] for water.

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WATER TABULATED EOS

$$\left. \begin{array}{l} T^i = 278\text{K} \dots 610\text{K}, \\ \varepsilon_{\alpha}^{\text{sat}}(T^i), \tau_{\alpha}^{\text{sat}}(T^i) \text{ found in the tables} \end{array} \right\} \Rightarrow \left\{ \begin{array}{l} \mathfrak{A} = \left\{ \left(T_i, \frac{1}{\varepsilon_{\text{vap}}^{\text{sat}}(T_i)} \right) \right\}_i \\ \mathfrak{B} = \left\{ \left(T_i, \frac{\varepsilon_{\text{liq}}^{\text{sat}}(T_i)}{\varepsilon_{\text{vap}}^{\text{sat}}(T_i)} \right) \right\}_i \\ \mathfrak{C} = \left\{ \left(T_i, \frac{1}{\tau_{\text{vap}}^{\text{sat}}(T_i)} \right) \right\}_i \\ \mathfrak{D} = \left\{ \left(T_i, \frac{\tau_{\text{liq}}^{\text{sat}}(T_i)}{\tau_{\text{vap}}^{\text{sat}}(T_i)} \right) \right\}_i \end{array} \right\}$$

$\hat{\varepsilon}_{\alpha}^{\text{sat}}$ and $\hat{\tau}_{\alpha}^{\text{sat}}$ defined by using a least square approximation of \mathfrak{A} , \mathfrak{B} , \mathfrak{C} and \mathfrak{D} :

$$T \mapsto \varepsilon_{\text{vap}}^{\text{sat}} \approx \hat{\varepsilon}_{\text{vap}}^{\text{sat}} \stackrel{\text{def}}{=} \frac{1}{\sum_{k=0}^6 a_k T^k}$$

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