Modelling and Simulation of Liquid-Vapor Phase Transition

A Boiling Crisis Study Contribution

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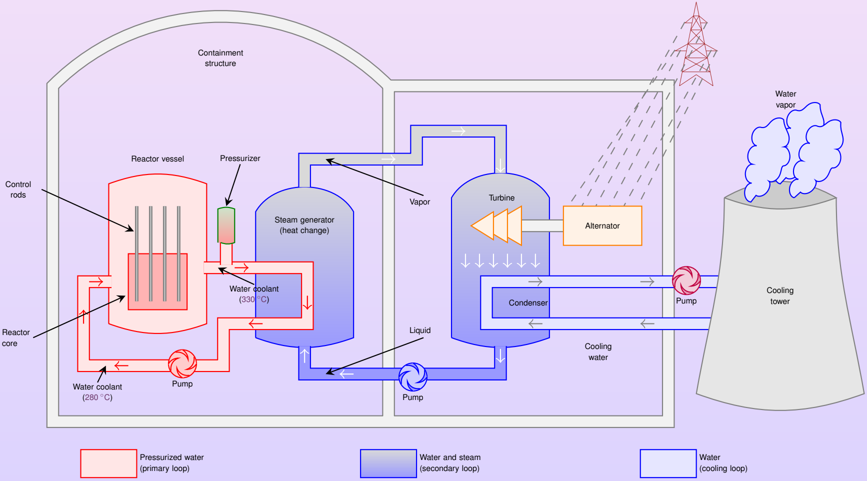
Orsay, 22nd October 2008

OUTLINE

Outline

Pressurized Water Reactor



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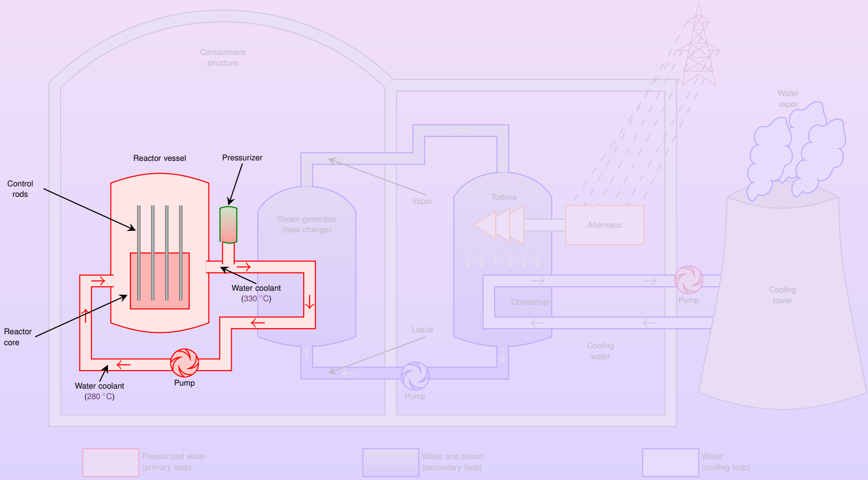

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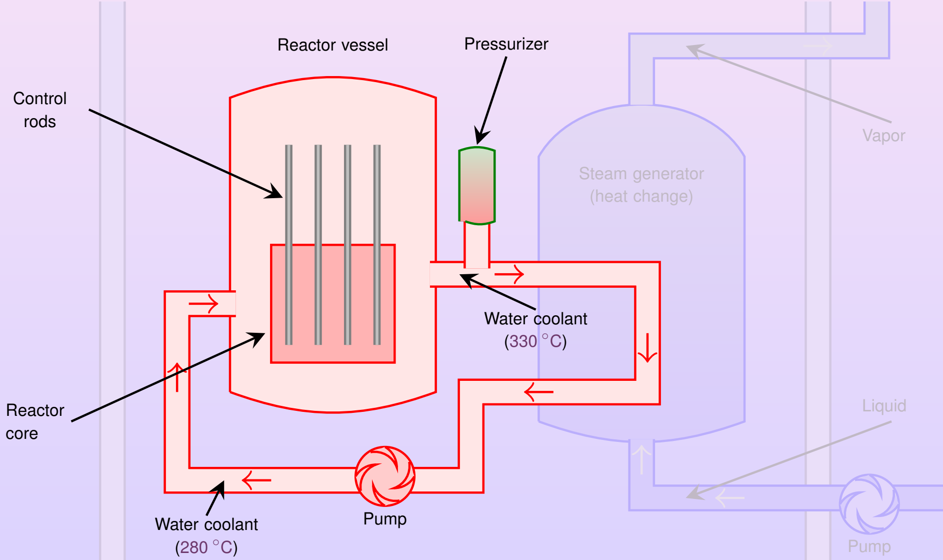
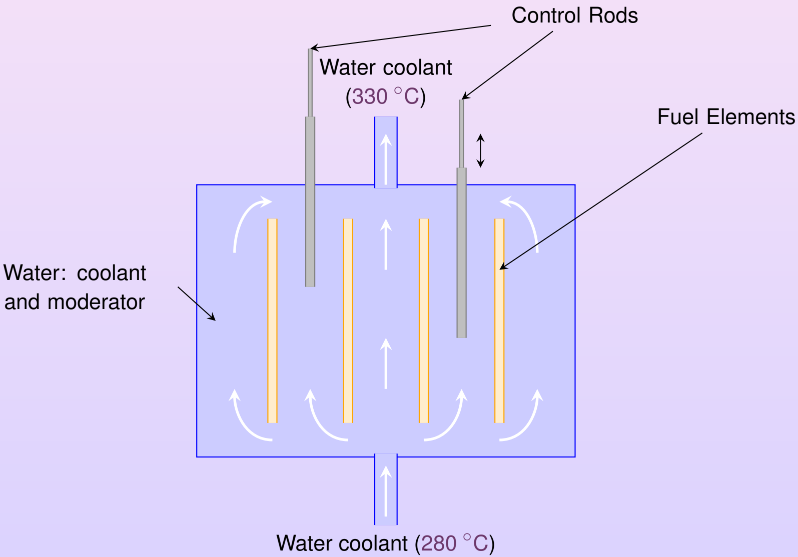


Core of a Pressurized Water Reactor



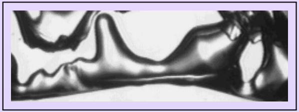
Boiling Crisis

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

OMEGA - CEA GRENOBLE

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"INGREDIENTS" OF THE MODEL

- ✔ System of PDEs for the mouvement of the fluid,
- Phase transition (pressure and/or temperature variations),
- Heat Diffusion,
- Surface Tension,
- Gravity.

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Outline

EULER SYSTEM

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

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

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

EULER SYSTEM

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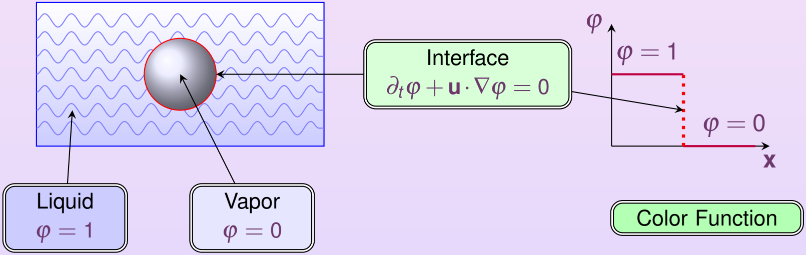
OUTLINE

1. Context
2. **Model**
   - Equation of state
   - Muvement Equations
3. Numerical Approximation
   - Numerical Method
   - Numerical Tests
4. Conclusion

Liquid-Vapor Interface



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

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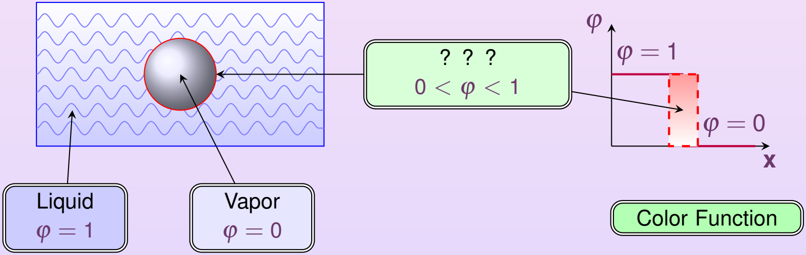

$$(\rho, \varepsilon) \mapsto P = \begin{cases} P^{\text{liq}} & \text{if } \varphi = 1; \\ ??? & \text{if } 0 < \varphi < 1; \\ P^{\text{vap}} & \text{if } \varphi = 0. \end{cases}$$

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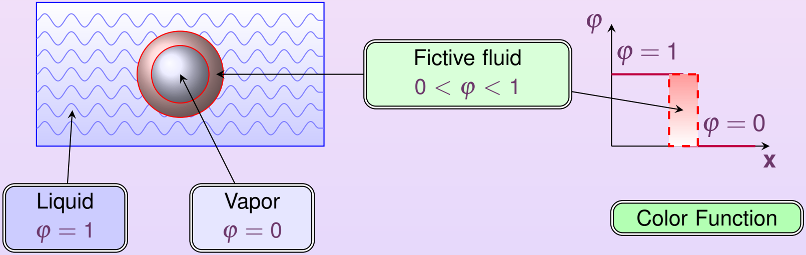

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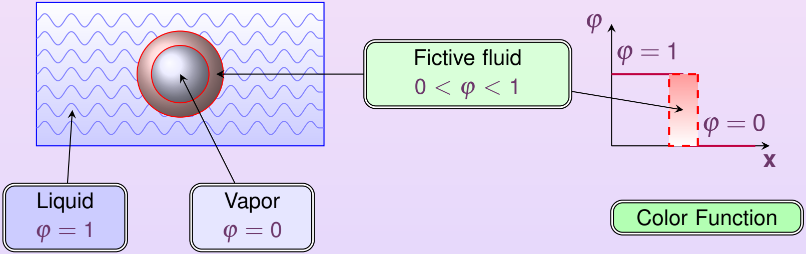

Goal: define a global pressure law such that

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

EOS of each Phase $\alpha = 1,2$

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

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

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

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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. $y\tau_1 = z\tau$;
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EOS WITH PHASE CHANGE

ENTROPY WITHOUT PH.CH.

$$(\mathbf{w}, z, y, \psi) \mapsto \sigma$$

ENTROPY AT EQUILIBRIUM

$$\mathbf{w} \mapsto s^{\mathrm{eq}}$$

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

Optimization Problem:

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

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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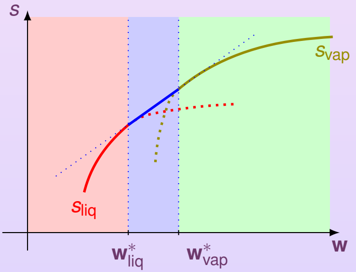

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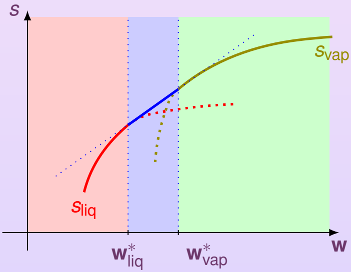

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EOS with Phase Change

Entropy without Ph.Ch.

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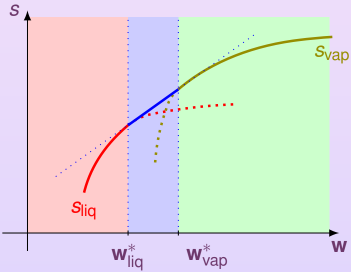
Entropy at equilibrium

$$\mathbf{w} \mapsto s^{\mathrm{eq}}$$



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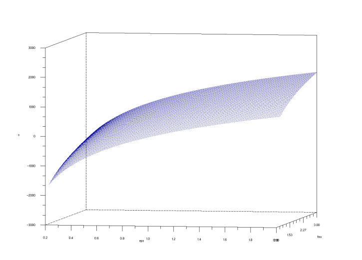
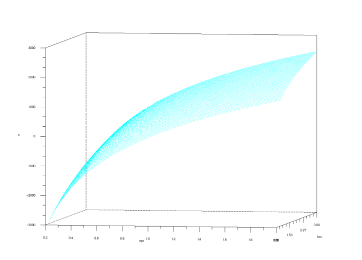
Concave Hull with two Perfect Gases

$(\tau, \varepsilon) \mapsto s_{\text{liq}}$



$(\tau, \varepsilon) \mapsto s_{\text{vap}}$



Concave Hull with two Perfect Gases

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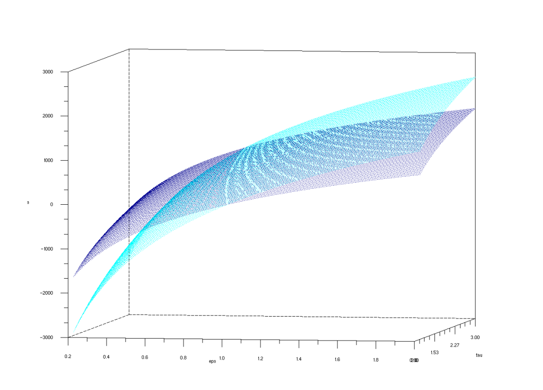

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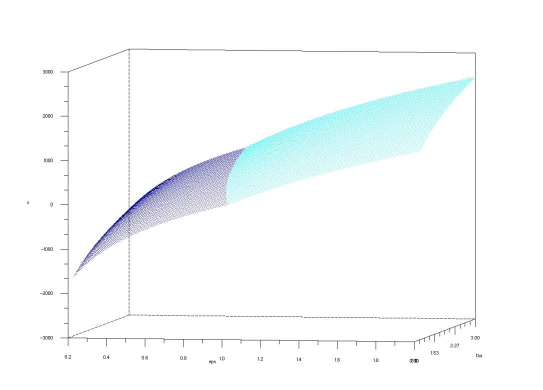

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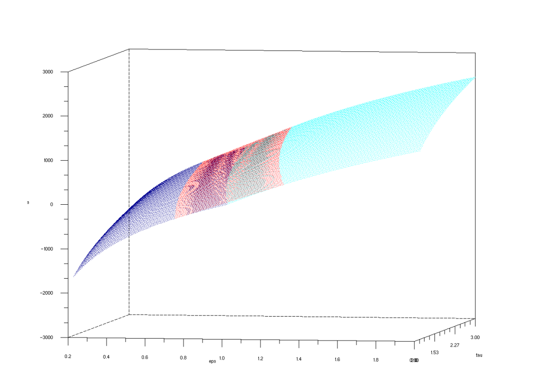

CONCAVE HULL WITH TWO PERFECT GASES

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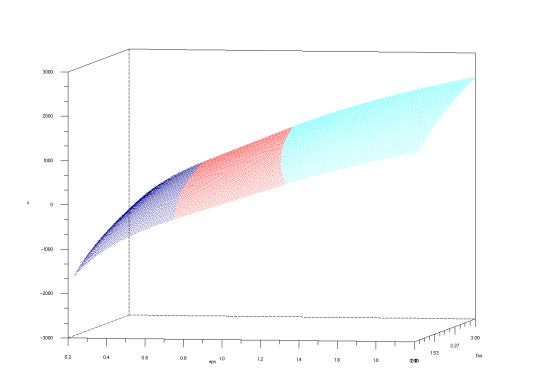

From $\mathbf{w} \mapsto s^{\mathrm{eq}}$ to $\mathbf{w} \mapsto P^{\mathrm{eq}}$

For all $\widetilde{\mathbf{w}}$ fixed, we seek $(\mathbf{w}^*_{\mathrm{liq}}, \mathbf{w}^*_{\mathrm{vap}}, y^*)$ as the solution of the system

$$\begin{cases} P_{\mathrm{liq}}(\mathbf{w}_{\mathrm{liq}}) = P_{\mathrm{vap}}(\mathbf{w}_{\mathrm{vap}}) \\ T_{\mathrm{liq}}(\mathbf{w}_{\mathrm{liq}}) = T_{\mathrm{vap}}(\mathbf{w}_{\mathrm{vap}}) \\ g_{\mathrm{liq}}(\mathbf{w}_{\mathrm{liq}}) = g_{\mathrm{vap}}(\mathbf{w}_{\mathrm{vap}}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{\mathrm{liq}} + (1-y)\mathbf{w}_{\mathrm{vap}} \end{cases}$$

1. if $y^* \in]0,1[$ then $\widetilde{\mathbf{w}}$ is an **equilibrium mixture state**

$$s^{\mathrm{eq}}(\widetilde{\mathbf{w}}) = y^* s_{\mathrm{liq}}(\mathbf{w}^*_{\mathrm{liq}}) + (1-y^*) s_{\mathrm{vap}}(\mathbf{w}^*_{\mathrm{vap}}),$$
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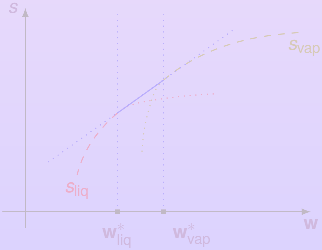
2. if the system has no solution or $y^* \notin]0,1[$ then $\widetilde{\mathbf{w}}$ is a **monophasique pure state**

$$s^{\mathrm{eq}}(\widetilde{\mathbf{w}}) = \max\{s_{\mathrm{liq}}(\widetilde{\mathbf{w}}), s_{\mathrm{vap}}(\widetilde{\mathbf{w}})\},$$
$$P^{\mathrm{eq}}(\widetilde{\mathbf{w}}) = P_{\alpha}(\widetilde{\mathbf{w}}).$$



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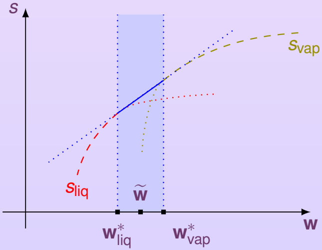
2. if the system has no solution or $y^* \notin]0,1[$ then $\widetilde{\mathbf{w}}$ is a **monophasique pure state**

$$s^{\mathrm{eq}}(\widetilde{\mathbf{w}}) = \max\{s_{\mathrm{liq}}(\widetilde{\mathbf{w}}), s_{\mathrm{vap}}(\widetilde{\mathbf{w}})\},$$

$$P^{\mathrm{eq}}(\widetilde{\mathbf{w}}) = P_{\alpha}(\widetilde{\mathbf{w}}).$$



From $\mathbf{w} \mapsto s^{\text{eq}}$ to $\mathbf{w} \mapsto P^{\text{eq}}$

For all $\widetilde{\mathbf{w}}$ fixed, we seek $(\mathbf{w}^*_{\text{liq}}, \mathbf{w}^*_{\text{vap}}, y^*)$ as the solution of the system

$$\begin{cases} P_{\text{liq}}(\mathbf{w}_{\text{liq}}) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ T_{\text{liq}}(\mathbf{w}_{\text{liq}}) = T_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ g_{\text{liq}}(\mathbf{w}_{\text{liq}}) = g_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{\text{liq}} + (1-y)\mathbf{w}_{\text{vap}} \end{cases}$$

1. if $y^* \in]0,1[$ then $\widetilde{\mathbf{w}}$ is an **equilibrium mixture state**

$$s^{\text{eq}}(\widetilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}^*_{\text{liq}}) + (1-y^*) s_{\text{vap}}(\mathbf{w}^*_{\text{vap}}),$$

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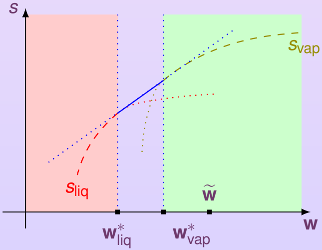

FROM $\mathbf{w} \mapsto s^{\mathrm{eq}}$ TO $\mathbf{w} \mapsto P^{\mathrm{eq}}$

For all $\widetilde{\mathbf{w}}$ fixed, we seek $(\mathbf{w}^*_{\mathrm{liq}}, \mathbf{w}^*_{\mathrm{vap}}, y^*)$ as the solution of the system

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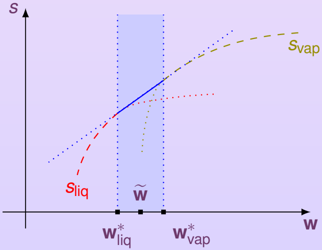

From $\mathbf{w} \mapsto s^{\text{eq}}$ to $\mathbf{w} \mapsto P^{\text{eq}}$

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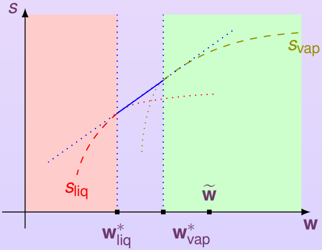

ANALYTICAL EOS

(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

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

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

T SOLUTION OF

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

Water Example

Analytical EOS

(τ,ε) fixed

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

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

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

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

Water Example

Analytical EOS

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Water Example

Analytical EOS

(τ, ε) fixed

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least square approximation

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

T SOLUTION OF

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

Water Example

Tabulated EOS

(τ, ε) fixed

T solution of

$$\frac{\tau - \tau_2^{\mathrm{sat}}(T)}{\tau_1^{\mathrm{sat}}(T) - \tau_2^{\mathrm{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\mathrm{sat}}(T)}{\varepsilon_1^{\mathrm{sat}}(T) - \varepsilon_2^{\mathrm{sat}}(T)} \quad \text{with} \quad \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha^{\mathrm{sat}}(T) \quad \text{tabulated}$$

$$\wr\wr$$

$$\frac{\tau - \widehat{\tau}_2^{\mathrm{sat}}(T)}{\widehat{\tau}_1^{\mathrm{sat}}(T) - \widehat{\tau}_2^{\mathrm{sat}}(T)} = \frac{\varepsilon - \widehat{\varepsilon}_2^{\mathrm{sat}}(T)}{\widehat{\varepsilon}_1^{\mathrm{sat}}(T) - \widehat{\varepsilon}_2^{\mathrm{sat}}(T)} \quad \text{with} \quad \begin{pmatrix} \widehat{\tau} \\ \widehat{\varepsilon} \end{pmatrix}_\alpha^{\mathrm{sat}}(T)$$

Water Examples

TABULATED EOS

(τ, ε) fixed

T SOLUTION OF

$$\frac{\tau - \tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T) - \tau_2^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T) - \varepsilon_2^{\text{sat}}(T)}$$ with $\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T)$ tabulated

$\wr\wr$

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least square approximations

Water Examples

TABULATED EOS

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least square approximations

Water Examples

OUTLINE

Dynamic Liquid-Vapor Phase Change

Euler System

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

Properties [G. Allaire, G. Faccanoni, S. Kokh]

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

❶ $c(\mathbf{w}) > 0$, ❷ $s^{\text{eq}}_{\tau\varepsilon}(\mathbf{w}) > 0$

❶ Euler system: strict hyperbolicity ($\neq$ p-system),

❷ Riemann problem: multitude of entropy (Lax) solutions [R. Menikoff, B. J. Plohr], uniqueness of Liu solution.

Dynamic Liquid-Vapor Phase Change

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DYNAMIC LIQUID-VAPOR PHASE CHANGE

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OUTLINE

How to simulate the Liu solution

- Exact Riemann Solver (cf. [A. Voß] for Van der Waals EOS)
- Viscous Solver (the Liu solution is the only solution that has a viscous profile) (cf. [S. Jaouen] for Perfect Gas EOS with $c_{v_{\text{liq}}} = c_{v_{\text{vap}}}$)
- 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],…

OUTLINE

1. Context
2. Model
   - Equation of state
   - Muvement Equations
3. Numerical Approximation
   - Numerical Method
   - Numerical Tests
4. Conclusion

Relaxation Approach

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

Relaxation Approach

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

Relaxation Approach

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Equilibrium System

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P^{\text{eq}}\,\mathbb{I}) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + P^{\text{eq}})\mathbf{u}) = 0 \end{cases}$$

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

Relaxation Approach

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

Augmented System

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P \mathbb{I}) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + P)\mathbf{u}) = 0 \end{cases}$$

$$P(\rho, \varepsilon, z, y, \psi) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

Equilibrium System

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In the interface

$$\begin{cases} \partial_t z + \mathbf{u}\cdot\mathbf{grad}\, z = \\ \partial_t y + \mathbf{u}\cdot\mathbf{grad}\, y = \\ \partial_t \psi + \mathbf{u}\cdot\mathbf{grad}\, \psi = \end{cases}$$

$$P(\rho,\varepsilon,z,y,\psi) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

Equilibrium System

$$\begin{cases} \partial_t\rho + \operatorname{div}(\rho\mathbf{u}) = 0 \\ \partial_t(\rho\mathbf{u}) + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u} + P^{\mathrm{eq}}\mathbb{I}) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + P^{\mathrm{eq}})\mathbf{u}) = 0 \end{cases}$$

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

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

Augmented System

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P\mathbb{I}) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + P)\mathbf{u}) = 0 \end{cases}$$

In the interface

$$\begin{cases} \partial_t z + \mathbf{u}\cdot \mathbf{grad}\, z = \dfrac{1}{\mu_z}\left(\dfrac{P_2}{T_2} - \dfrac{P_1}{T_1}\right) \\ \partial_t y + \mathbf{u}\cdot \mathbf{grad}\, y = \dfrac{1}{\mu_y}\left(\dfrac{g_1}{T_1} - \dfrac{g_2}{T_2}\right)\dfrac{1}{\rho} \\ \partial_t \psi + \mathbf{u}\cdot \mathbf{grad}\, \psi = \dfrac{1}{\mu_\psi}\left(\dfrac{1}{T_1} - \dfrac{1}{T_2}\right)\varepsilon \end{cases}$$

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

Equilibrium System

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P^{\text{eq}}\mathbb{I}) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + P^{\text{eq}})\mathbf{u}) = 0 \end{cases}$$

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

Relaxation Approach

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

Augmented System

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P\mathbb{I}) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + P)\mathbf{u}) = 0 \end{cases}$$

In the interface
$$\begin{cases} \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = \dfrac{1}{\mu_z}\left(\dfrac{P_2}{T_2} - \dfrac{P_1}{T_1}\right) \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, y = \dfrac{1}{\mu_y}\left(\dfrac{g_1}{T_1} - \dfrac{g_2}{T_2}\right)\dfrac{1}{\rho} \\ \partial_t \psi + \mathbf{u} \cdot \mathbf{grad}\, \psi = \dfrac{1}{\mu_\psi}\left(\dfrac{1}{T_1} - \dfrac{1}{T_2}\right)\varepsilon \end{cases}$$

$$P(\rho,\varepsilon,z,y,\psi) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

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

Equilibrium System

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P^{\text{eq}}\mathbb{I}) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + P^{\text{eq}})\mathbf{u}) = 0 \end{cases}$$

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

Remark: $\cancel{\partial_t \psi + \mathbf{u} \cdot \mathbf{grad}\, \psi = 0} \rightsquigarrow T_1 = T_2$.

NUMERICAL SCHEME

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

$\mathbf{V}_i^n \longrightarrow \mathbf{V}_i^{n+1}$

❶ $\mu_j = +\infty$

$\Downarrow$

$$\partial_t \mathbf{V} + \operatorname{div} \mathbf{G}(\mathbf{V}) = \mathbf{S}(\mathbf{V})$$

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

❷ $\mu_j = 0$

$\Downarrow$

$$\mathbf{R}(\mathbf{V}) = \mathbf{0}$$

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

Numerical Scheme

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

$\mathbf{V}_i^n \longrightarrow \mathbf{V}_i^{n+1}$

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Num. Scheme: op. splitting
Conv.: [G. Allaire and all.]
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Heat: 2D implicit

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Numerical Scheme

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

$\mathbf{V}_i^n \longrightarrow \mathbf{V}_i^{n+1/2} \longrightarrow \mathbf{V}_i^{n+1}$

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$$\partial_t \mathbf{V} + \operatorname{div} \mathbf{G}(\mathbf{V}) = \mathbf{S}(\mathbf{V})$$

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

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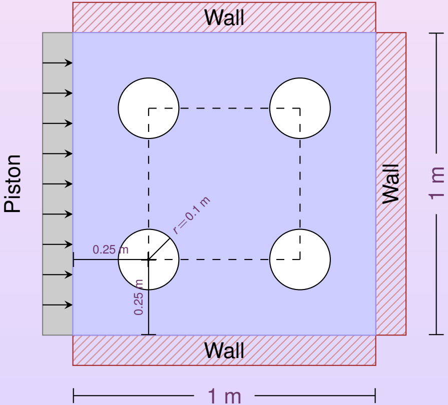
$\Downarrow$

$$\mathbf{R}(\mathbf{V}) = \mathbf{0}$$

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

Outline

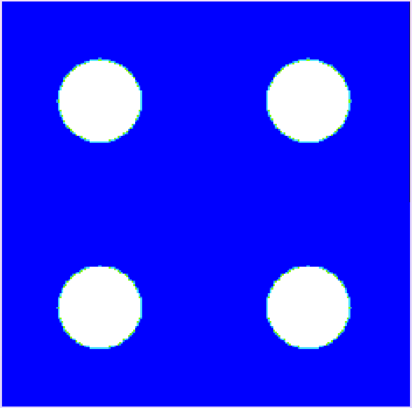
Compression of Vapor Bubbles



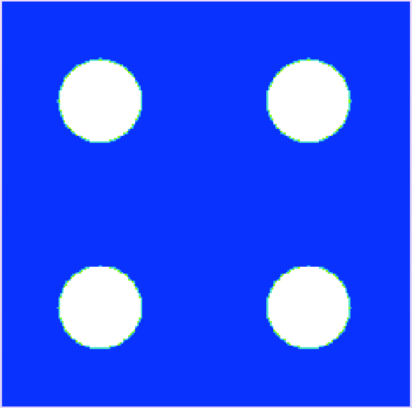
Compression of 4 Vapor Bubbles involving two Stiffened Gases for water and steam. The piston moves towards right at constant speed $u_{\mathrm{p}} = 30$ m/s.

Compression of Vapor Bubbles

Mass Fraction y



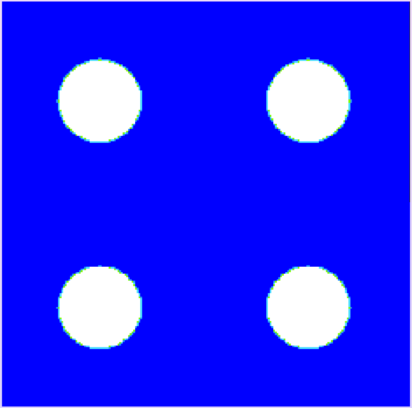
Density ρ



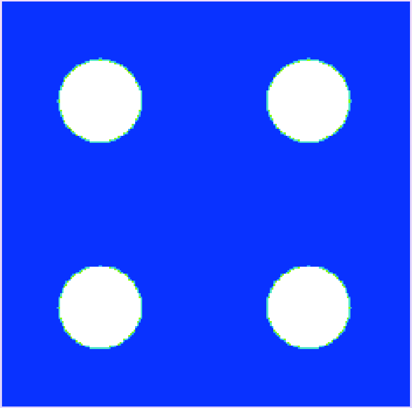
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



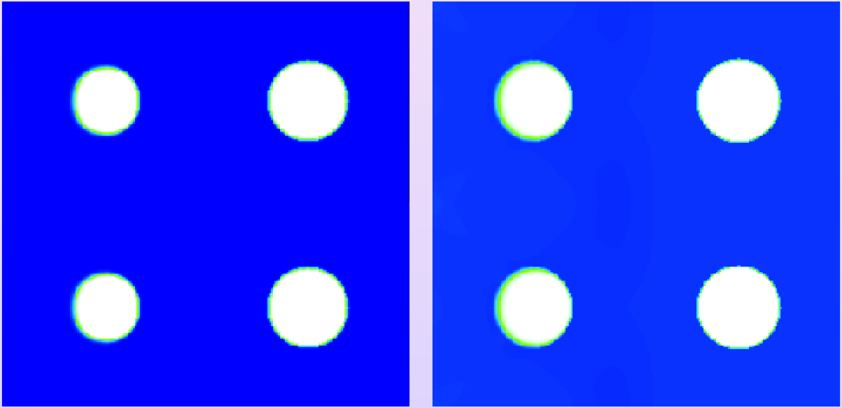
Density ρ



Geometry Play Skip

Compression of Vapor Bubbles

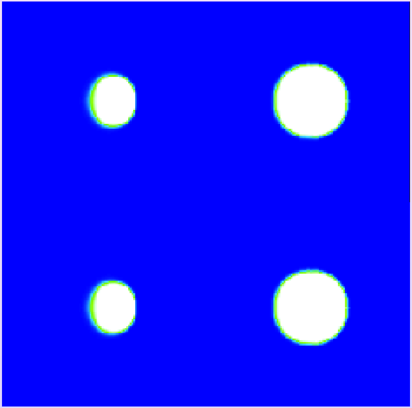
Mass Fraction y Density ρ



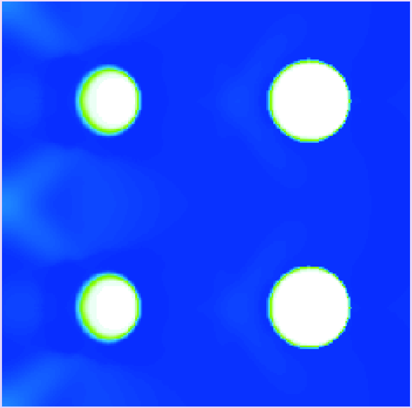
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



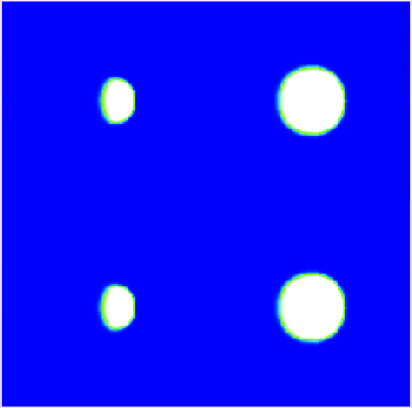
Density ρ



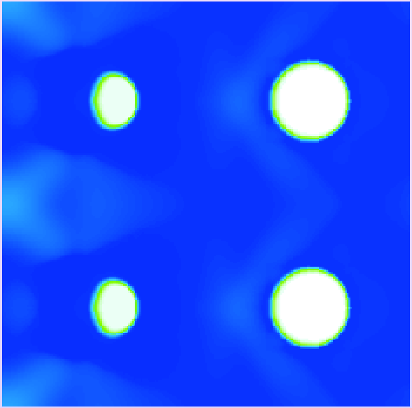
◂ Geometry ▸ Play ▸▸ Skip

Compression of Vapor Bubbles

Mass Fraction y



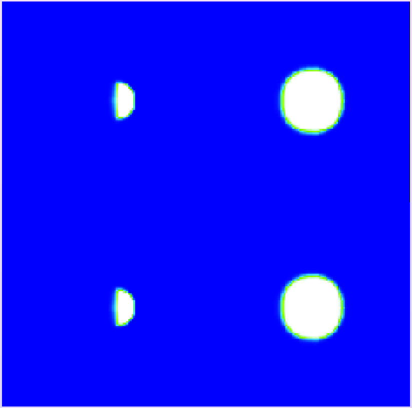
Density ρ



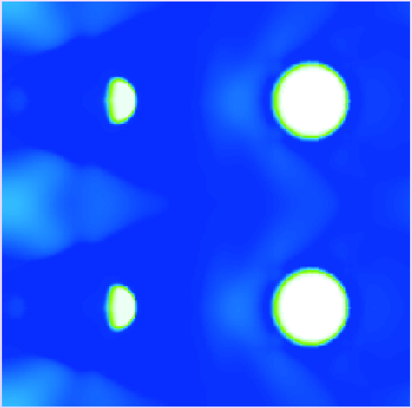
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



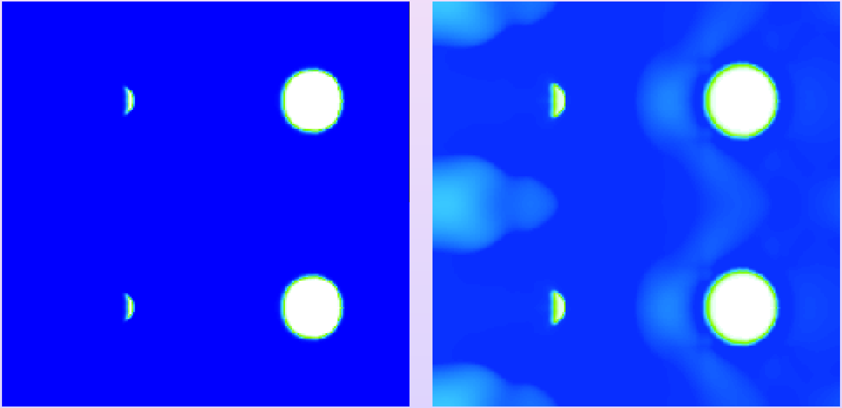
Density ρ



Geometry Play Skip

Compression of Vapor Bubbles

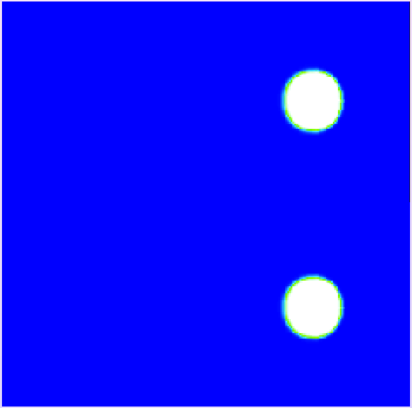
Mass Fraction y Density ρ



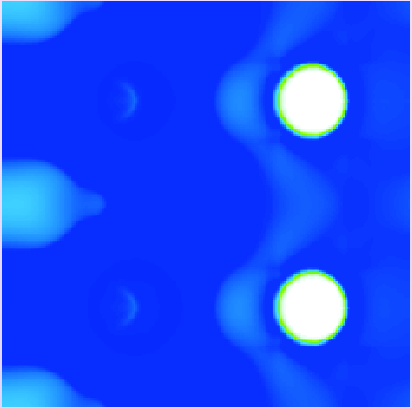
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



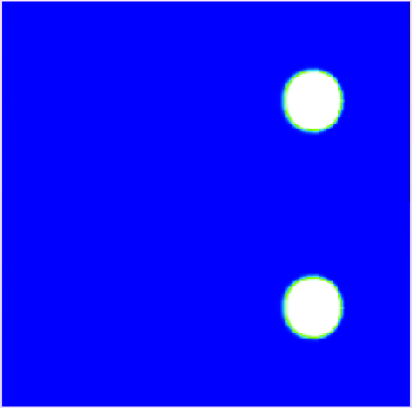
Density ρ



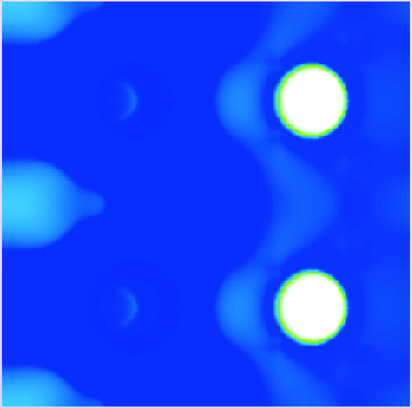
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y

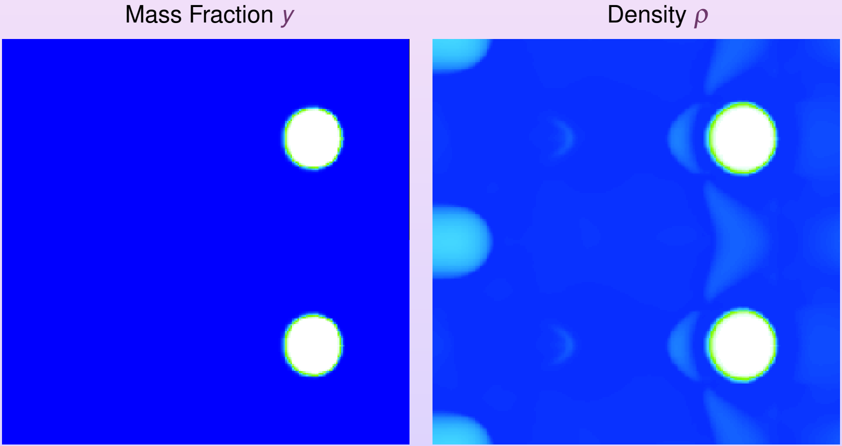


Density ρ



Geometry Play Skip

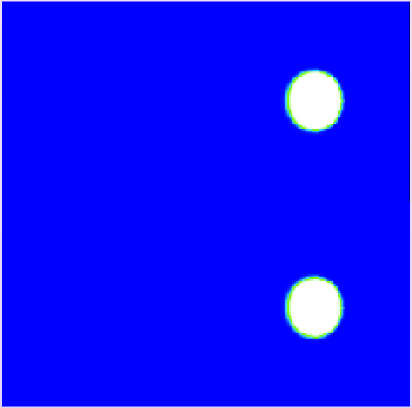
Compression of Vapor Bubbles



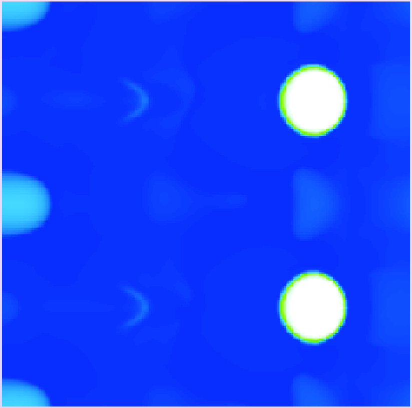
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



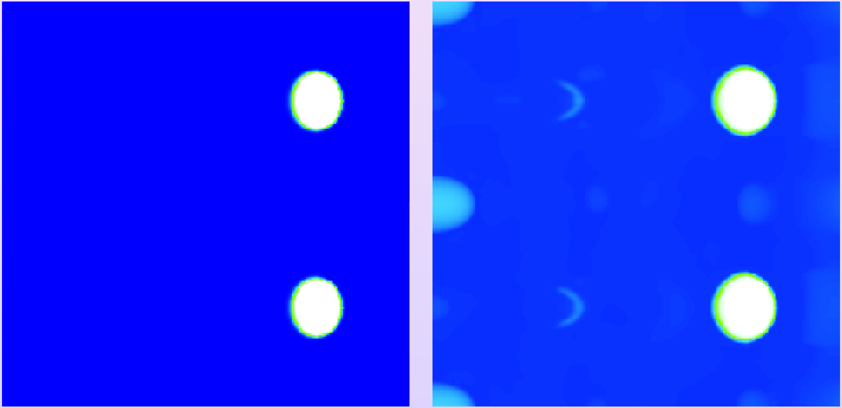
Density ρ



Geometry Play Skip

Compression of Vapor Bubbles

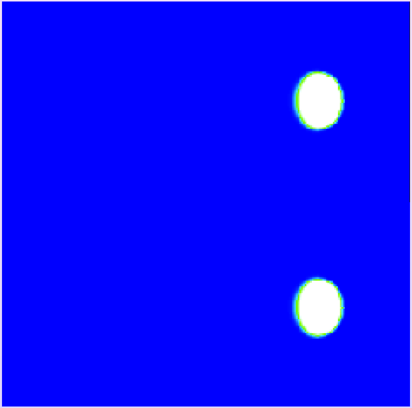
Mass Fraction y Density ρ



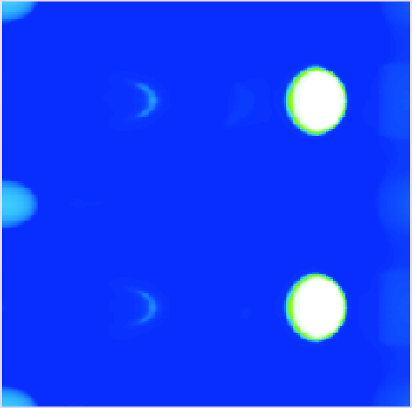
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



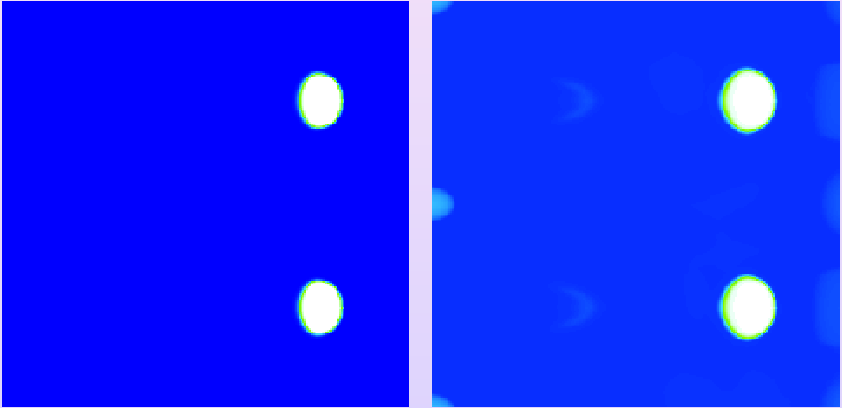
Density ρ



Geometry Play Skip

Compression of Vapor Bubbles

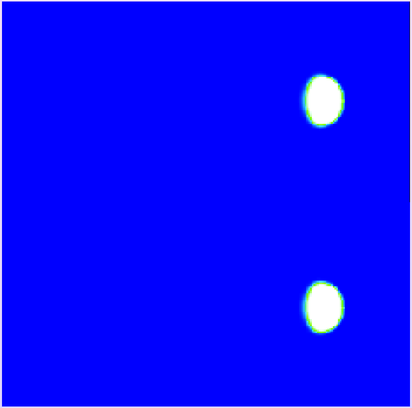
Mass Fraction y Density ρ



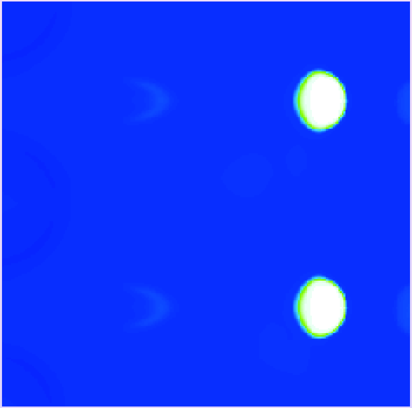
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



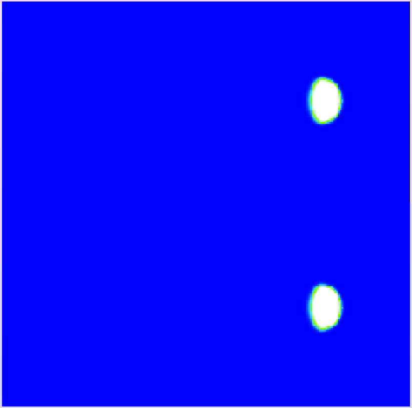
Density ρ



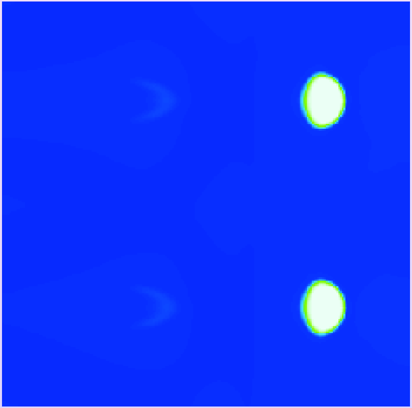
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



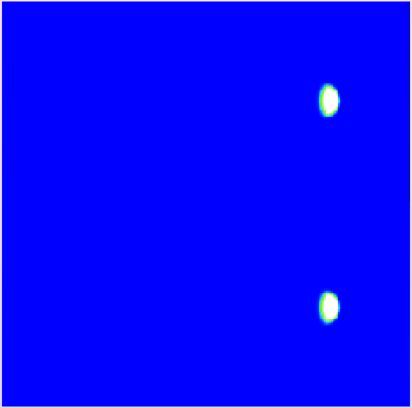
Density ρ



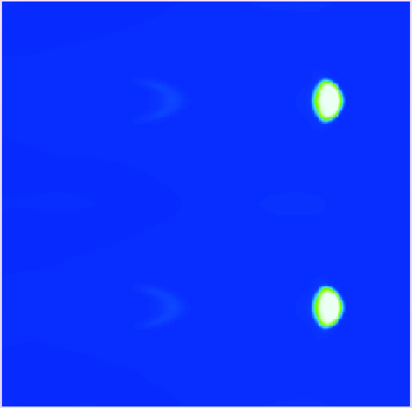
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



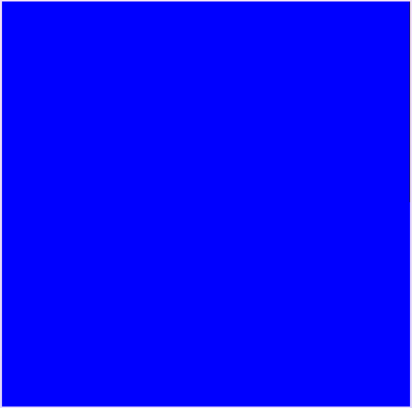
Density ρ



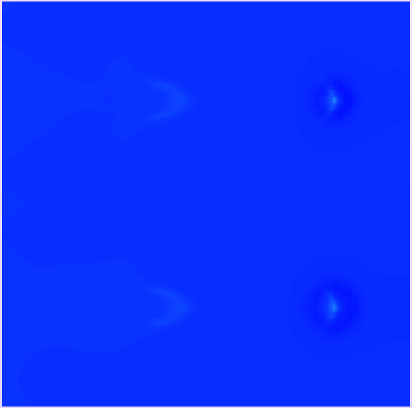
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



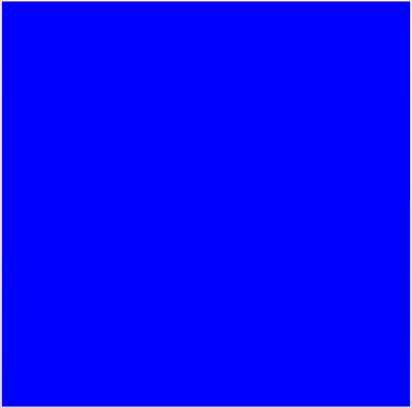
Density ρ



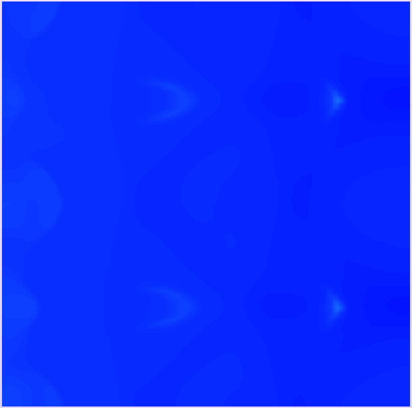
Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y



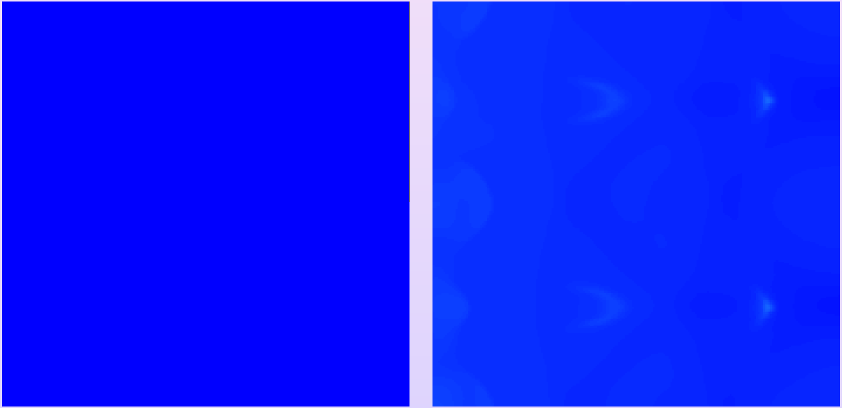
Density ρ



Geometry Play Skip

Compression of Vapor Bubbles

Mass Fraction y Density ρ

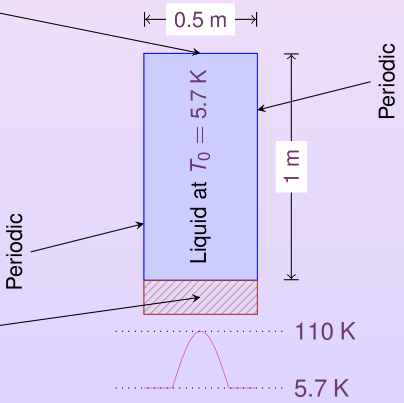


Geometry Play Skip

NUCLEATING BUBBLE

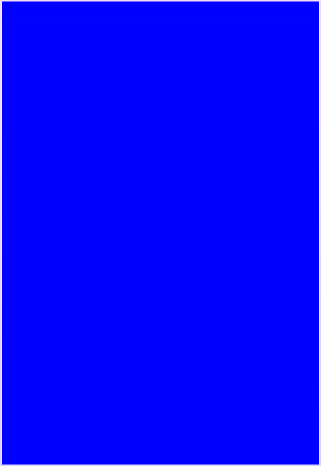
Pression and temperature imposed
$P = P^{\text{ref}} > P^{\text{sat}}(T_0)$,
$T = T_0$

Wall, temperature imposed



Nucleating Bubble

Mass Fraction y

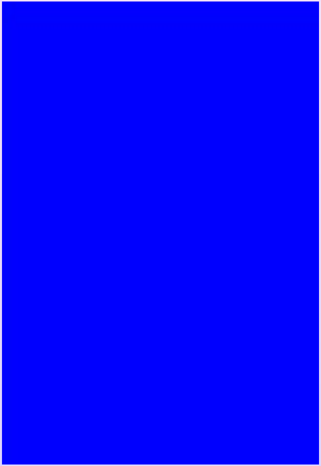


Temperature T

Geometry Play Skip

NUCLEATING BUBBLE

Mass Fraction y

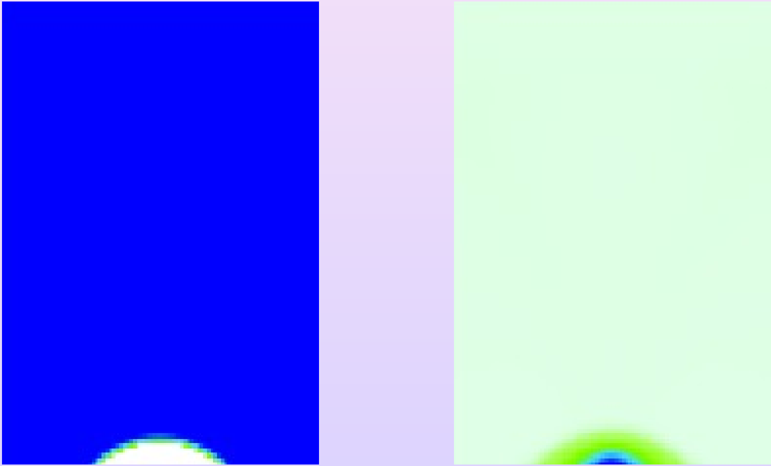


Temperature T

Geometry Play Skip

Nucleating Bubble

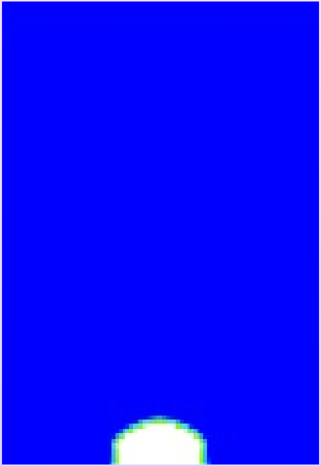
Mass Fraction y Temperature T



Geometry Play Skip

Nucleating Bubble

Mass Fraction y

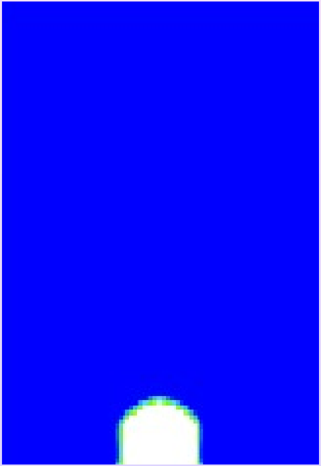


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

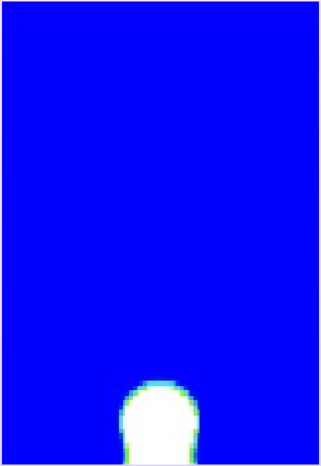


Temperature T

◀ Geometry ▶ Play ▶▶ Skip

Nucleating Bubble

Mass Fraction y

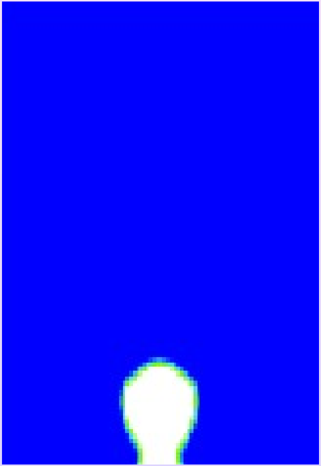


Temperature T

Geometry Play Skip

NUCLEATING BUBBLE

Mass Fraction y



Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

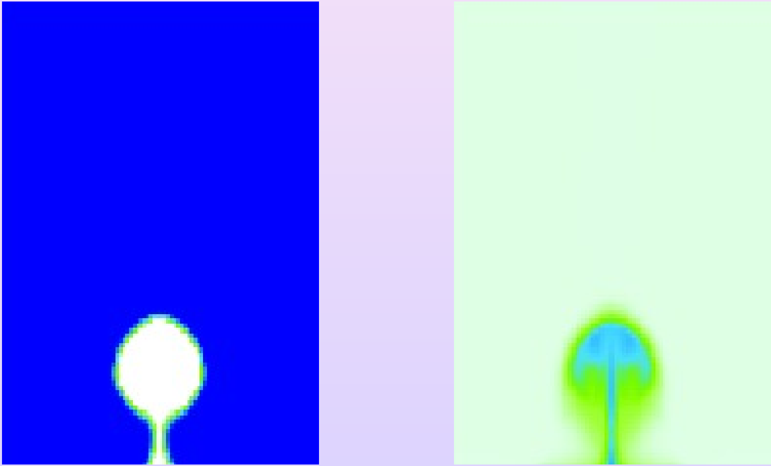
Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

Temperature T



◀ Geometry ▶ Play ▶▶ Skip

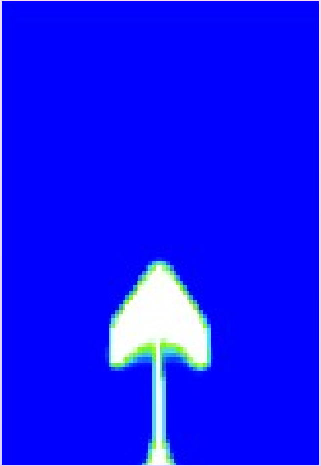
Nucleating Bubble

Mass Fraction y Temperature T

Geometry Play Skip

NUCLEATING BUBBLE

Mass Fraction y

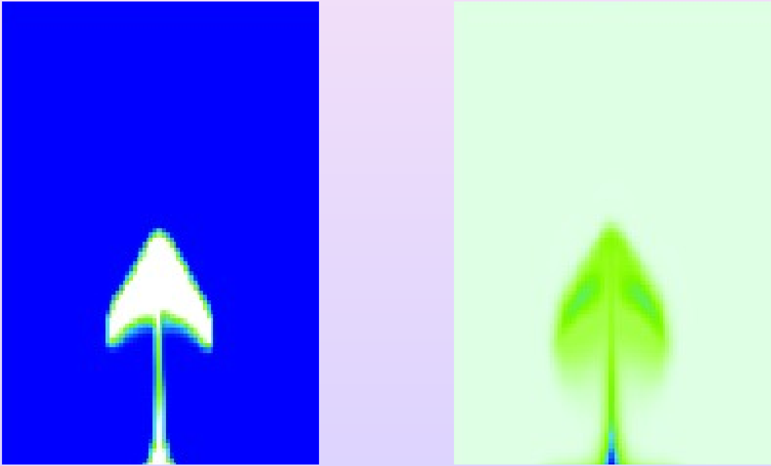


Temperature T

◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLE

Mass Fraction y Temperature T



◀ Geometry ▶ Play ▶▶ Skip

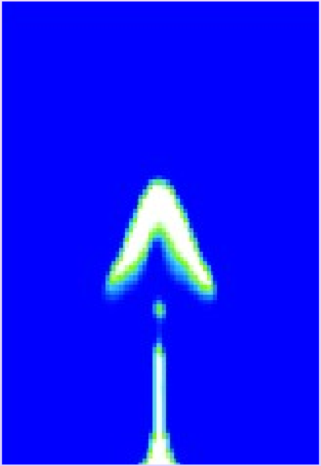
Nucleating Bubble

Mass Fraction y Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

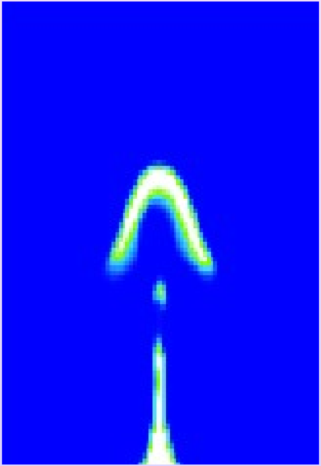


Temperature T

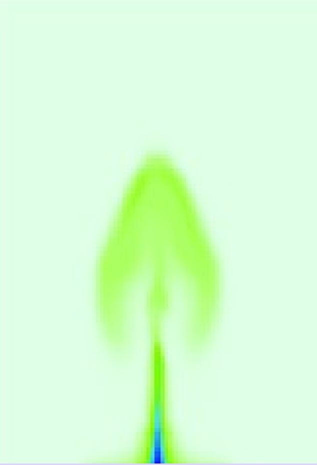
Geometry Play Skip

Nucleating Bubble

Mass Fraction y



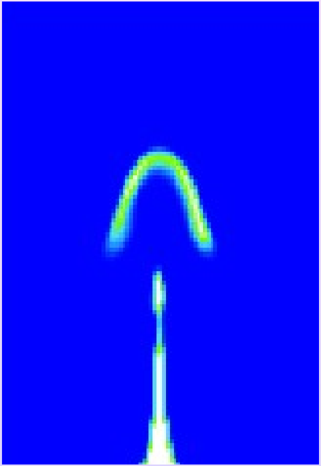
Temperature T



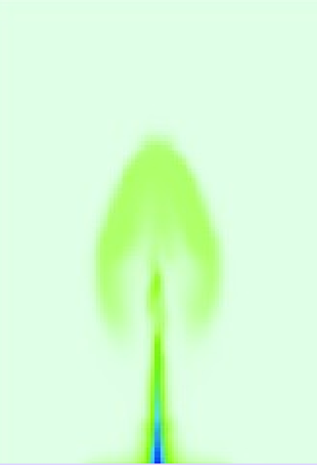
Geometry Play Skip

Nucleating Bubble

Mass Fraction y



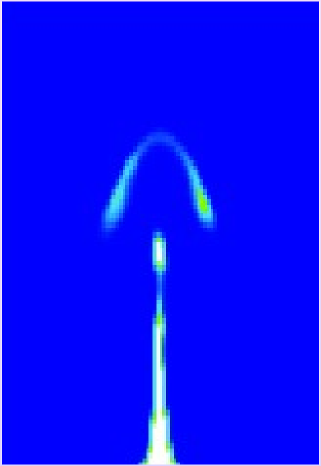
Temperature T



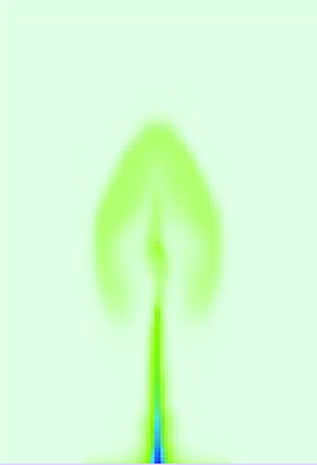
Geometry Play Skip

Nucleating Bubble

Mass Fraction y



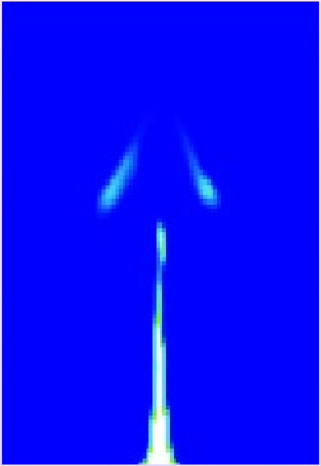
Temperature T



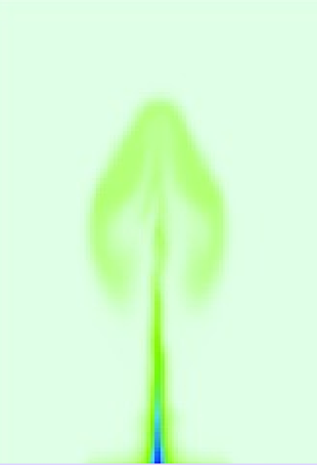
◀ Geometry ▶ Play ▶▶ Skip

Nucleating Bubble

Mass Fraction y



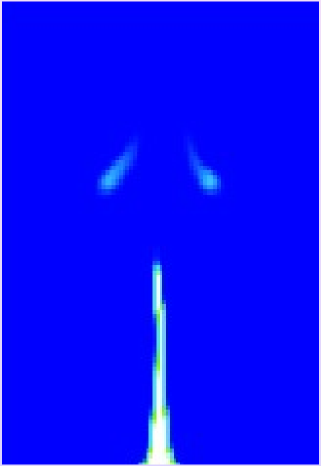
Temperature T



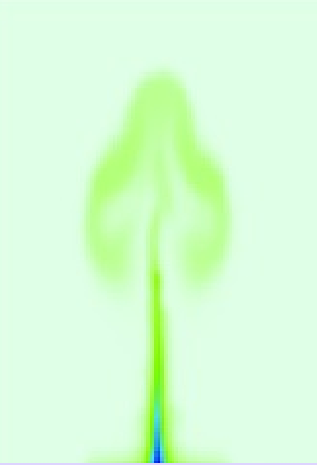
Geometry Play Skip

Nucleating Bubble

Mass Fraction y



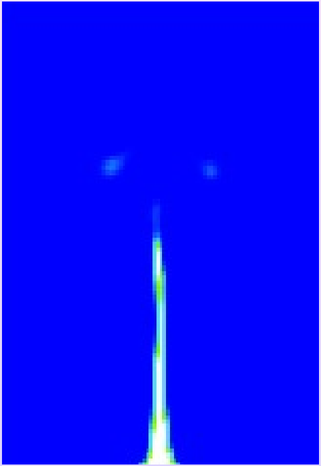
Temperature T



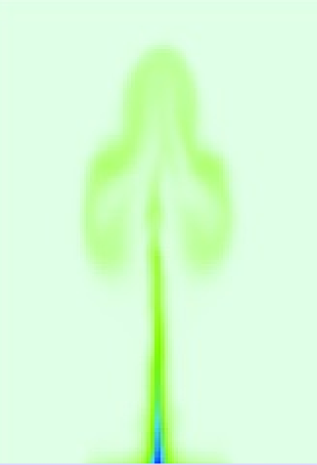
◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLE

Mass Fraction y



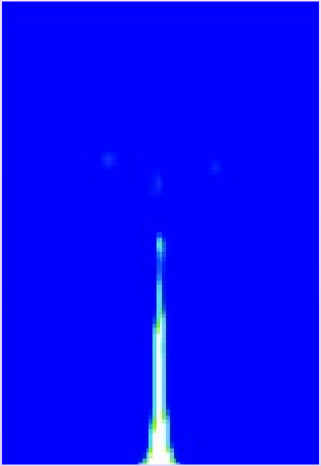
Temperature T



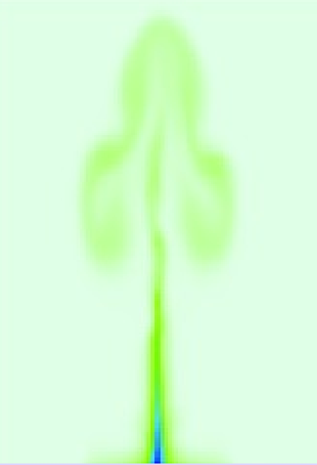
◀ Geometry ▶ Play ▶▶ Skip

NUCLEATING BUBBLE

Mass Fraction y



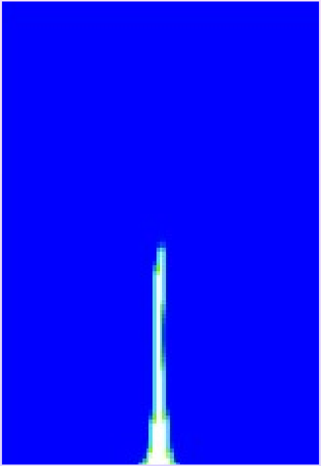
Temperature T



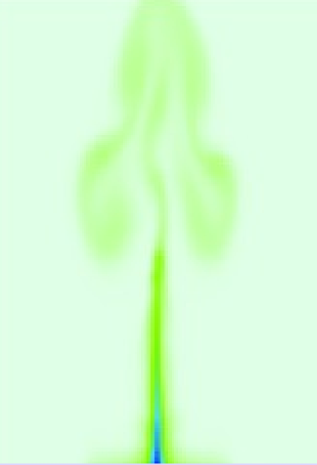
Geometry Play Skip

NUCLEATING BUBBLE

Mass Fraction y



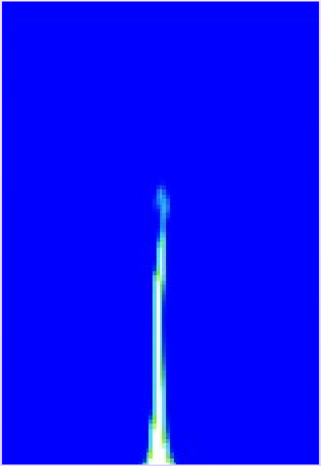
Temperature T



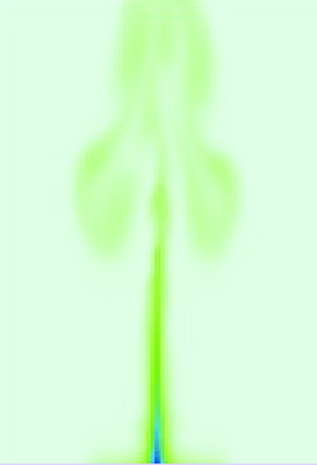
Geometry Play Skip

Nucleating Bubble

Mass Fraction y



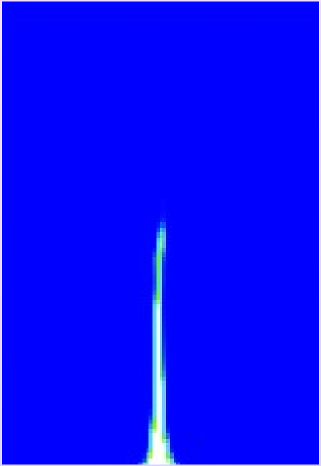
Temperature T



Geometry Play Skip

Nucleating Bubble

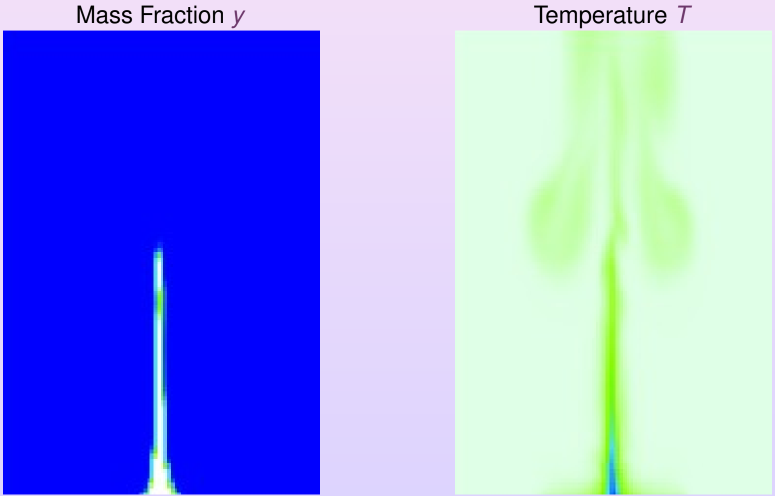
Mass Fraction y



Temperature T

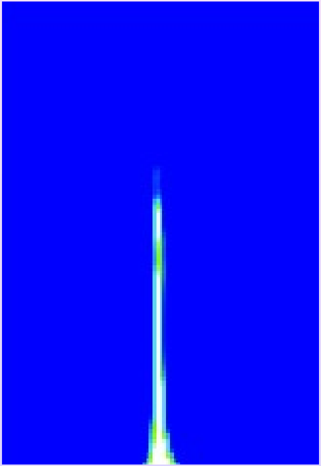
Geometry Play Skip

Nucleating Bubble



Geometry Play Skip

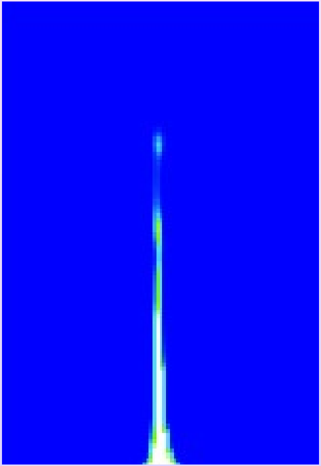
NUCLEATING BUBBLE



Geometry Play Skip

NUCLEATING BUBBLE

Mass Fraction y

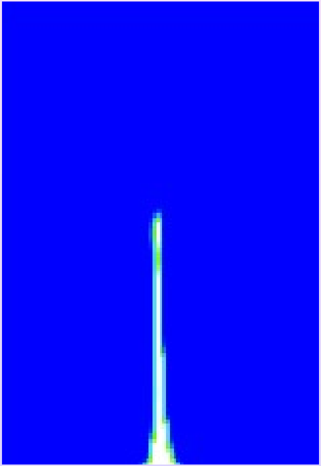


Temperature T

◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLE

Mass Fraction y

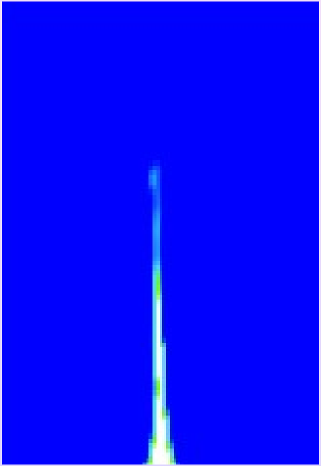


Temperature T

Geometry Play Skip

NUCLEATING BUBBLE

Mass Fraction y

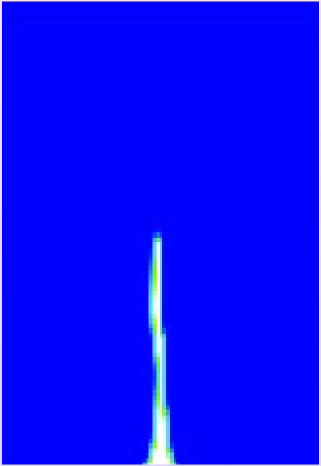


Temperature T

◀ Geometry ▶ Play ▶▶ Skip

Nucleating Bubble

Mass Fraction y

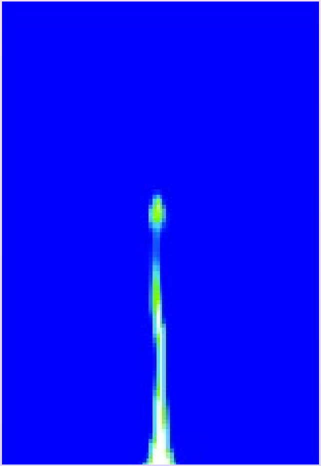


Temperature T

◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubble

Mass Fraction y

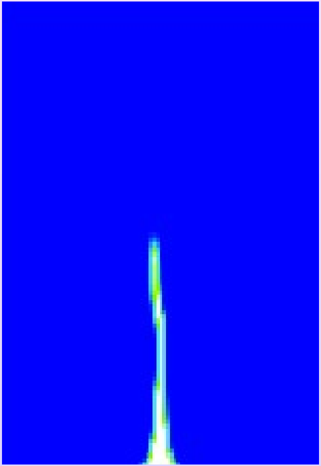


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

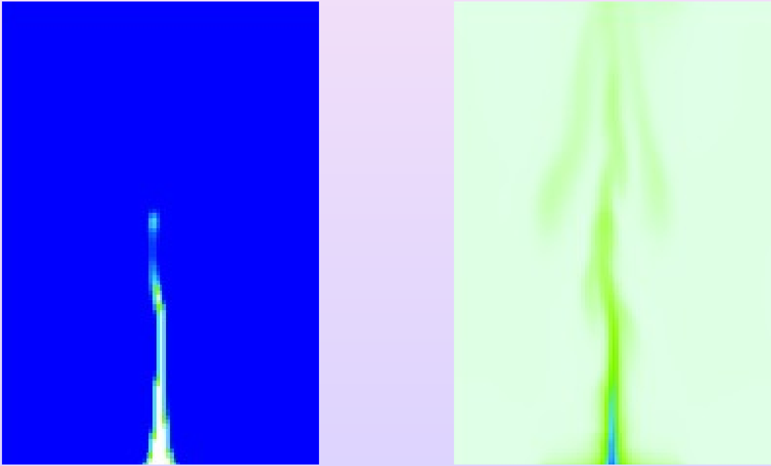


Temperature T

Geometry Play Skip

Nucleating Bubble

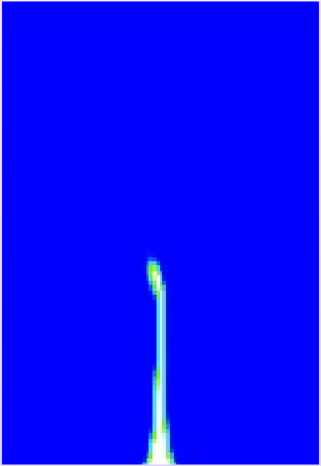
Mass Fraction y Temperature T



◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubble

Mass Fraction y

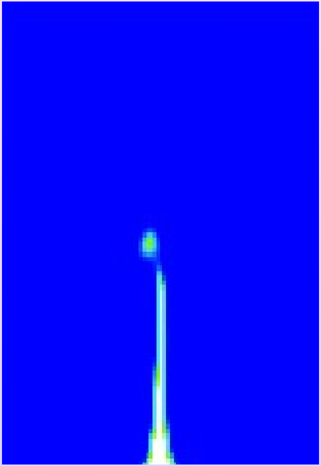


Temperature T

◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubble

Mass Fraction y

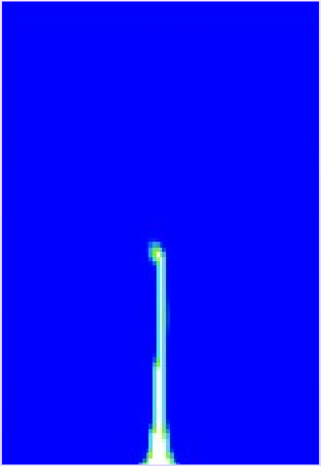


Temperature T

◀ Geometry ▶ Play ▶▶ Skip

Nucleating Bubble

Mass Fraction y

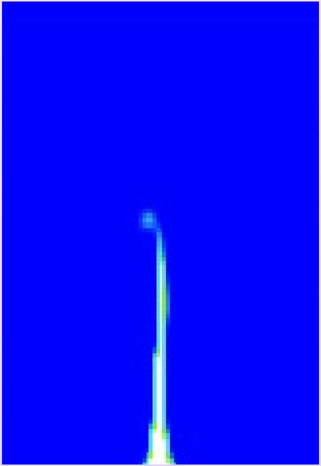


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

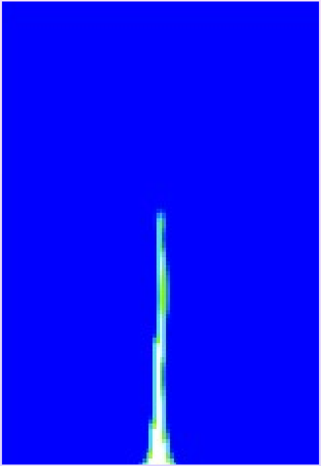


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

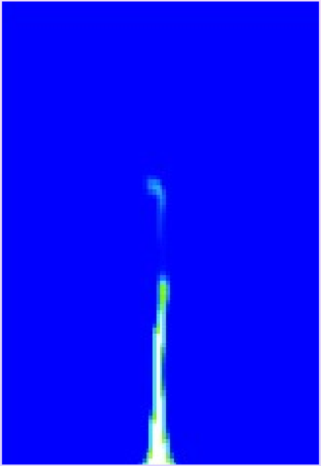


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

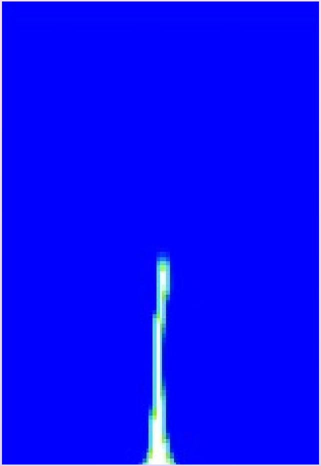


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

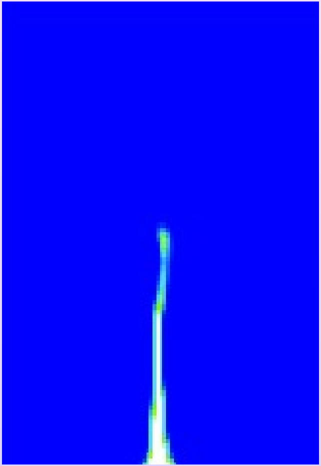


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

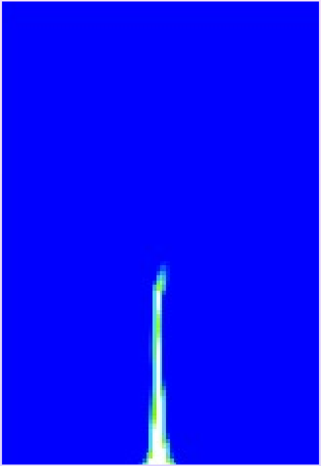


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

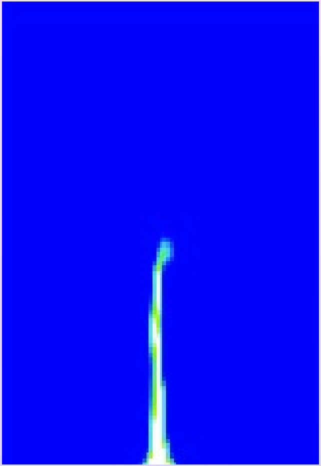


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

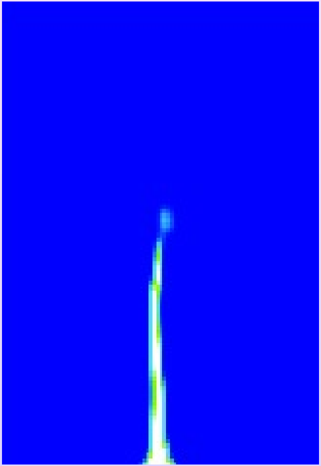


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

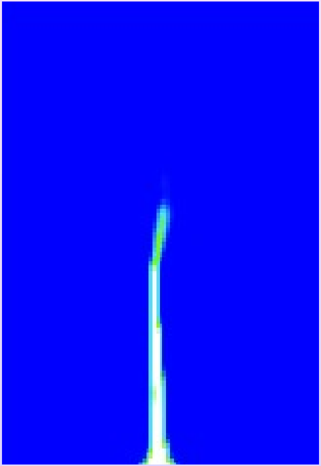


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

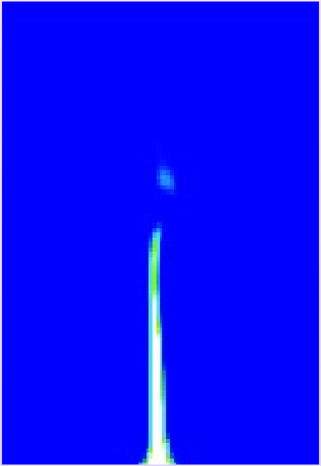


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

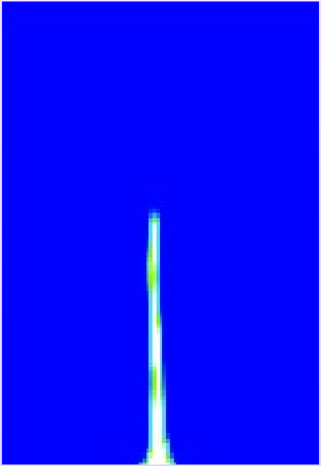


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

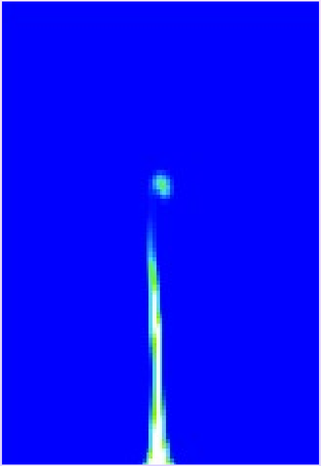


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

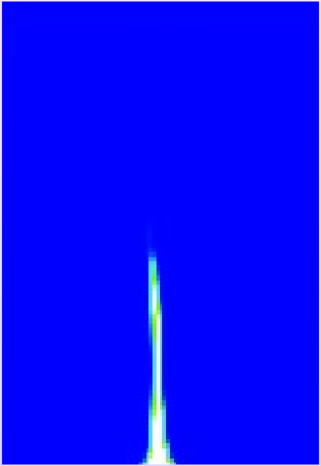


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

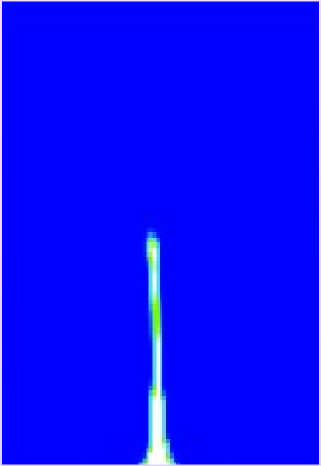


Temperature T

◀ Geometry ▶ Play ▶▶ Skip

Nucleating Bubble

Mass Fraction y

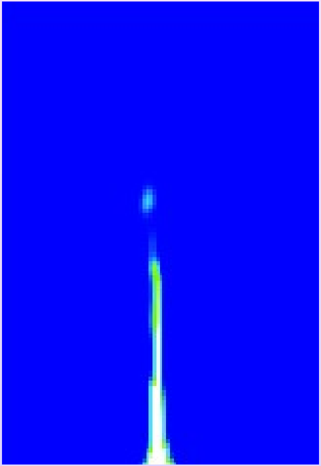


Temperature T

Geometry Play Skip

Nucleating Bubble

Mass Fraction y

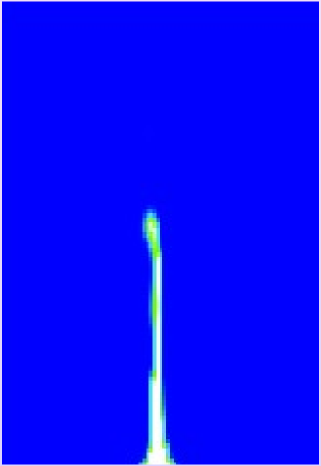


Temperature T

Geometry Play Skip

NUCLEATING BUBBLE

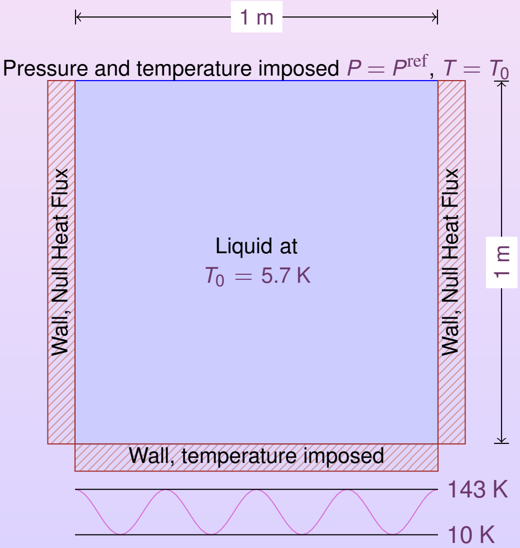
Mass Fraction y



Temperature T

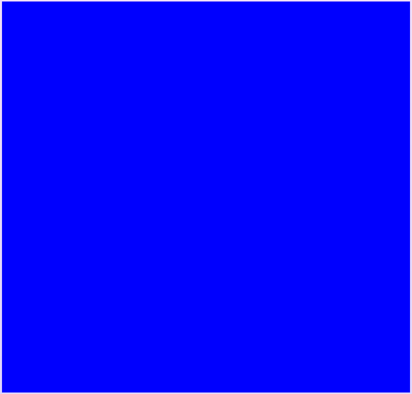
Geometry Play Skip

FILM


1 m
Pressure and temperature imposed $P = P^{\text{ref}}$, $T = T_0$
Wall, Null Heat Flux
Liquid at
$T_0 = 5.7$ K
Wall, Null Heat Flux
1 m
Wall, temperature imposed
143 K
10 K

Film

Mass Fraction y

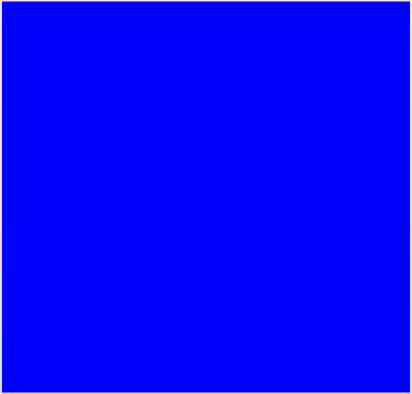


Temperature T

Geometry Play Skip

Film

Mass Fraction y

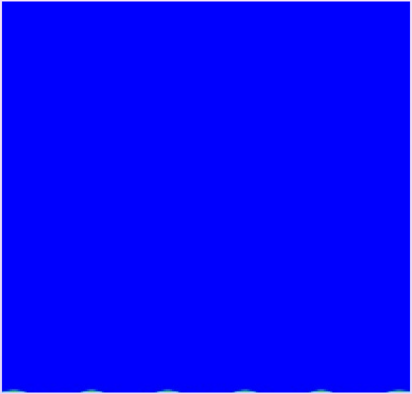


Temperature T

Geometry Play Skip

FILM

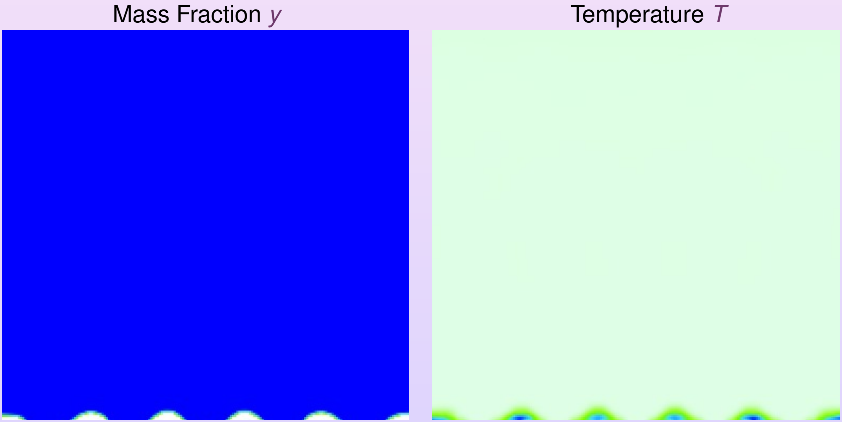
Mass Fraction y



Temperature T

◂ Geometry ▸ Play ▸▸ Skip

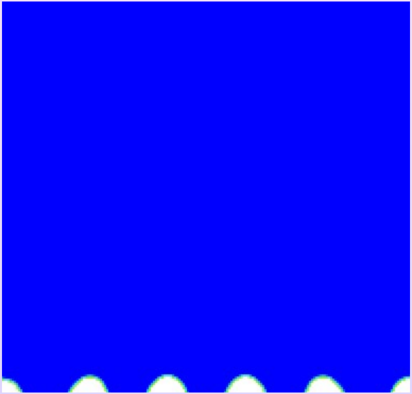
Film



◂ Geometry ▸ Play ▸▸ Skip

Film

Mass Fraction y

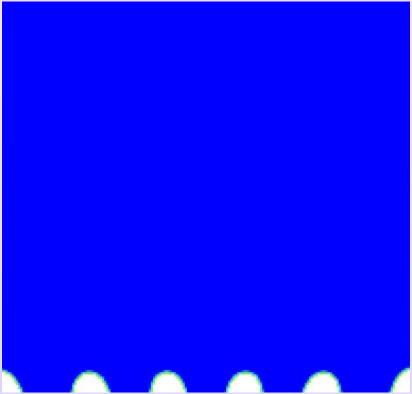


Temperature T

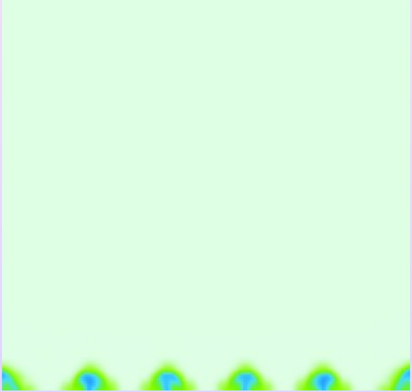
Geometry Play Skip

Film

Mass Fraction y



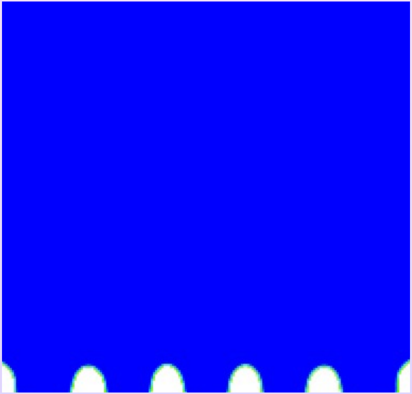
Temperature T



Geometry Play Skip

FILM

Mass Fraction y

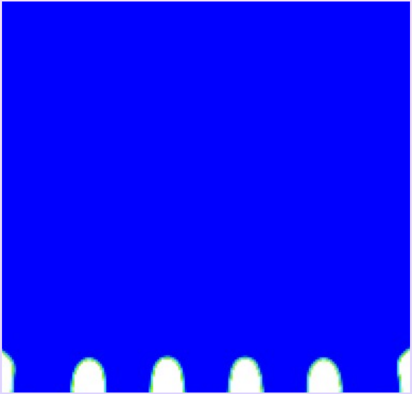


Temperature T

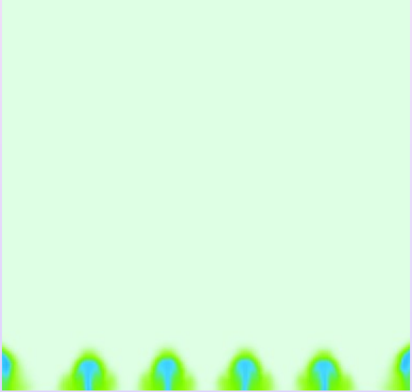
Geometry Play Skip

Film

Mass Fraction y



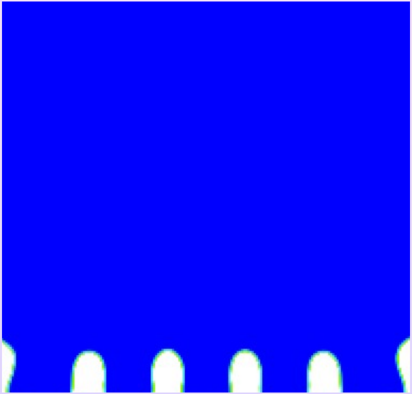
Temperature T

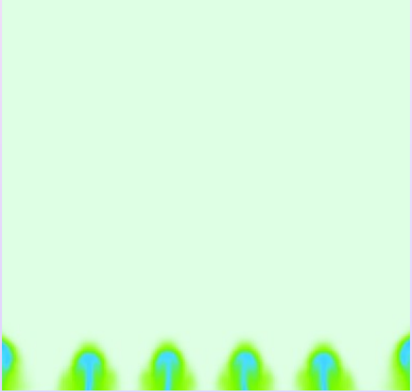


◂ Geometry ▸ Play ▸▸ Skip

FILM

Mass Fraction y Temperature T

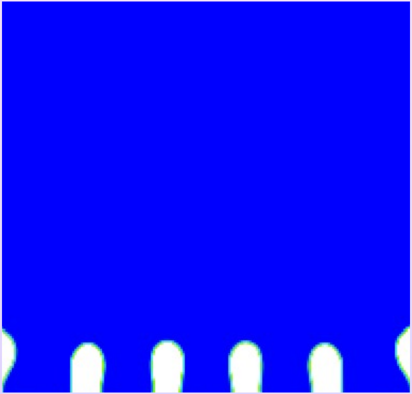




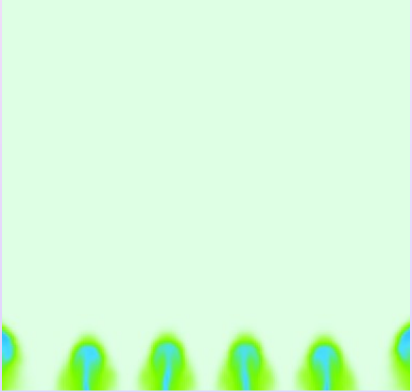
Geometry Play Skip

Film

Mass Fraction y



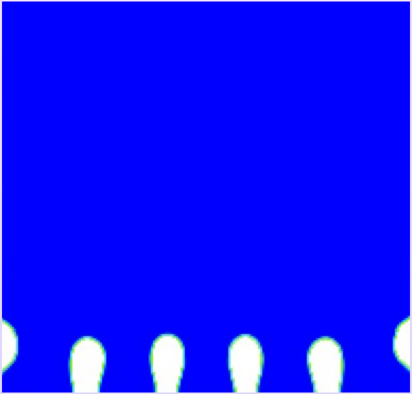
Temperature T



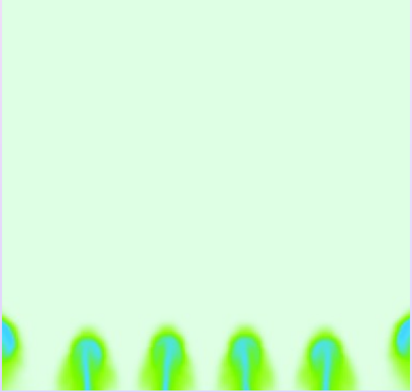
Geometry Play Skip

Film

Mass Fraction y



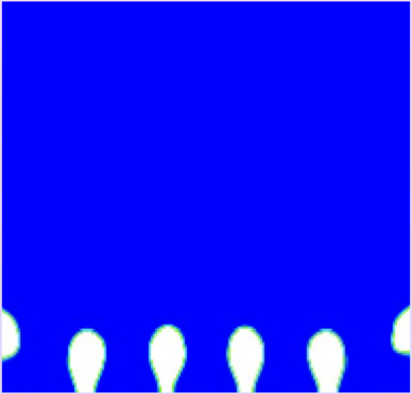
Temperature T



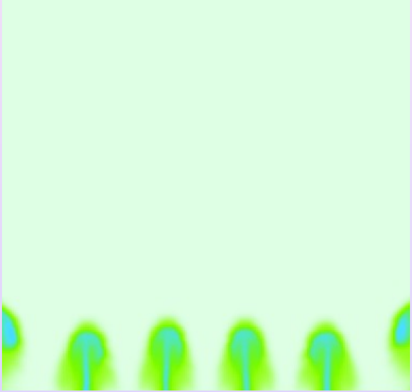
◀ Geometry ▶ Play ▶▶ Skip

FILM

Mass Fraction y



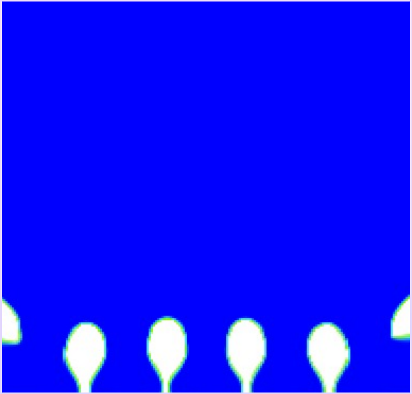
Temperature T



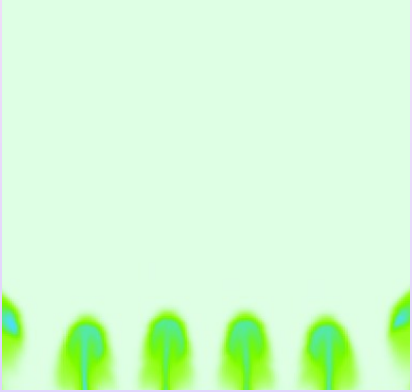
◂ Geometry ▸ Play ▸▸ Skip

Film

Mass Fraction y



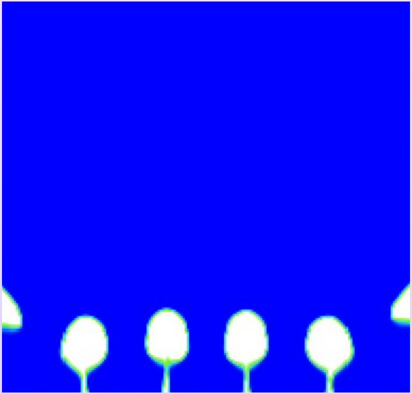
Temperature T



Geometry Play Skip

FILM

Mass Fraction y



Temperature T

Geometry Play Skip

FILM

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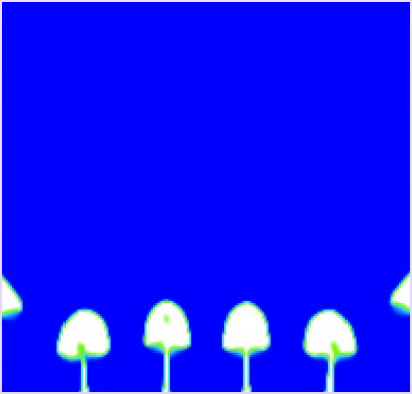

Temperature T

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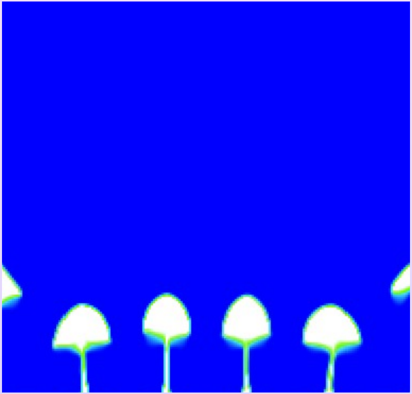
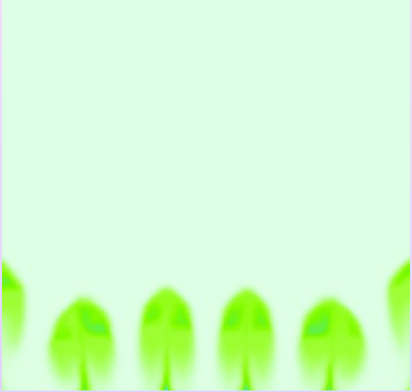


Temperature T



Geometry Play Skip

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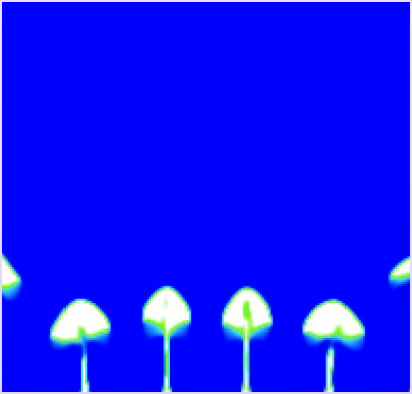

Temperature T

Geometry Play Skip

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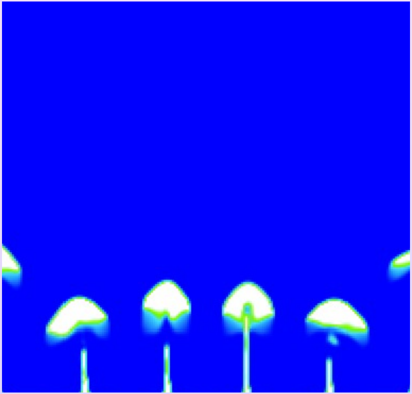

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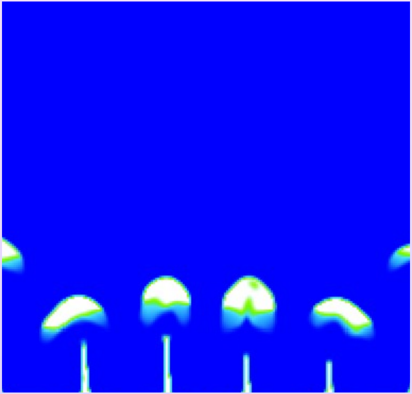

Temperature T

◂ Geometry ▸ Play ▸▸ Skip

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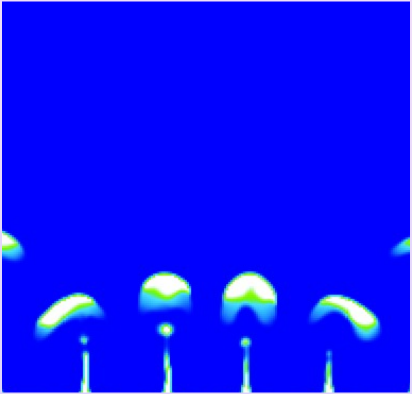

Temperature T

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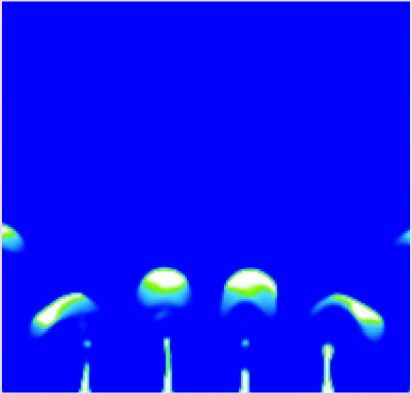

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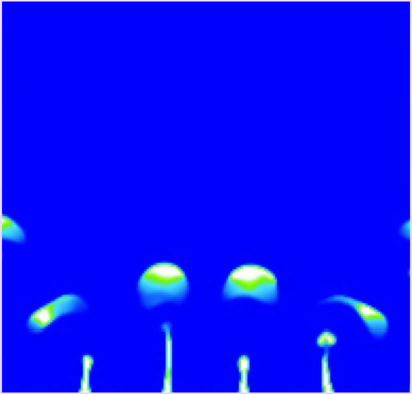

Temperature T

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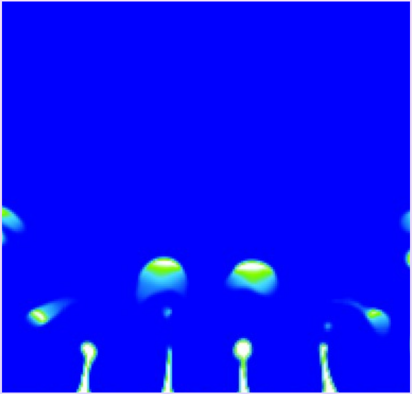

Temperature T

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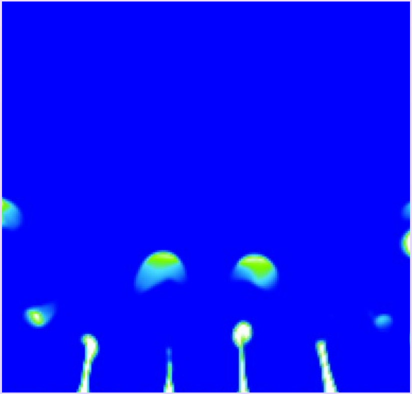

Temperature T

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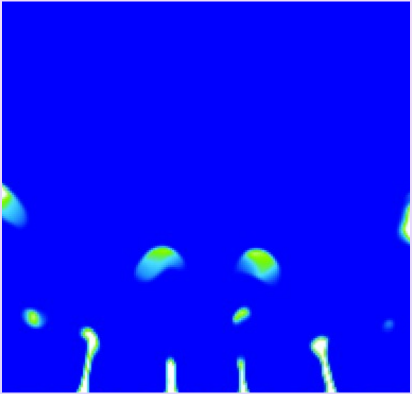

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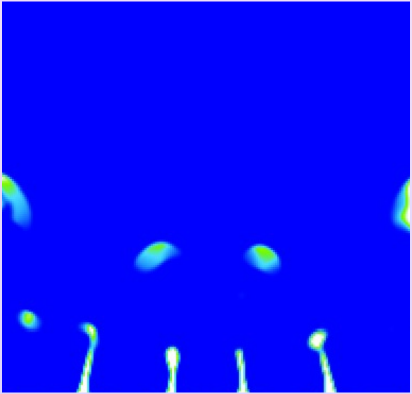

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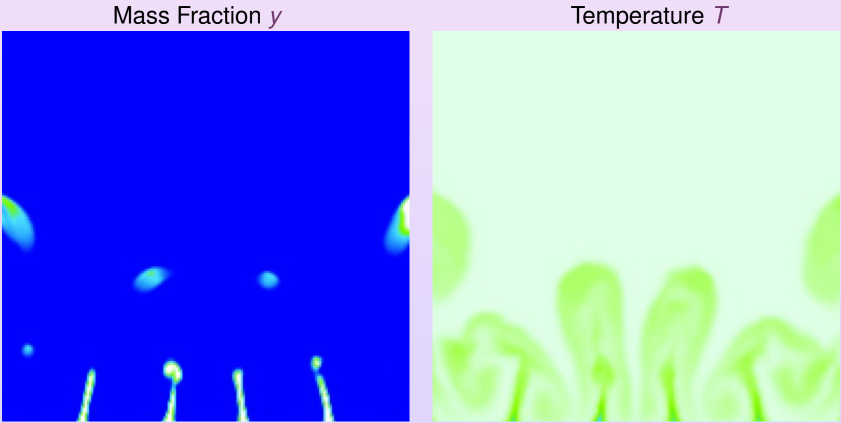

◂ Geometry ▸ Play ▸▸ Skip

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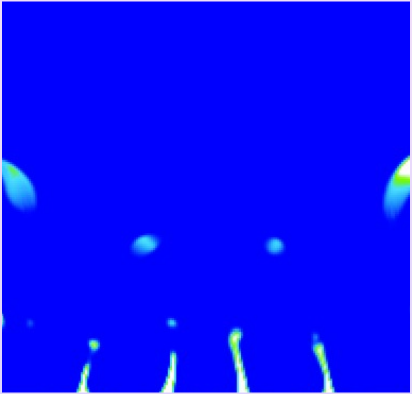

Temperature T

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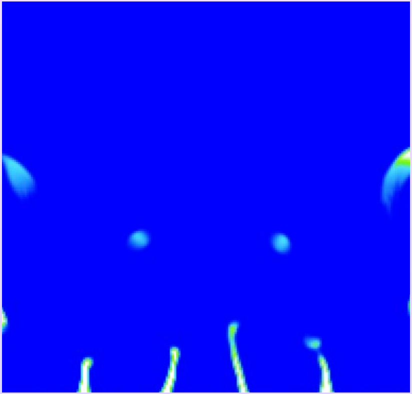

Temperature T

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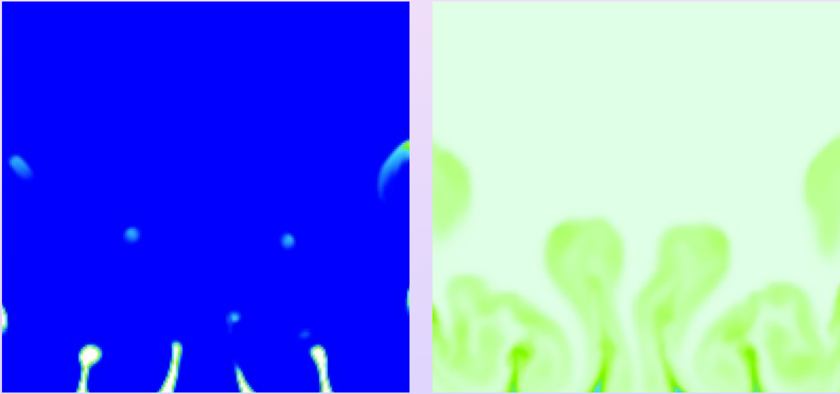
Mass Fraction y Temperature T



Geometry Play Skip

FILM

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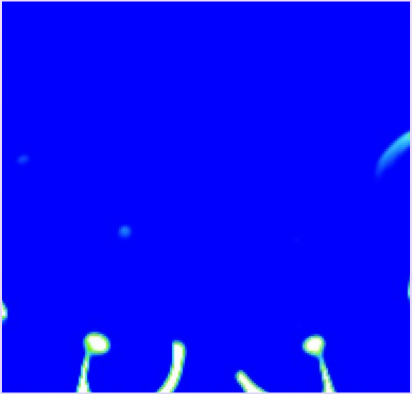

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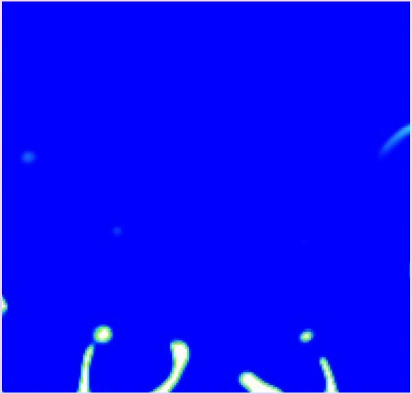

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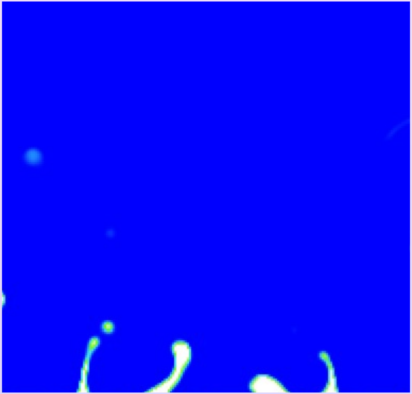

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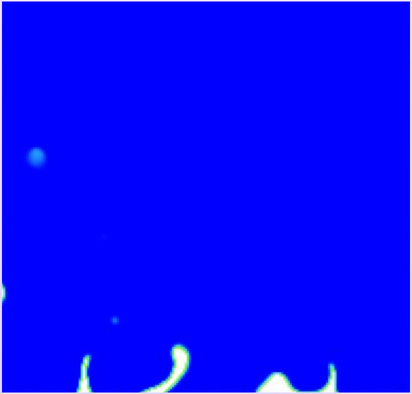

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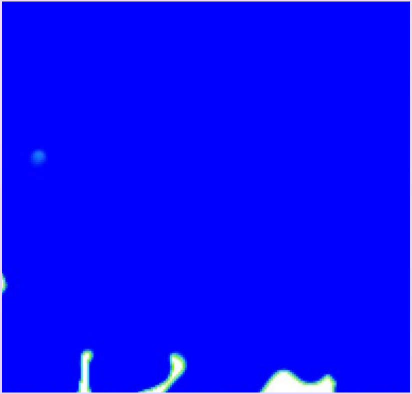

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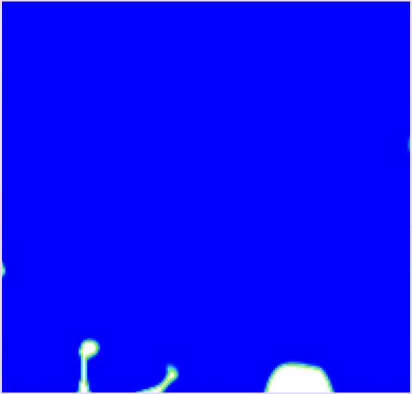

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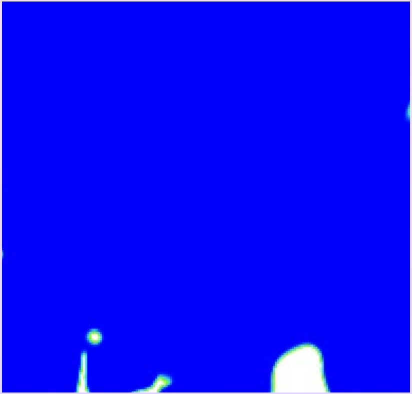

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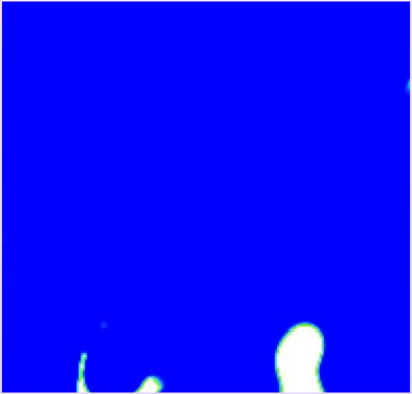

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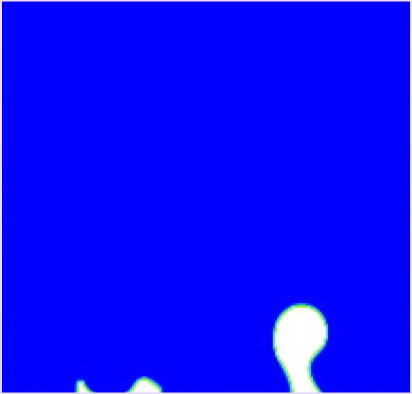

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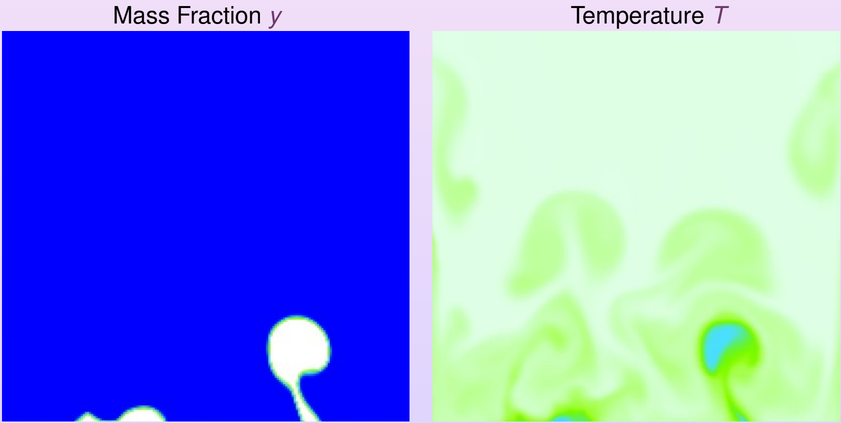

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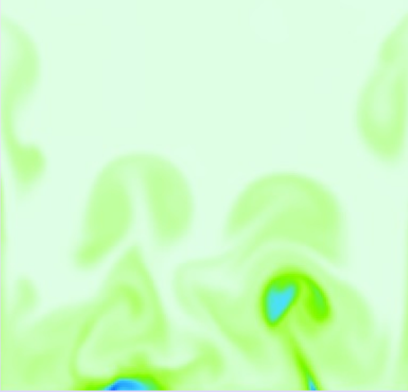

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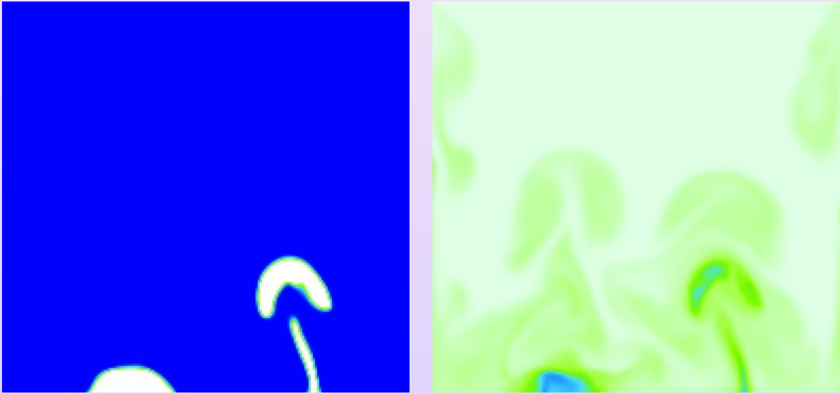

◂ Geometry ▸ Play ▸▸ Skip

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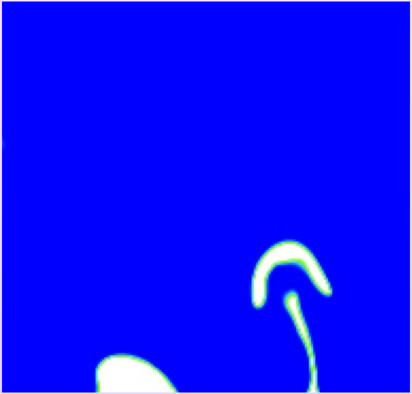

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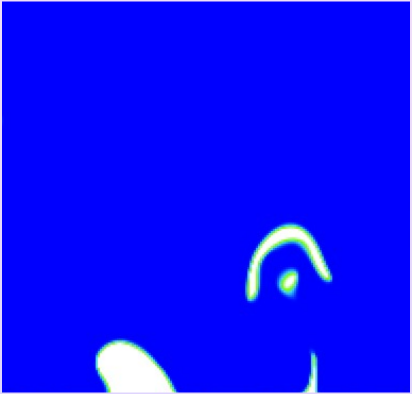

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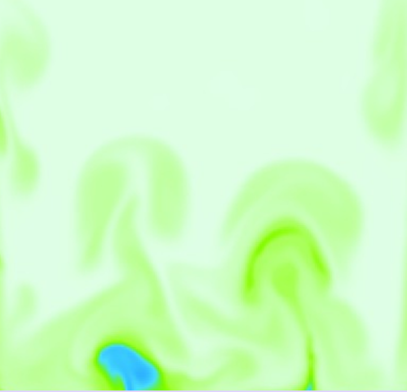

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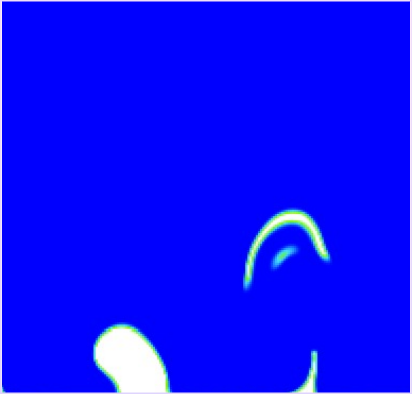

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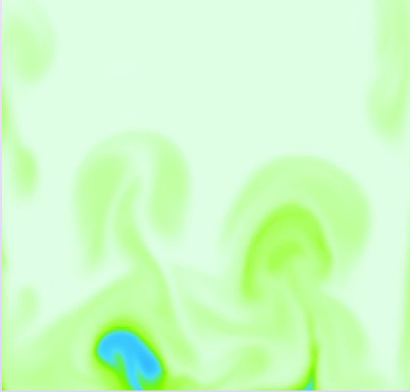

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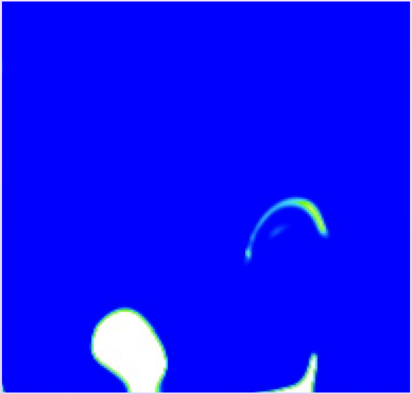

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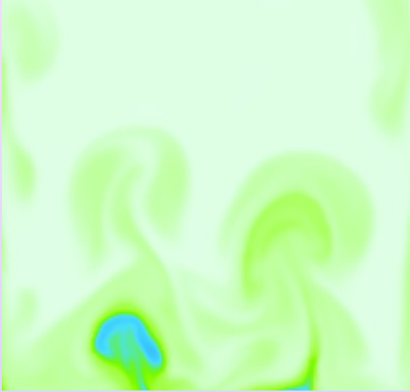

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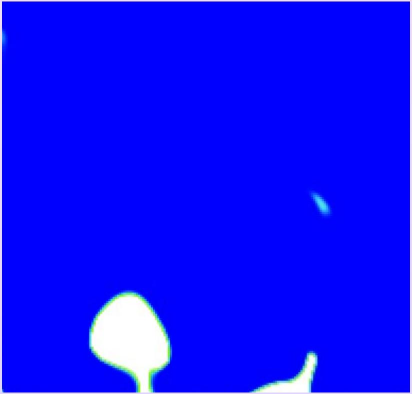

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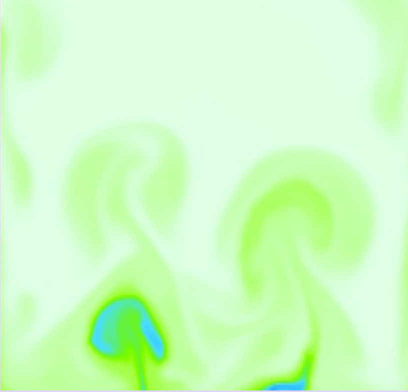

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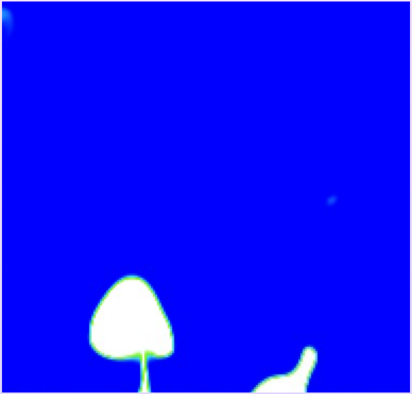

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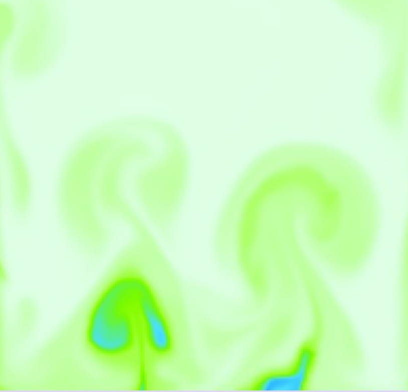

◂ Geometry ▸ Play ▸▸ Skip

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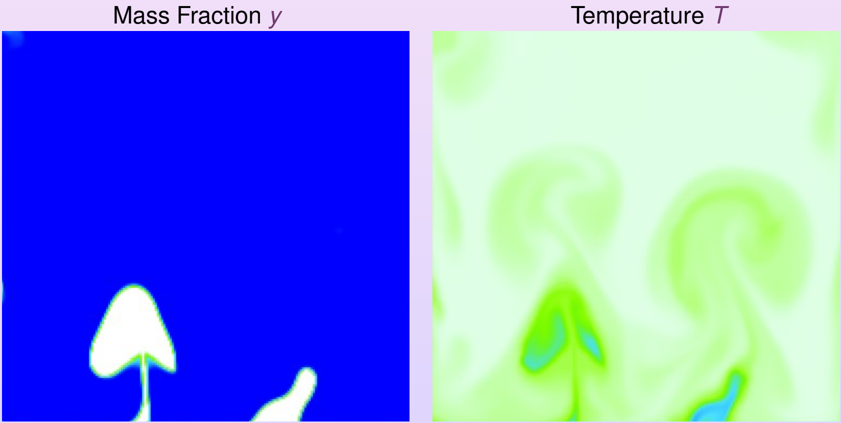

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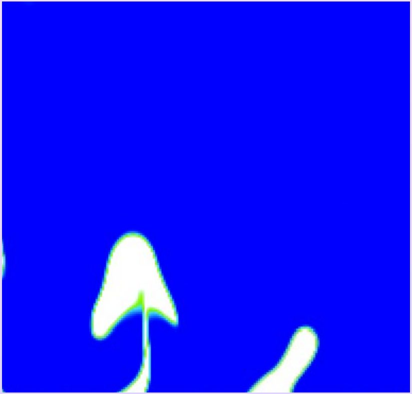

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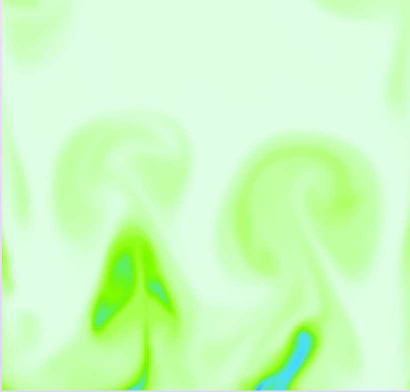

◀ Geometry ▶ Play ▶▶ Skip

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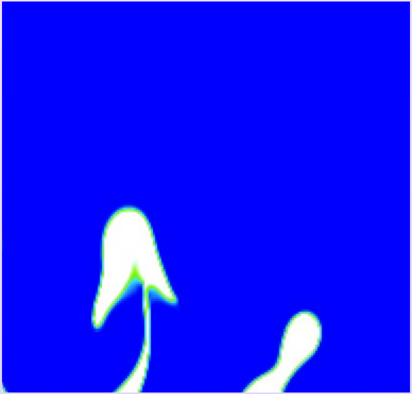

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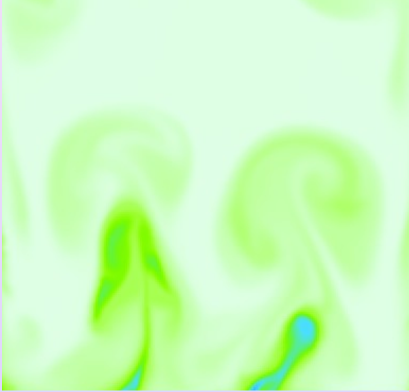

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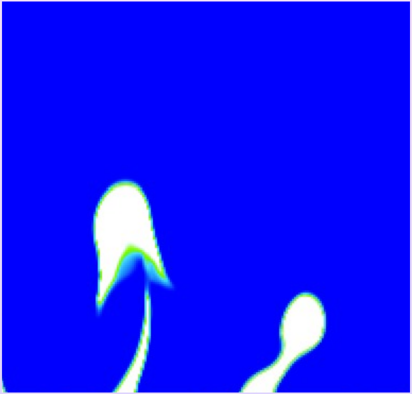

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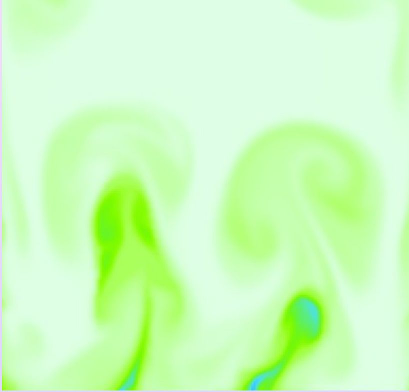

◂ Geometry ▸ Play ▸▸ Skip

Outline

1. Context
2. Model
   - Equation of state
   - Muvement Equations
3. Numerical Approximation
   - Numerical Method
   - 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)]
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Table: Parameters proposed by [Le Metayer] for water.

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$$\left.\begin{array}{l} T^i = 278\text{K} \dots 610\text{K}, \\ g_1(P, T^i) = g_2(P, T^i) \Rightarrow P^{\text{sat}}(T^i) \end{array}\right\} \Rightarrow \mathfrak{A} = \left\{ \left(T^i, P^{\text{sat}}(T^i) \right) \right\}_{i=0}^{83}$$

$\widehat{P}^{\text{sat}}$ defined by using a least square approximation of $\mathfrak{A}$:

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$$\left.\begin{aligned} &T^i = 278\text{K}\dots 610\text{K},\\ &g_1(P,T^i) = g_2(P,T^i) \Rightarrow P^{\text{sat}}(T^i)\end{aligned}\right\} \Rightarrow \mathfrak{A} = \left\{\left(T^i, P^{\text{sat}}(T^i)\right)\right\}_{i=0}^{83}$$

$\widehat{P}^{\text{sat}}$ defined by using a least square approximation of $\mathfrak{A}$:

$$T\mapsto P^{\text{sat}}(T)\approx\widehat{P}^{\text{sat}}(T)\stackrel{\text{def}}{=}\exp\left(\sum_{k=-8}^{k=8} a_k T^k\right)$$

Water Tabulated EOS

		Volume (m^3/kg)		Internal Energy (kJ/kg)	
T (K)	P^{sat} (MPa)	τ_{liq}^{sat}	τ_{vap}^{sat}	ε_{liq}^{sat}	ε_{vap}^{sat}
275	0,00069845	0,0010001	181,60	7,7590	2377,5
278	0,00086349	0,0010001	148,48	20,388	2381,6
281	0,0010621	0,0010002	122,01	32,996	2385,7
284	0,0012999	0,0010004	100,74	45,586	2389,8
287	0,0015835	0,0010008	83,560	58,162	2393,9
290	0,0019200	0,0010012	69,625	70,727	2398,0
293	0,0023177	0,0010018	58,267	83,284	2402,1
296	0,0027856	0,0010025	48,966	95,835	2406,2
299	0,0033342	0,0010032	41,318	108,38	2410,3
302	0,0039745	0,0010041	35,002	120,92	2414,4
305	0,0047193	0,0010050	29,764	133,46	2418,4
308	0,0055825	0,0010060	25,403	146	2422,5
...	...	...	...	...	...

Source: `http://webbook.nist.gov/chemistry/fluid/`

Water Tabulated EOS

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

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

$$T \mapsto \varepsilon_{\text{vap}}^{\text{sat}} \approx \widehat{\varepsilon}_{\text{vap}}^{\text{sat}} \stackrel{\text{def}}{=} \frac{1}{\sum_{k=0}^{6} a_k T^k} \qquad T \mapsto \varepsilon_{\text{liq}}^{\text{sat}} \approx \widehat{\varepsilon}_{\text{liq}}^{\text{sat}} \stackrel{\text{def}}{=} \widehat{\varepsilon}_{\text{vap}}^{\text{sat}}(T) \sum_{k=0}^{6} b_k T^k$$

$$T \mapsto \tau_{\text{vap}}^{\text{sat}} \approx \widehat{\tau}_{\text{vap}}^{\text{sat}} \stackrel{\text{def}}{=} \frac{1}{\sum_{k=0}^{8} c_k T^k} \qquad T \mapsto \tau_{\text{liq}}^{\text{sat}} \approx \widehat{\tau}_{\text{liq}}^{\text{sat}} \stackrel{\text{def}}{=} \widehat{\tau}_{\text{vap}}^{\text{sat}}(T) \sum_{k=0}^{9} d_k T^k$$

Speed of sound

$$c^2 \stackrel{\text{def}}{=} \tau^2 \left(P^{\text{eq}} \left.\frac{\partial P^{\text{eq}}}{\partial \varepsilon}\right|_{\tau} - \left.\frac{\partial P^{\text{eq}}}{\partial \tau}\right|_{\varepsilon} \right) = \underbrace{\boxed{-\tau^2 T^{\text{eq}}}}^{\leq 0} \overbrace{\boxed{\begin{bmatrix} P^{\text{eq}}, & -1 \end{bmatrix} \begin{bmatrix} s^{\text{eq}}_{\varepsilon\varepsilon} & s^{\text{eq}}_{\tau\varepsilon} \\ s^{\text{eq}}_{\tau\varepsilon} & s^{\text{eq}}_{\tau\tau} \end{bmatrix} \begin{bmatrix} P^{\text{eq}} \\ -1 \end{bmatrix}}}^{\leq 0}$$

Hessian matrix of $\mathbf{w} \mapsto s^{\text{eq}}$

- for all $\mathbf{w}$ pure phase state

$$\mathbf{v}^T \, \mathrm{d}^2 s^{\text{eq}}(\mathbf{w}) \, \mathbf{v} < 0 \quad \forall \, \mathbf{v} \neq 0,$$

- for all $\mathbf{w}$ equilibrium mixture state

$$\exists \, \mathbf{v}(\mathbf{w}) \neq 0 \ \text{ s.t. } (\mathbf{v}(\mathbf{w}))^T \, \mathrm{d}^2 s^{\text{eq}}(\mathbf{w}) \, \mathbf{v}(\mathbf{w}) = 0.$$

Speed of sound

$$c^2 \stackrel{\text{def}}{=} \tau^2 \left(P^{\text{eq}} \left.\frac{\partial P^{\text{eq}}}{\partial \varepsilon}\right|_{\tau} - \left.\frac{\partial P^{\text{eq}}}{\partial \tau}\right|_{\varepsilon} \right) = \underbrace{\boxed{-\tau^2 T^{\text{eq}}}}_{<0} \underbrace{\boxed{\begin{bmatrix} P^{\text{eq}}, & -1 \end{bmatrix} \begin{bmatrix} s^{\text{eq}}_{\varepsilon\varepsilon} & s^{\text{eq}}_{\tau\varepsilon} \\ s^{\text{eq}}_{\tau\varepsilon} & s^{\text{eq}}_{\tau\tau} \end{bmatrix} \begin{bmatrix} P^{\text{eq}} \\ -1 \end{bmatrix}}}_{\leq 0}$$

Hessian matrix of $\mathbf{w} \longmapsto s^{\text{eq}}$

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SPEED OF SOUND

$$c^2 \stackrel{\text{def}}{=} \tau^2 \left(P^{\mathrm{eq}} \left.\frac{\partial P^{\mathrm{eq}}}{\partial \varepsilon}\right|_{\tau} - \left.\frac{\partial P^{\mathrm{eq}}}{\partial \tau}\right|_{\varepsilon} \right) = \underbrace{\boxed{-\tau^2 T^{\mathrm{eq}}}}_{<0} \overbrace{\boxed{\begin{bmatrix} P^{\mathrm{eq}}, & -1 \end{bmatrix} \begin{bmatrix} s^{\mathrm{eq}}_{\varepsilon\varepsilon} & s^{\mathrm{eq}}_{\tau\varepsilon} \\ s^{\mathrm{eq}}_{\tau\varepsilon} & s^{\mathrm{eq}}_{\tau\tau} \end{bmatrix} \begin{bmatrix} P^{\mathrm{eq}} \\ -1 \end{bmatrix}}}^{\leq 0}$$

HESSIAN MATRIX OF $\mathbf{w} \mapsto s^{\mathrm{eq}}$

- for all **w** pure phase state

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Speed of sound

$$c^2 \stackrel{\text{def}}{=} \tau^2 \left(P^{\text{eq}} \left.\frac{\partial P^{\text{eq}}}{\partial \varepsilon}\right|_\tau - \left.\frac{\partial P^{\text{eq}}}{\partial \tau}\right|_\varepsilon \right) = \boxed{\underbrace{-\tau^2 T^{\text{eq}}}_{<0}} \overbrace{\boxed{\begin{bmatrix} P^{\text{eq}}, & -1 \end{bmatrix} \begin{bmatrix} s^{\text{eq}}_{\varepsilon\varepsilon} & s^{\text{eq}}_{\tau\varepsilon} \\ s^{\text{eq}}_{\tau\varepsilon} & s^{\text{eq}}_{\tau\tau} \end{bmatrix} \begin{bmatrix} P^{\text{eq}} \\ -1 \end{bmatrix}}}^{\leq 0}$$

Hessian matrix of $\mathbf{w} \mapsto s^{\text{eq}}$

- for all $\mathbf{w}$ pure phase state

$$\mathbf{v}^T \, \mathrm{d}^2 s^{\text{eq}}(\mathbf{w}) \, \mathbf{v} < 0 \quad \forall \, \mathbf{v} \neq 0,$$

- for all $\mathbf{w}$ equilibrium mixture state

$$\exists \, \mathbf{v}(\mathbf{w}) \neq 0 \;\text{ s.t. } (\mathbf{v}(\mathbf{w}))^T \, \mathrm{d}^2 s^{\text{eq}}(\mathbf{w}) \, \mathbf{v}(\mathbf{w}) = 0.$$

$$\boxed{\forall \mathbf{w} \text{ equilibrium mixture state, } \mathbf{v}(\mathbf{w}) \stackrel{?}{\equiv} [P^{\text{eq}}(\mathbf{w}), -1]}$$

Speed of sound

$$c^2 \overset{\text{def}}{=} \tau^2 \left(P^{\text{eq}} \left.\frac{\partial P^{\text{eq}}}{\partial \varepsilon}\right|_{\tau} - \left.\frac{\partial P^{\text{eq}}}{\partial \tau}\right|_{\varepsilon} \right) = \overset{<0}{\boxed{-\tau^2 T^{\text{eq}}}} \overset{\leq 0}{\boxed{\begin{bmatrix} P^{\text{eq}}, & -1 \end{bmatrix} \begin{bmatrix} s^{\text{eq}}_{\varepsilon\varepsilon} & s^{\text{eq}}_{\tau\varepsilon} \\ s^{\text{eq}}_{\tau\varepsilon} & s^{\text{eq}}_{\tau\tau} \end{bmatrix} \begin{bmatrix} P^{\text{eq}} \\ -1 \end{bmatrix}}}$$

Hessian matrix of $\mathbf{w} \mapsto s^{\text{eq}}$

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$$\mathbf{v}^T \, \mathrm{d}^2 s^{\text{eq}}(\mathbf{w}) \, \mathbf{v} < 0 \quad \forall \, \mathbf{v} \neq 0,$$

- for all $\mathbf{w}$ equilibrium mixture state

$$\exists \, \mathbf{v}(\mathbf{w}) \neq 0 \;\text{ s.t. }\; (\mathbf{v}(\mathbf{w}))^T \, \mathrm{d}^2 s^{\text{eq}}(\mathbf{w}) \, \mathbf{v}(\mathbf{w}) = 0.$$

$\forall \mathbf{w}$ equilibrium mixture state, $\mathbf{v}(\mathbf{w}) \overset{?}{\not\propto} [P^{\text{eq}}(\mathbf{w}), -1]$

Return

Isentropic curves