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Modelling and Simulation of Nucleate Boiling

A contribution to the study of the boiling crisis

Gloria Faccanoni[1] Grégoire Allaire[2] Samuel Kokh[3]

[1]IMATH – Université du Sud Toulon-Var (France)

[2]CMAP – École Polytechnique (France)

[3]DEN/DANS/DM2S/SFME/LETR – CEA Saclay (France)

Outline

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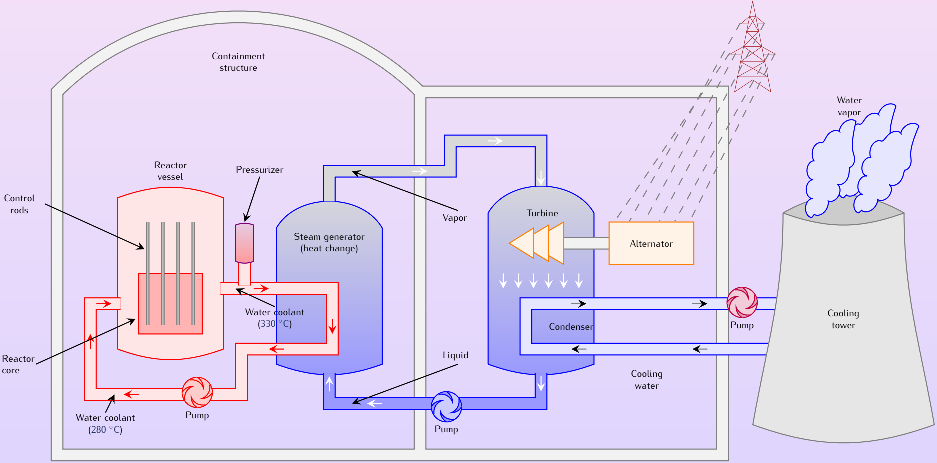
1. Context
2. Model
    - Equation of State
    - Conservation Laws
3. Numerical Approximation and Example
    - The Phase Change Equation
    - Numerical Scheme and Example
4. Conclusion

Pressurized Water Reactor

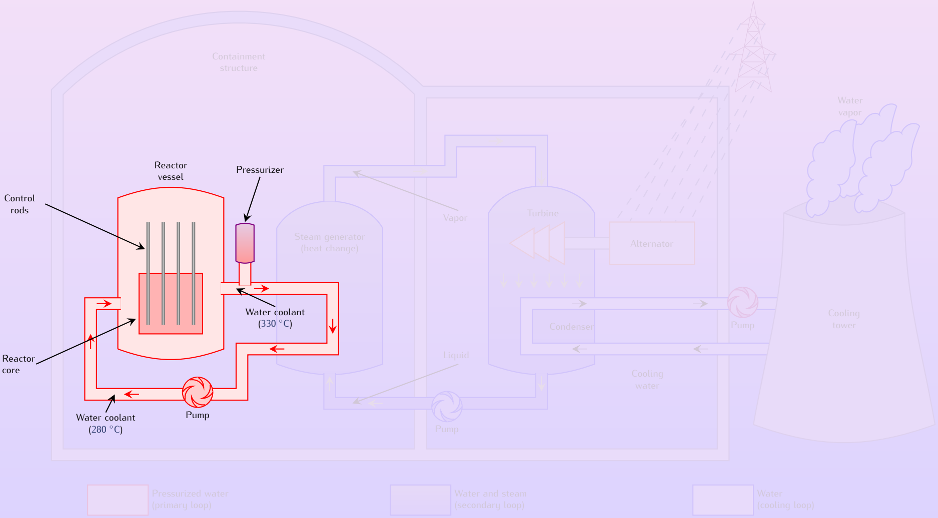


Pressurized water (primary loop)

Water and steam (secondary loop)

Water (cooling loop)

Pressurized Water Reactor



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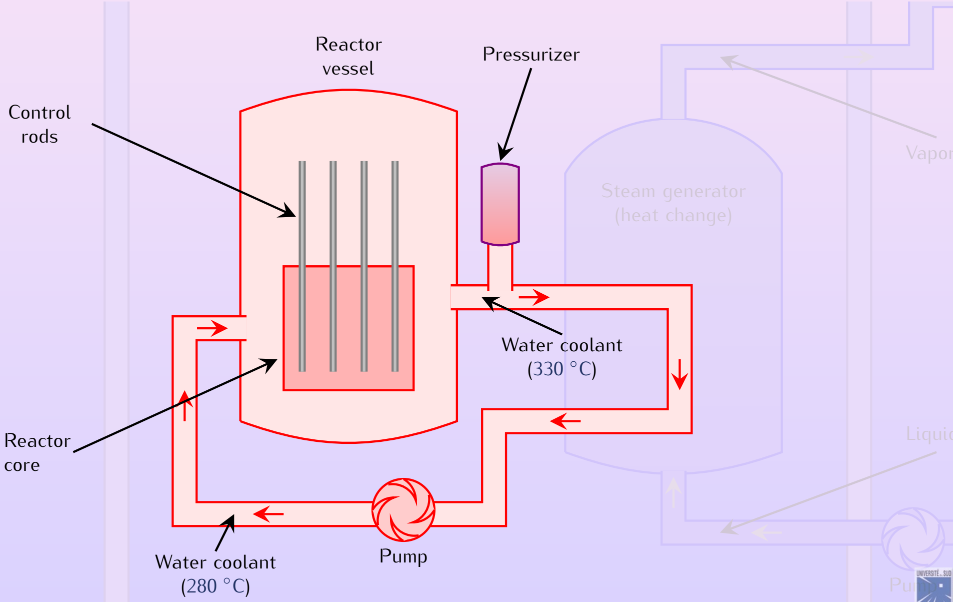
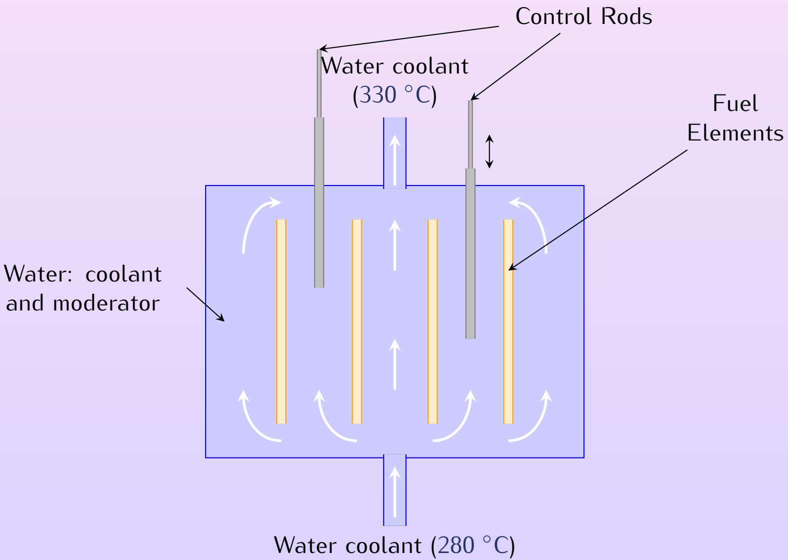


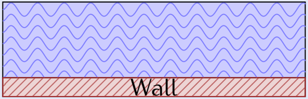
Core of a Pressurized Water Reactor



Boiling Crisis

Phenomenon

Liquid phase heated by a wall at a fixed temperature T^{wall}.
When T^{wall} increases, we switch from a **Nucleate Boiling** to a **Film Boiling**.



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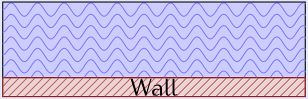

Nucleate Boiling

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

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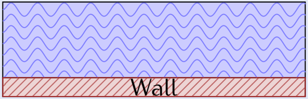

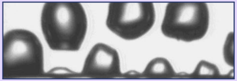

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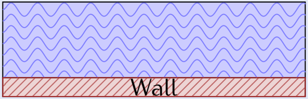

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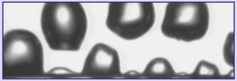

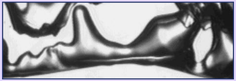

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"Ingredients" of the Model

- ✔ Simulating all bubbles (DNS),
- System of PDEs for the fluid flow (monophasic or diphasic),
- Phase transition (pressure and/or temperature variations),
- Heat Diffusion,
- Surface Tension,
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Euler System

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\begin{cases}
\partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0, \\
\partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\, \mathbb{I}) = \mathfrak{V}_{\mathrm{vf}} - \mathfrak{S}_{\mathrm{sf}}, \\
\partial_t \left(\varrho \left(\frac{|\mathbf{u}|^2}{2} + \varepsilon \right) \right) + \operatorname{div} \left(\varrho \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).
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- $(\mathbf{x}, t) \mapsto \varrho$ specific density,
- $(\mathbf{x}, t) \mapsto \varepsilon$ specific internal energy,
- $(\mathbf{x}, t) \mapsto \mathbf{u}$ velocity;
- $(\varrho, \varepsilon) \mapsto \mathfrak{V}_{\mathrm{vf}}$ body forces,
- $(\varrho, \varepsilon) \mapsto \mathfrak{S}_{\mathrm{sf}}$ surface forces,
- $(\varrho, \varepsilon) \mapsto \operatorname{div}(q)$ heat transfer.

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

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EOS of each Phase $\alpha = \text{liq}, \text{vap}$

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

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

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

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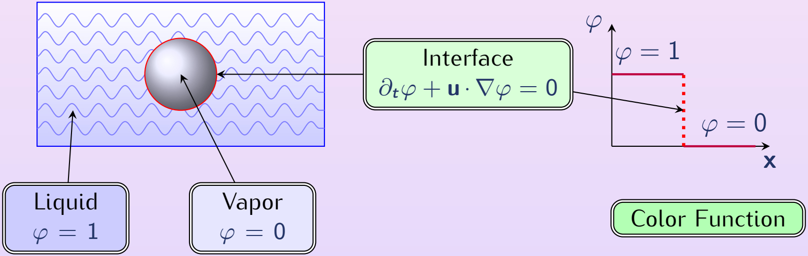
Liquid–Vapor Interface



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

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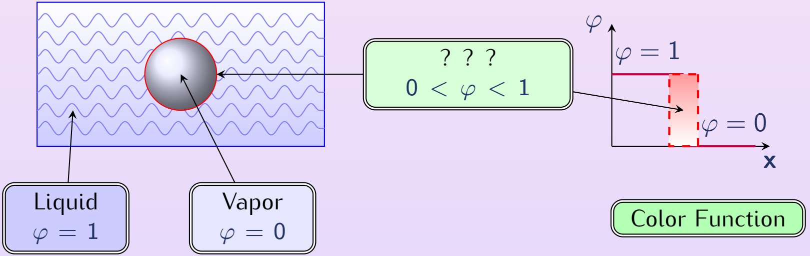

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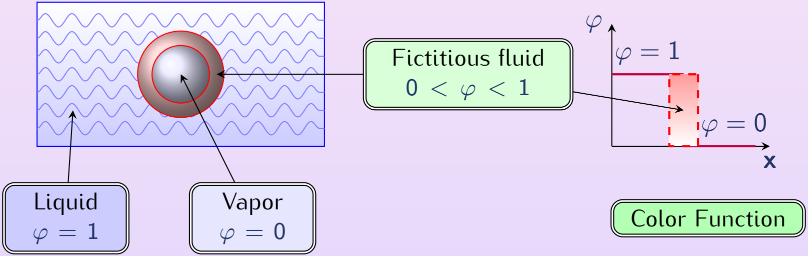

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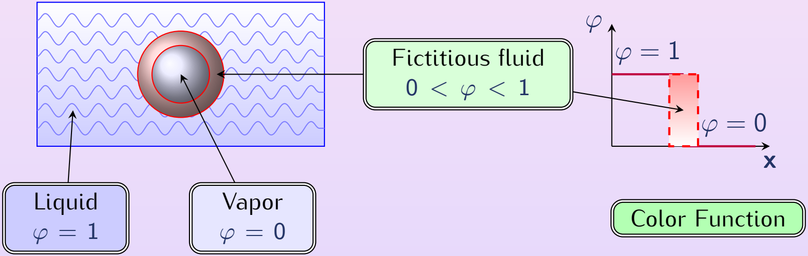

- **Goal: define a global pressure law such that**
  - $(\varrho, \varepsilon, \mathbf{u}, P)$ are continuous (3 zones)
  - the interface position and the phase change are implicit (i.e. $\not\varphi$)
  - coherence with classical thermodynamics [H. Callen]

EOS of a Mixture

- $\mathbf{w} \stackrel{\text{def}}{=} y\mathbf{w}_{\text{liq}} + (1-y)\mathbf{w}_{\text{vap}}$;
- y mass fraction;
- z volume fraction s.t. $y\tau_{\text{liq}} = z\tau$;
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$$P = \left(\left.\frac{\partial\sigma}{\partial\varepsilon}\right|_{\tau;y,z,\psi}\right)^{-1} \left.\frac{\partial\sigma}{\partial\tau}\right|_{\varepsilon;y,z,\psi}$$

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Entropy at equilibrium

$$\mathbf{w} \mapsto s^{\text{eq}}(\mathbf{w}) = \sigma(\mathbf{w}, z^{\text{eq}}(\mathbf{w}), y^{\text{eq}}(\mathbf{w}), \psi^{\text{eq}}(\mathbf{w}))$$

Definition [H. Callen, Ph. Helluy ...]

Optimization Problem:

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

Optimality Condition: $\begin{cases} T_1(z,y,\psi) = T_2(z,y,\psi) \\ P_1(z,y,\psi) = P_2(z,y,\psi) \\ g_1(z,y,\psi) = g_2(z,y,\psi) \end{cases}$ Solution: (z^*, y^*, ψ^*)

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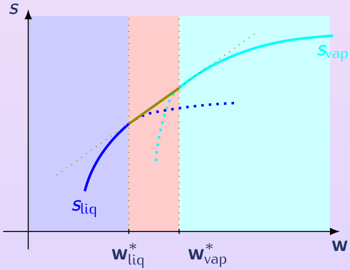

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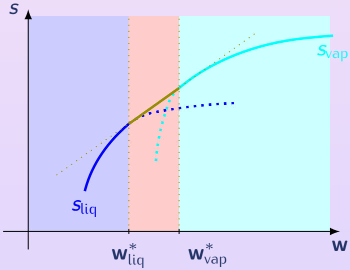

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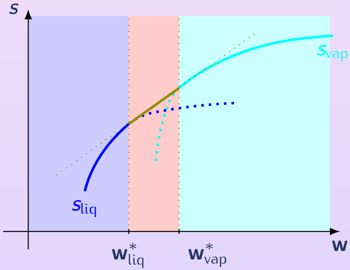

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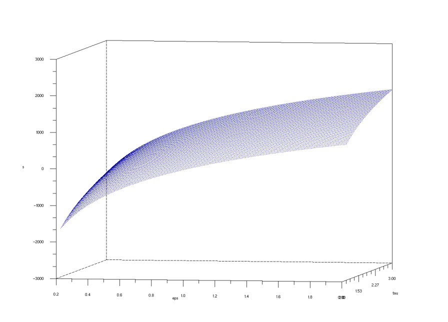

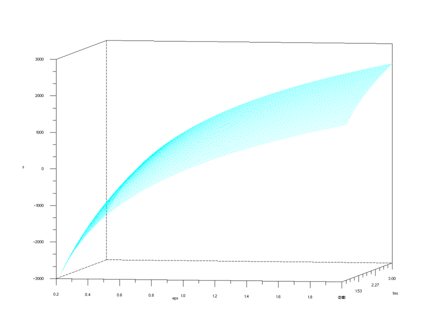

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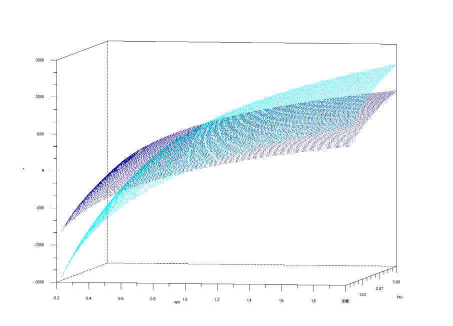

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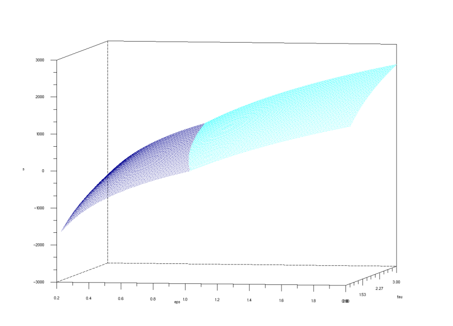

Concave Hull with two Perfect Gases

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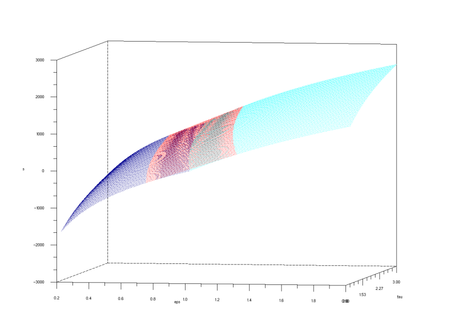

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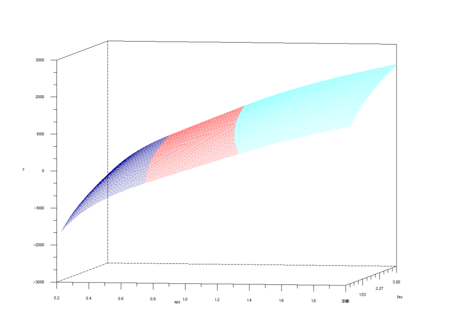

From $\mathbf{w} \mapsto s^{eq}$ to $\mathbf{w} \mapsto P^{eq}$

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

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

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

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

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

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

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

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

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\begin{cases}
P_{liq}(\mathbf{w}_{liq}) = P_{vap}(\mathbf{w}_{vap}) \\
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\end{cases}
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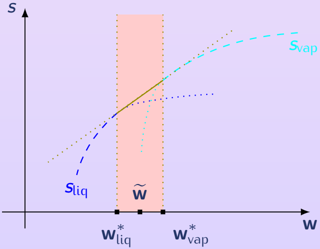

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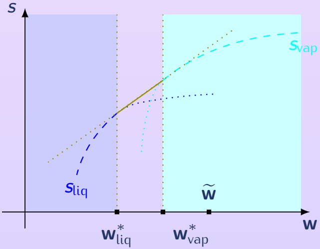

From $\mathbf{w} \mapsto s^{\text{eq}}$ to $\mathbf{w} \mapsto P^{\text{eq}}$

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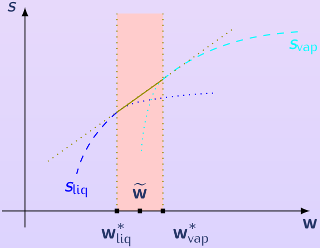

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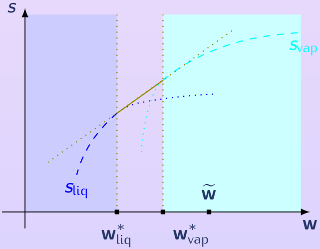

Outline

Dynamic Liquid–Vapor Phase Change

Euler System

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

Mathematical Properties

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

1. Euler system: strict hyperbolicity (≃ p-system);
2. Riemann problem: multitude of entropy (Lax) solutions [R. Menikoff, B. J. Plohr], uniqueness of Liu solution.

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Mathematical Properties

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

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

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1. Context
2. Model
   - Equation of State
   - Conservation Laws
3. Numerical Approximation and Example
   - The Phase Change Equation
   - Numerical Scheme and Example
4. Conclusion

Summary of the Model

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

$$\begin{cases} g_1(\mathbf{w}_1)=g_2(\mathbf{w}_2) \\ P_1(\mathbf{w}_1)=P_2(\mathbf{w}_2) \\ T_1(\mathbf{w}_1)=T_2(\mathbf{w}_2) \\ \mathbf{w}=y\mathbf{w}_1+(1-y)\mathbf{w}_2 \end{cases}$$

Euler System

$\mathbf{w} \mapsto P^{\text{eq}}$

Phase Change Equation

$$\frac{\tau-\tau_{\text{vap}}^{\text{sat}}}{\tau_{\text{liq}}^{\text{sat}}-\tau_{\text{vap}}^{\text{sat}}}=\frac{\varepsilon-\varepsilon_{\text{vap}}^{\text{sat}}}{\varepsilon_{\text{liq}}^{\text{sat}}-\varepsilon_{\text{vap}}^{\text{sat}}}$$

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

Euler System

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Phase Change Equation

$$\frac{\tau - \tau_{vap}^{sat}}{\tau_{liq}^{sat} - \tau_{vap}^{sat}} = \frac{\varepsilon - \varepsilon_{vap}^{sat}}{\varepsilon_{liq}^{sat} - \varepsilon_{vap}^{sat}}$$

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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

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

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

T SOLUTION OF

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

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

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least square approximation

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

T solution of

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

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/`

Tabulated EOS

(τ, ε) fixed

T solution of

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

$$\wr\wr$$

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

$$\wr\wr$$

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

least square approximations

Tabulated EOS

(τ, ε) fixed

T solution of

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

$\wr\wr$ ← least square approximations

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

Outline

Numerical Scheme based on Relaxation Approach

$\sigma(y, z, \psi, \tau, \varepsilon)$ —Optimization→ $s^{\text{eq}}(\tau, \varepsilon)$

Off Equilibrium

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \operatorname{grad} z = \\ \partial_t y + \mathbf{u} \cdot \operatorname{grad} y = \\ \partial_t \psi + \mathbf{u} \cdot \operatorname{grad} \psi = \end{cases}$$

$\xrightarrow[\mu_j \to \infty]{}$

Equilibrium

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

$$P^{\text{eq}}(\varrho, \varepsilon) = \frac{s^{\text{eq}}_\tau}{s^{\text{eq}}_\varepsilon}$$

Two Steps:

1. Hydrodynamic (+ gravity, surface tension, heat diffusion, ...)
2. Projection by solving the Phase-Change Equation

Numerical Scheme based on Relaxation Approach

$\sigma(y, z, \psi, \tau, \varepsilon)$ —Optimization→ $s^{eq}(\tau, \varepsilon)$

Off Equilibrium

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = \mu_z(z - z^{eq}) \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, y = \mu_y(y - y^{eq}) \\ \partial_t \psi + \mathbf{u} \cdot \mathbf{grad}\, \psi = \mu_\psi(\psi - \psi^{eq}) \end{cases}$$

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

$\xrightarrow{\mu_j \to \infty}$

Equilibrium

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

$$P^{eq}(\varrho, \varepsilon) = \frac{s^{eq}_\tau}{s^{eq}_\varepsilon}$$

Two Steps:

1. Hydrodynamic (+ gravity, surface tension, heat diffusion, …)
2. Projection by solving the Phase-Change Equation

Numerical Scheme based on Relaxation Approach

$\sigma(y, z, \psi, \tau, \varepsilon)$ —Optimization→ $s^{eq}(\tau, \varepsilon)$

Off Equilibrium

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = 0 \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, y = 0 \\ \partial_t \psi + \mathbf{u} \cdot \mathbf{grad}\, \psi = 0 \end{cases}$$

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

$\mu_j \to \infty$

Equilibrium

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

$$P^{eq}(\varrho, \varepsilon) = \frac{s^{eq}_\tau}{s^{eq}_\varepsilon}$$

Two Steps:

1. Hydrodynamic (+ gravity, surface tension, heat diffusion, ...)
2. Projection by solving the Phase-Change Equation

Numerical Scheme based on Relaxation Approach

$\sigma(y,z,\psi,\tau,\varepsilon)$ —Optimization→ $s^{eq}(\tau,\varepsilon)$

Off Equilibrium

$$\begin{cases}\partial_t\varrho + \operatorname{div}(\varrho\mathbf{u}) = 0\\ \partial_t(\varrho\mathbf{u}) + \operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u} + P\,\mathbb{I}) = 0\\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0\\ \partial_t z + \mathbf{u}\cdot\mathbf{grad}\,0 = \mu_z(z - z^{eq})\\ \partial_t y + \mathbf{u}\cdot\mathbf{grad}\,0 = \mu_y(y - y^{eq})\\ \partial_t\psi + \mathbf{u}\cdot\mathbf{grad}\,0 = \mu_\psi(\psi - \psi^{eq})\end{cases}$$

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

$\xrightarrow{\mu_j\to\infty}$

Equilibrium

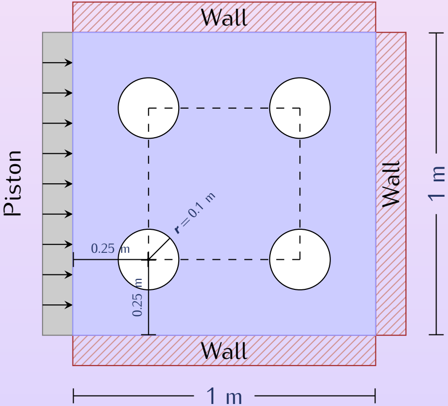
$$\begin{cases}\partial_t\varrho + \operatorname{div}(\varrho\mathbf{u}) = 0\\ \partial_t(\varrho\mathbf{u}) + \operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u} + P^{eq}\,\mathbb{I}) = 0\\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P^{eq})\mathbf{u}) = 0\end{cases}$$

$$P^{eq}(\varrho,\varepsilon) = \frac{s^{eq}_\tau}{s^{eq}_\varepsilon}$$

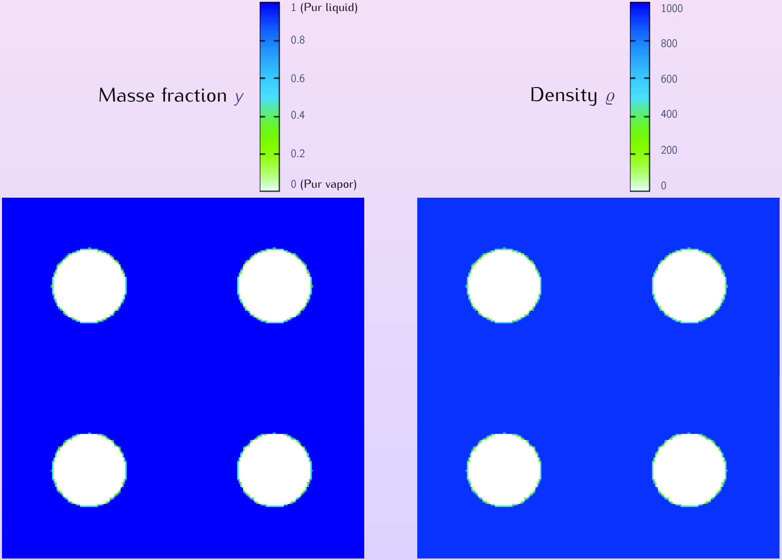
Two Steps:

1. Hydrodynamic (+ gravity, surface tension, heat diffusion, ...)
2. Projection by solving the Phase-Change Equation

Compression of Vapor Bubbles

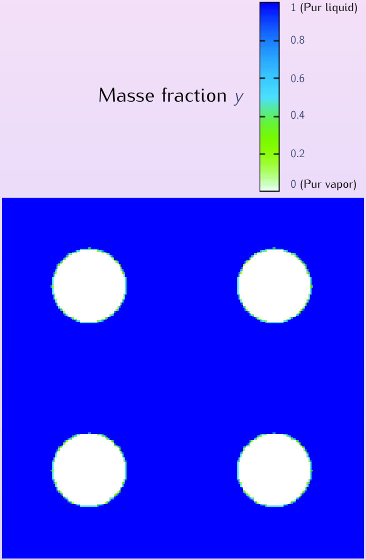


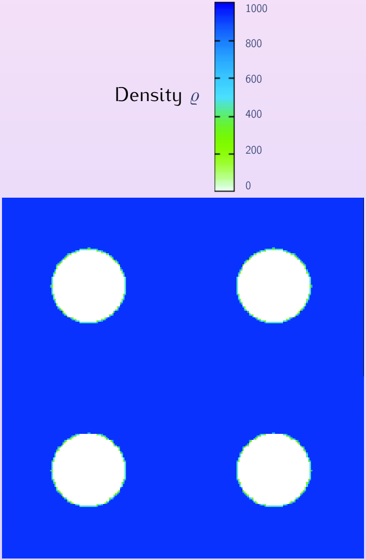
Compression of Vapor Bubbles



◂ Geometry ▸ Play ▸▸ Skip

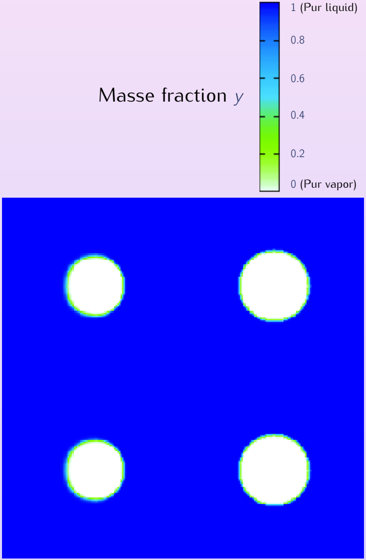
Compression of Vapor Bubbles

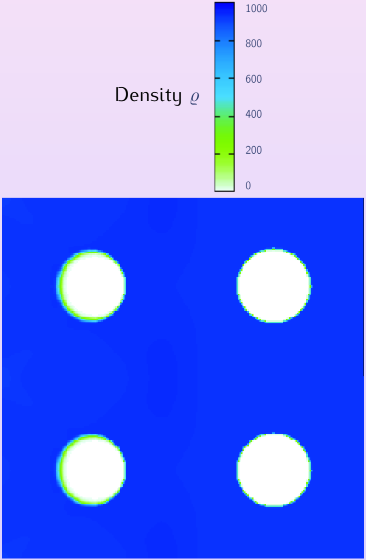




Geometry Play Skip

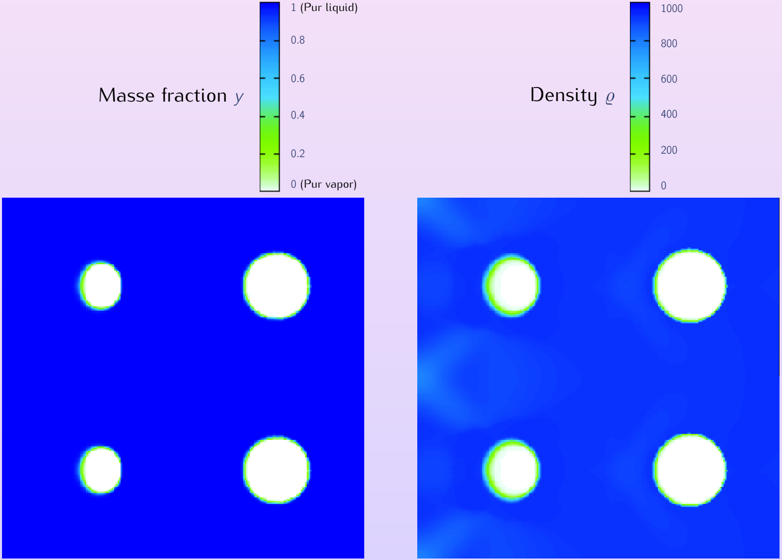
Compression of Vapor Bubbles





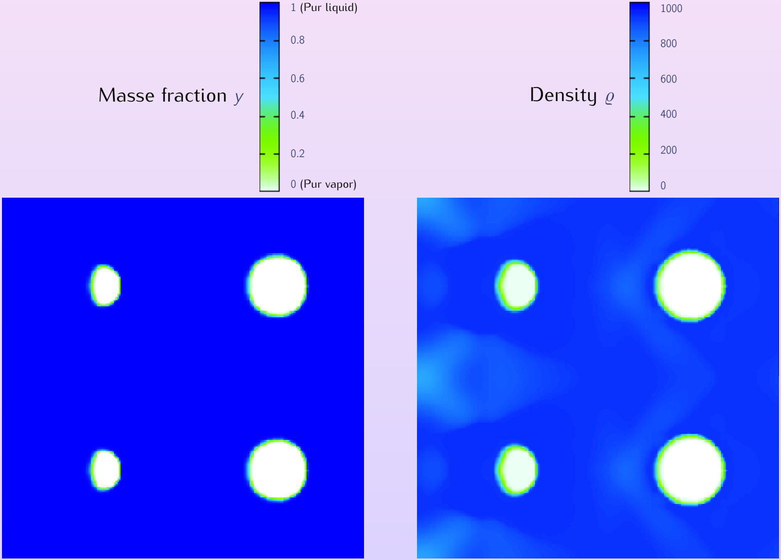
Geometry Play Skip

Compression of Vapor Bubbles



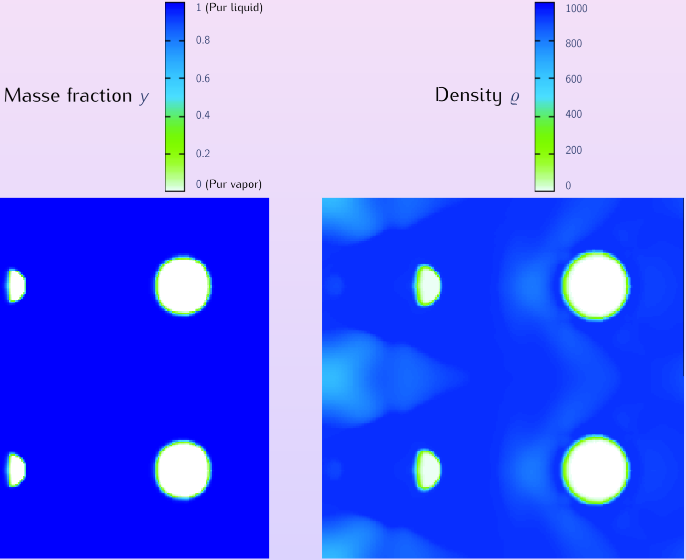
Geometry Play Skip

Compression of Vapor Bubbles



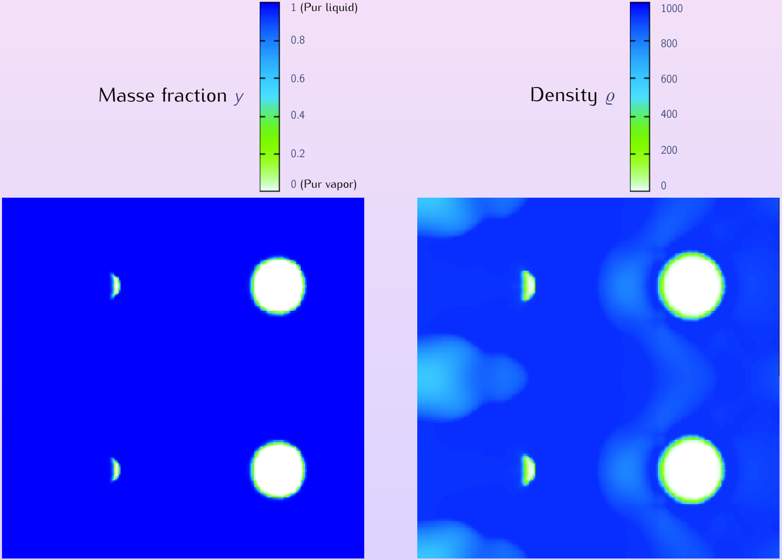
Geometry Play Skip

Compression of Vapor Bubbles



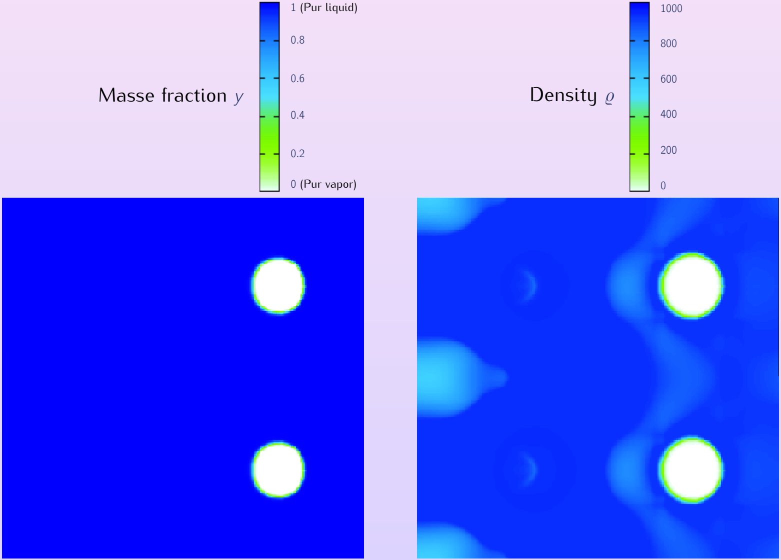
Geometry Play Skip

Compression of Vapor Bubbles



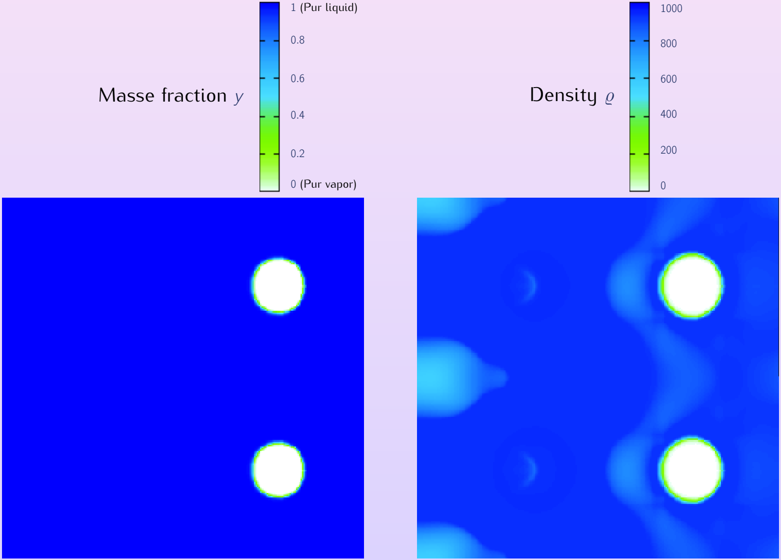
Geometry Play Skip

Compression of Vapor Bubbles



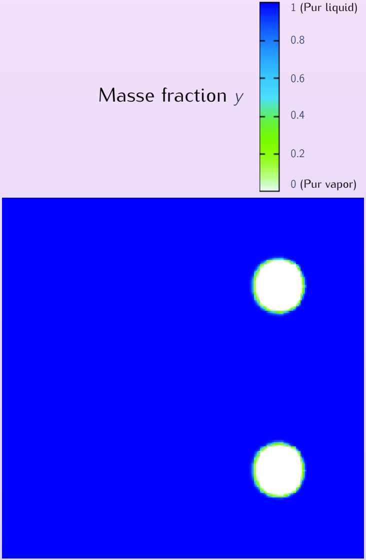
Geometry Play Skip

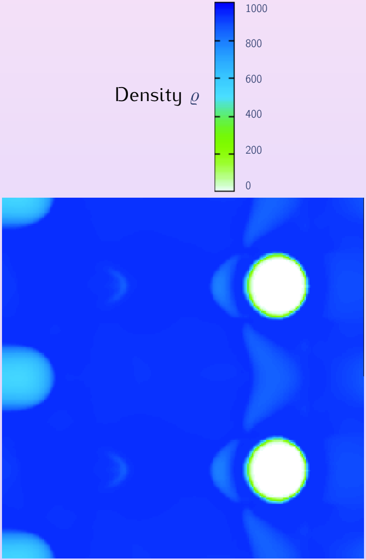
Compression of Vapor Bubbles



Geometry Play Skip

Compression of Vapor Bubbles

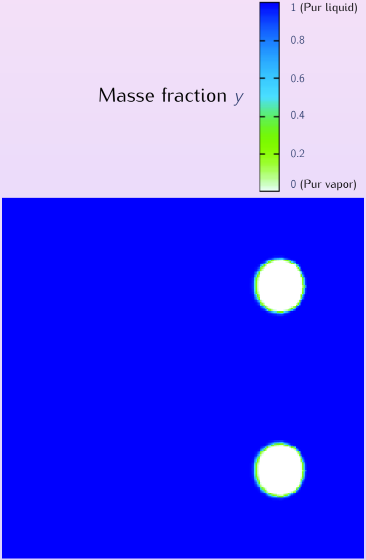




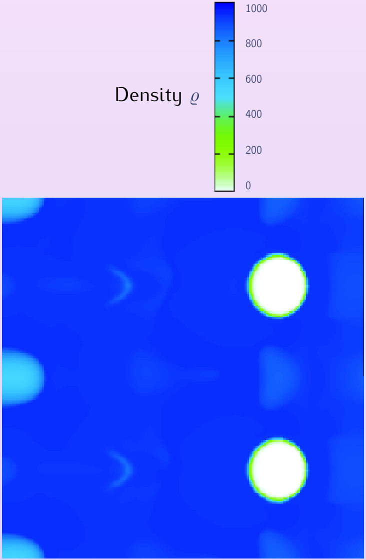
◀ Geometry ▶ Play ▶▶ Skip

Compression of Vapor Bubbles

Masse fraction y

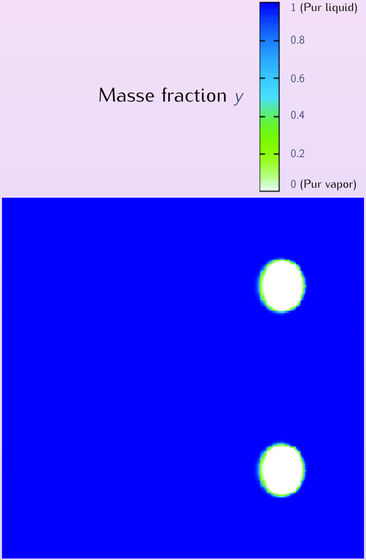


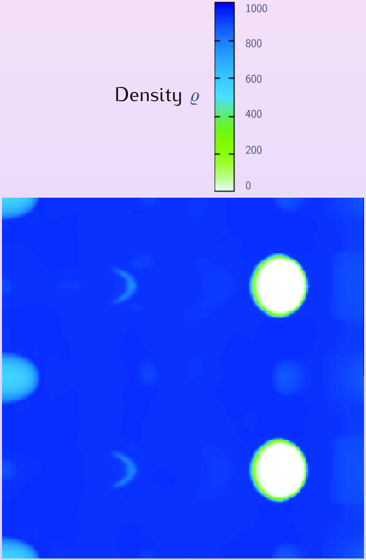
Density ϱ



Geometry Play Skip

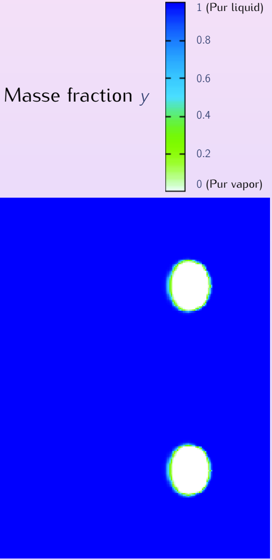
Compression of Vapor Bubbles

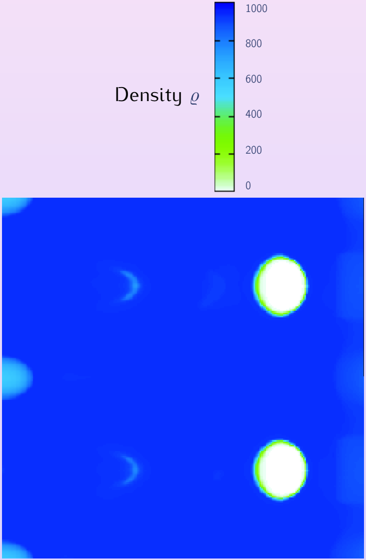




Geometry Play Skip

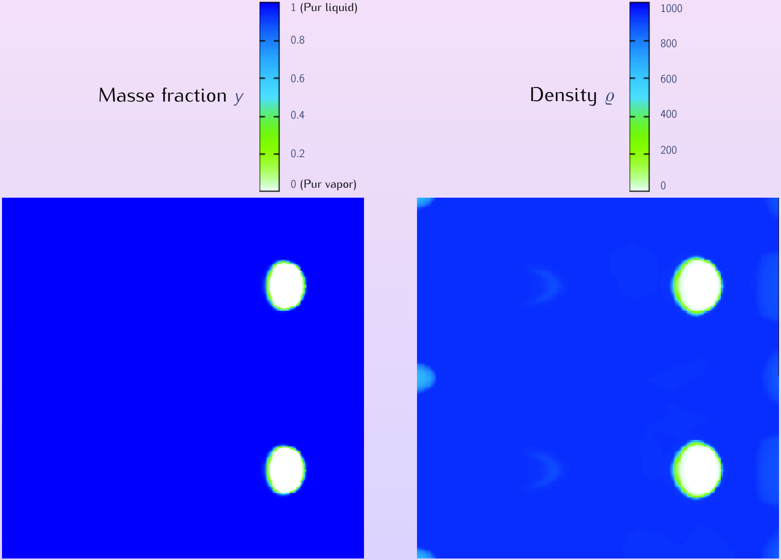
Compression of Vapor Bubbles





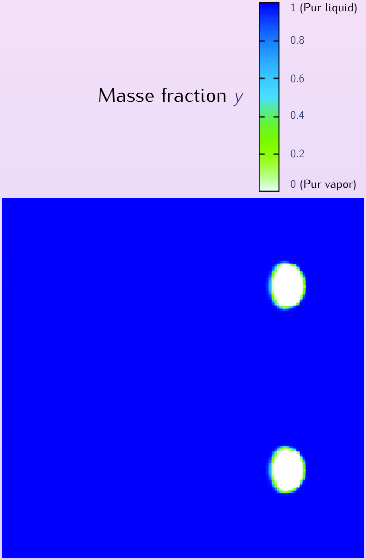
Geometry Play Skip

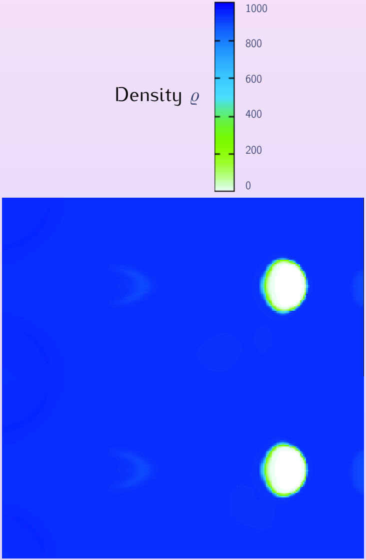
Compression of Vapor Bubbles



◂ Geometry ▸ Play ▸▸ Skip

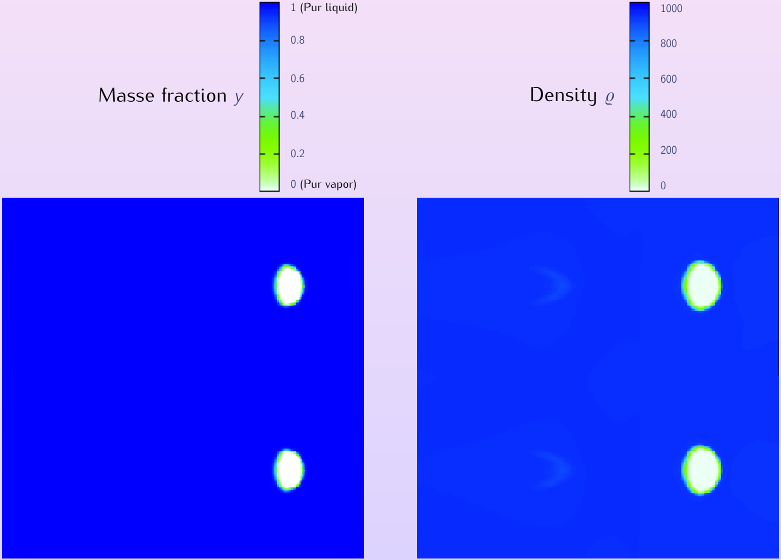
Compression of Vapor Bubbles





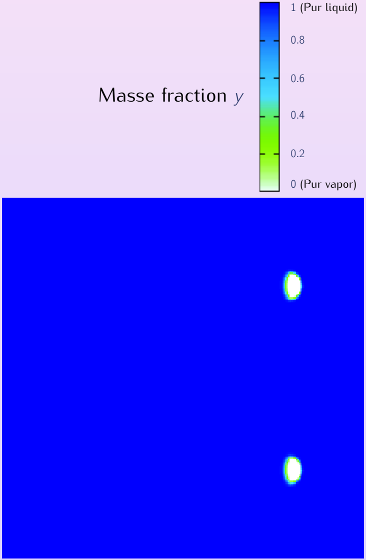
Geometry Play Skip

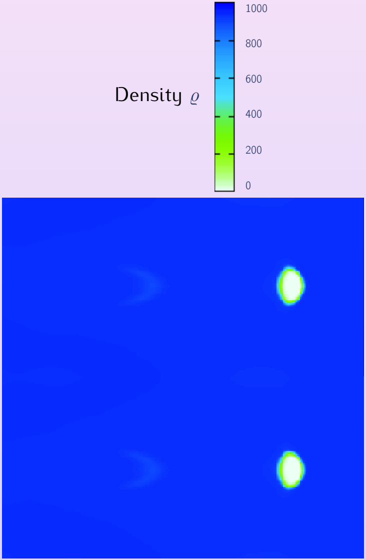
Compression of Vapor Bubbles



Geometry Play Skip

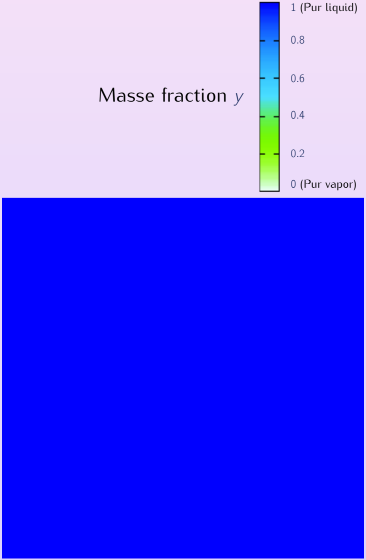
Compression of Vapor Bubbles

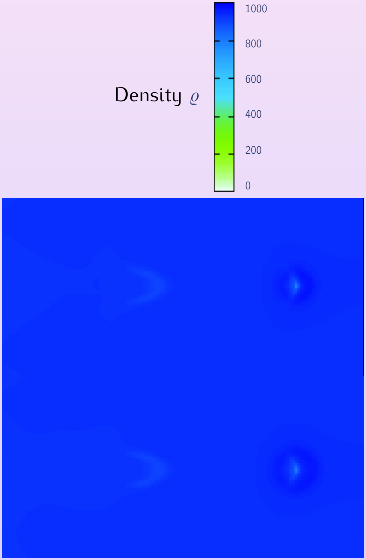




Geometry Play Skip

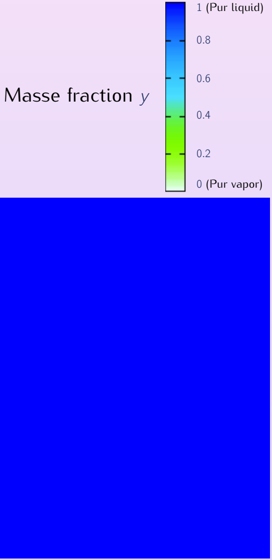
Compression of Vapor Bubbles

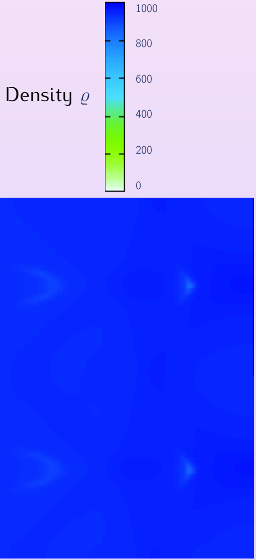




Geometry Play Skip

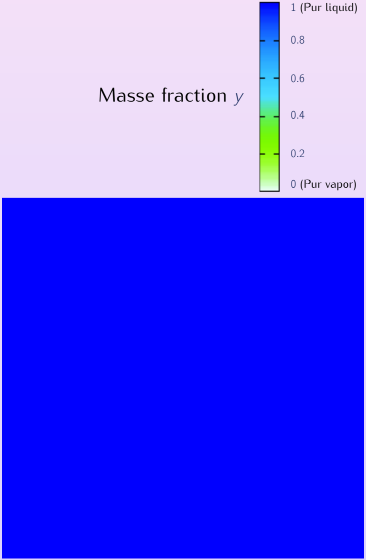
COMPRESSION OF VAPOR BUBBLES

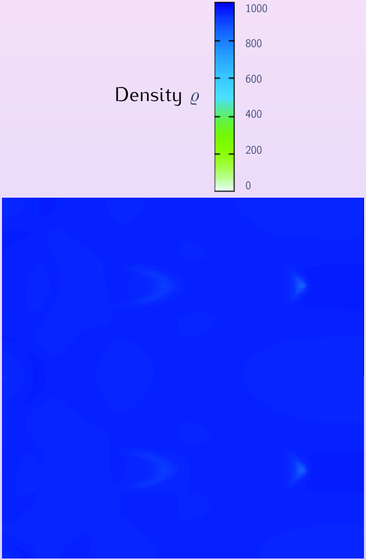




◂ Geometry ▸ Play ▸▸ Skip

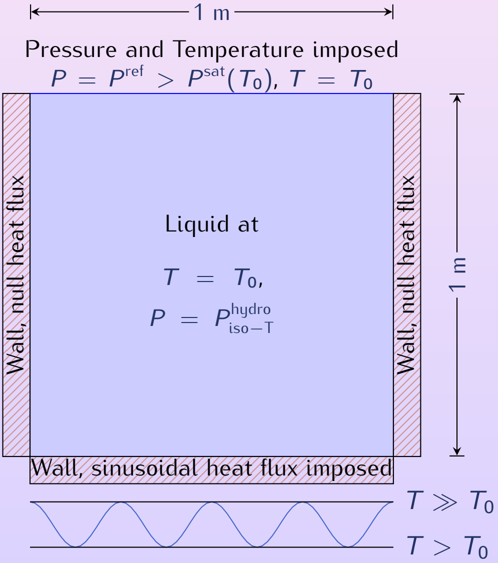
Compression of Vapor Bubbles



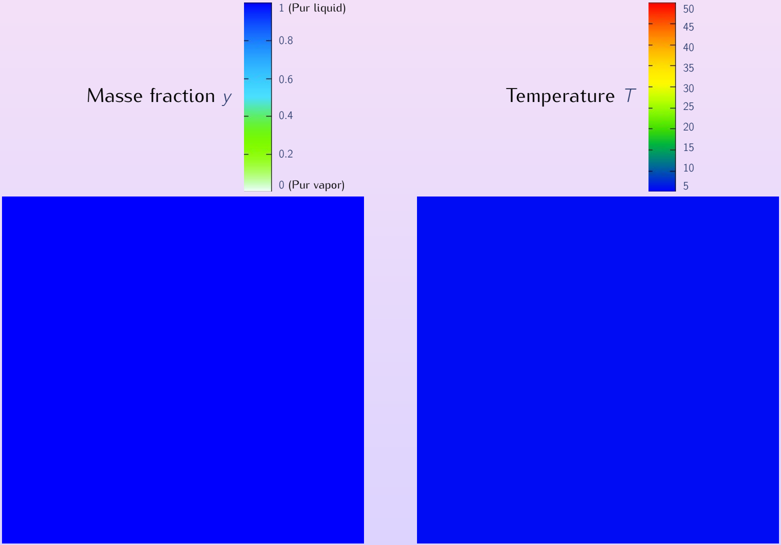


Geometry Play Skip

Transition to a Film Boiling

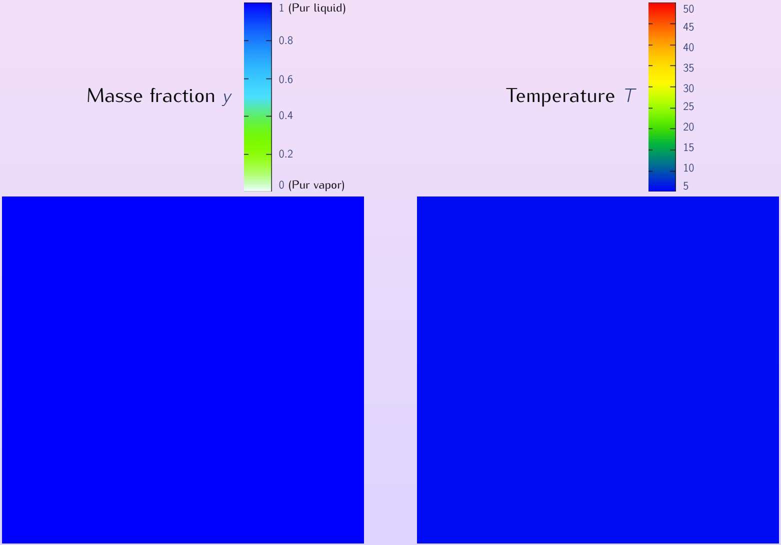


Transition to a Film Boiling



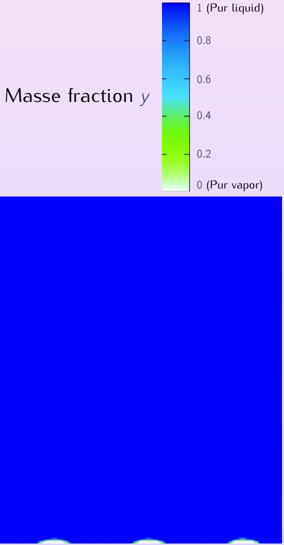
Geometry Play Skip

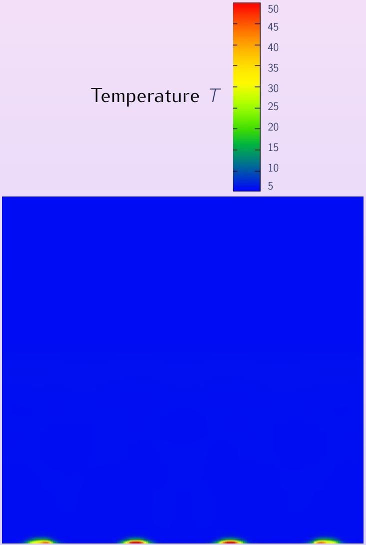
Transition to a Film Boiling



◂ Geometry ▸ Play ▸▸ Skip

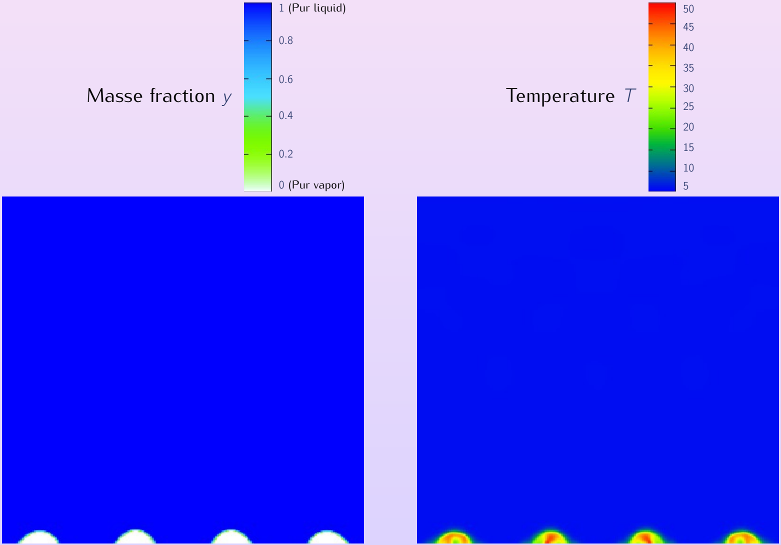
Transition to a Film Boiling





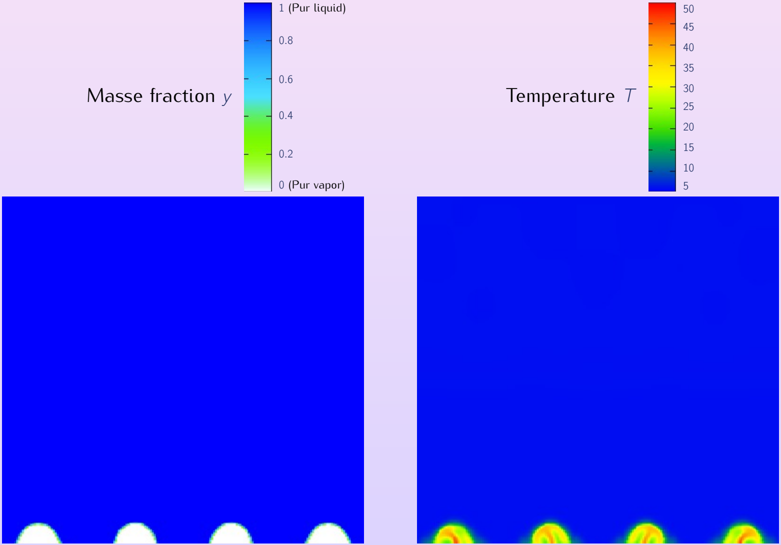
Geometry Play Skip

Transition to a Film Boiling



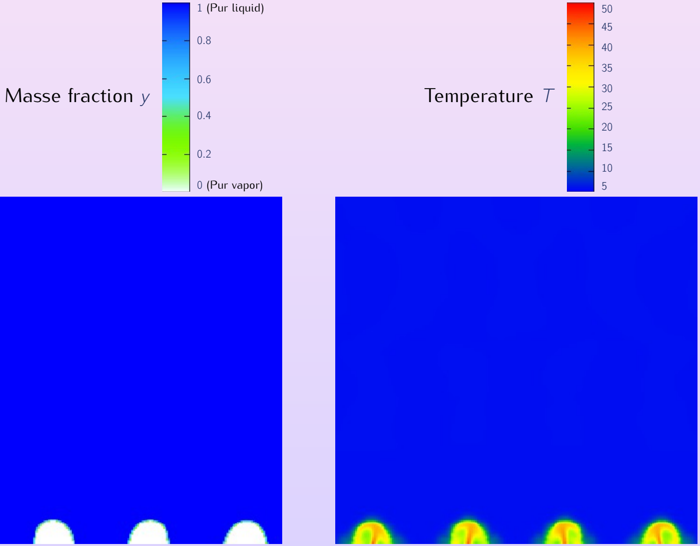
Geometry Play Skip

Transition to a Film Boiling



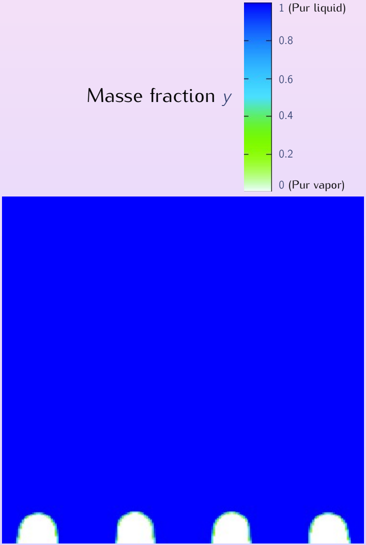
Geometry Play Skip

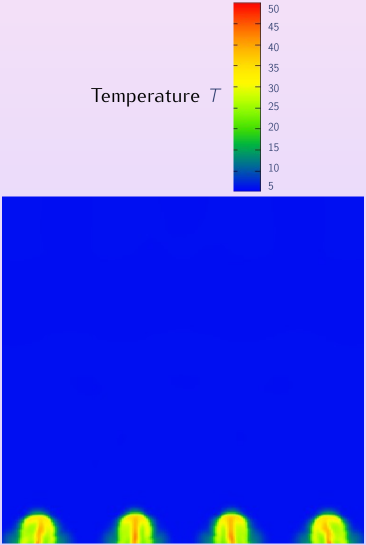
Transition to a Film Boiling



◂ Geometry ▸ Play ▸▸ Skip

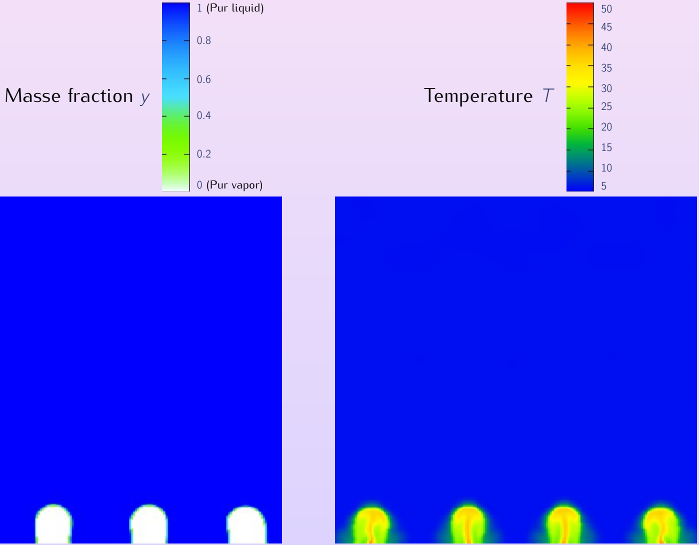
Transition to a Film Boiling





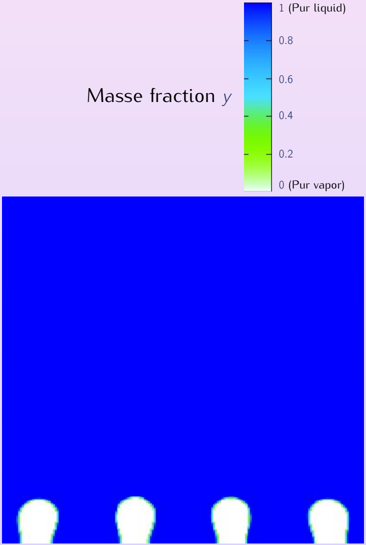
Geometry Play Skip

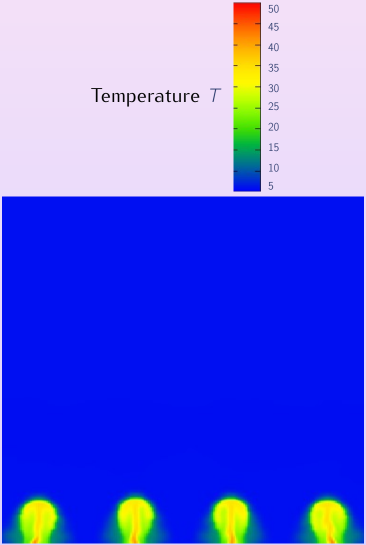
Transition to a Film Boiling



◀ Geometry ▶ Play ▶▶ Skip

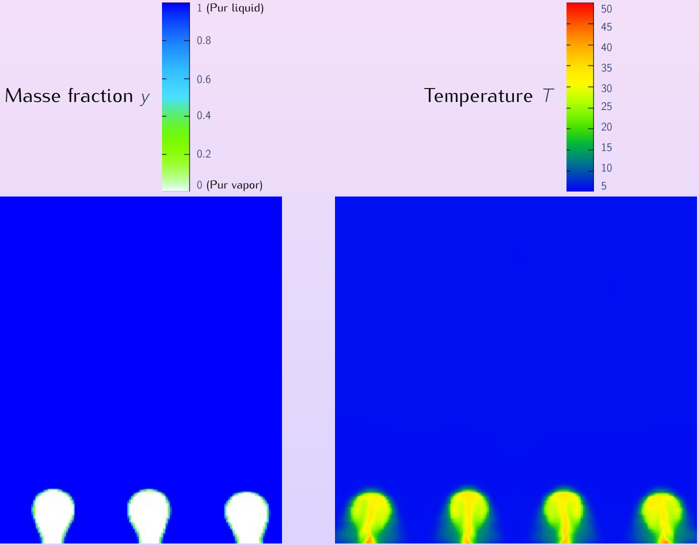
Transition to a Film Boiling





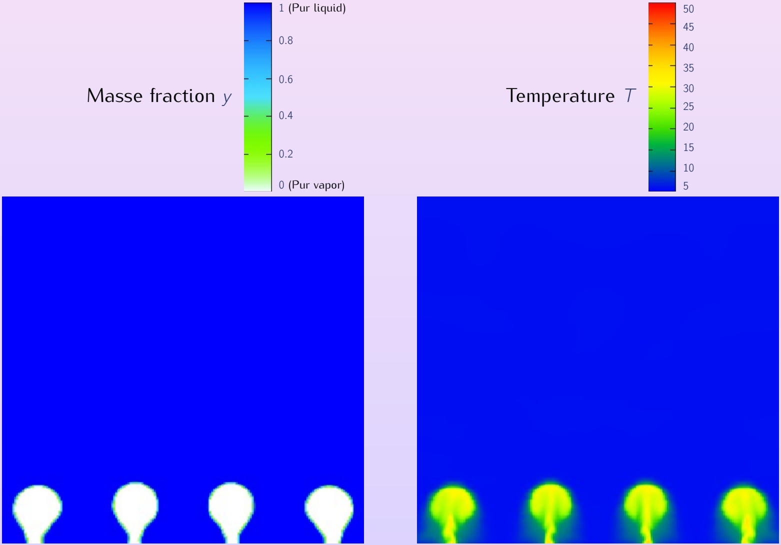
Geometry Play Skip

Transition to a Film Boiling



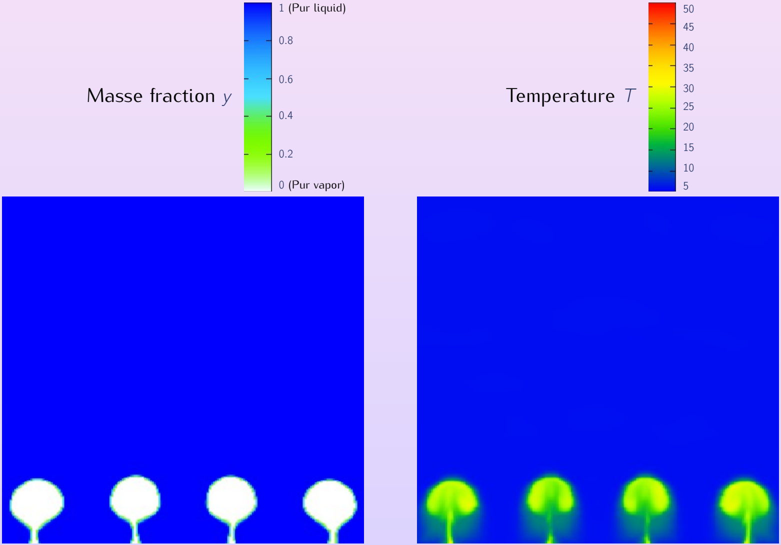
Geometry Play Skip

Transition to a Film Boiling



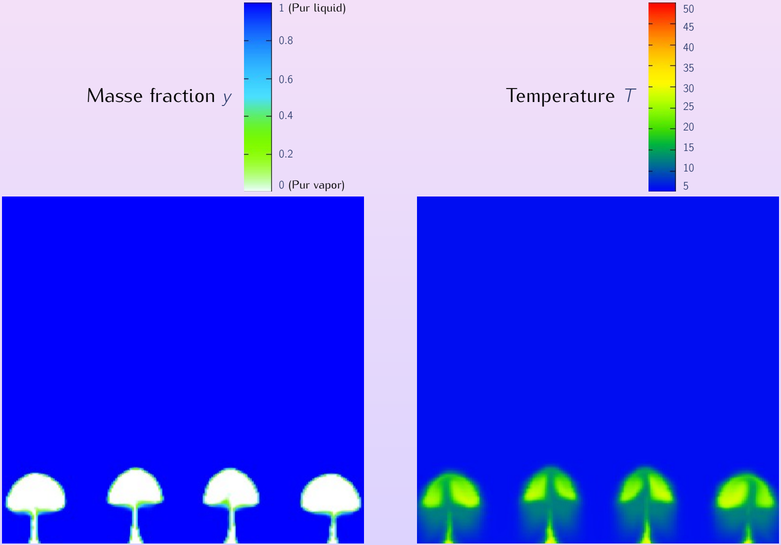
Geometry Play Skip

Transition to a Film Boiling



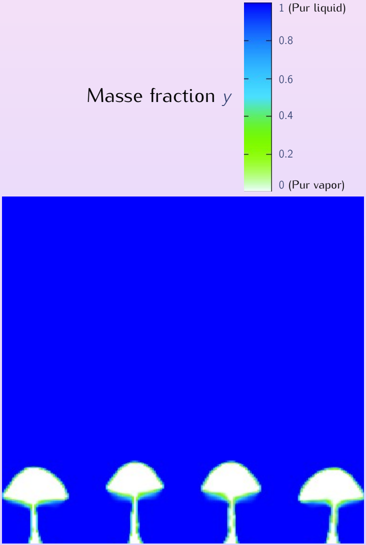
Geometry Play Skip

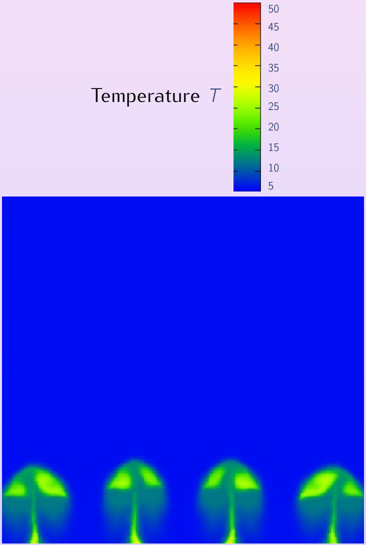
Transition to a Film Boiling



Geometry Play Skip

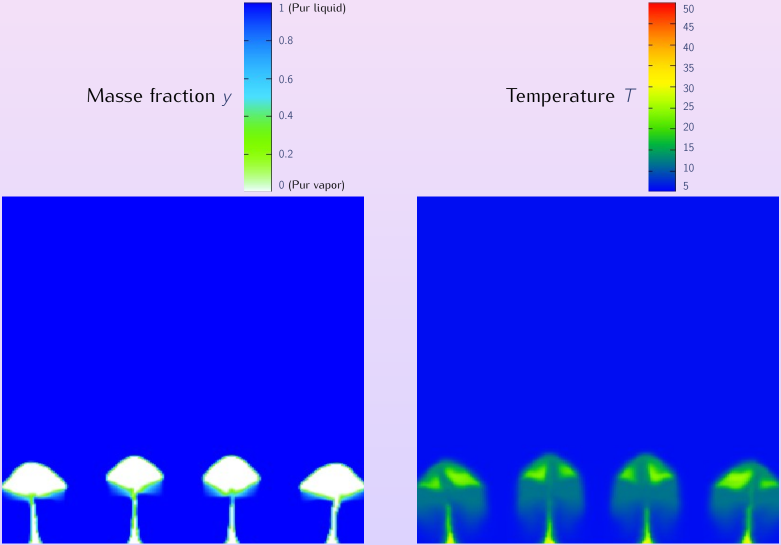
Transition to a Film Boiling





Geometry Play Skip

Transition to a Film Boiling



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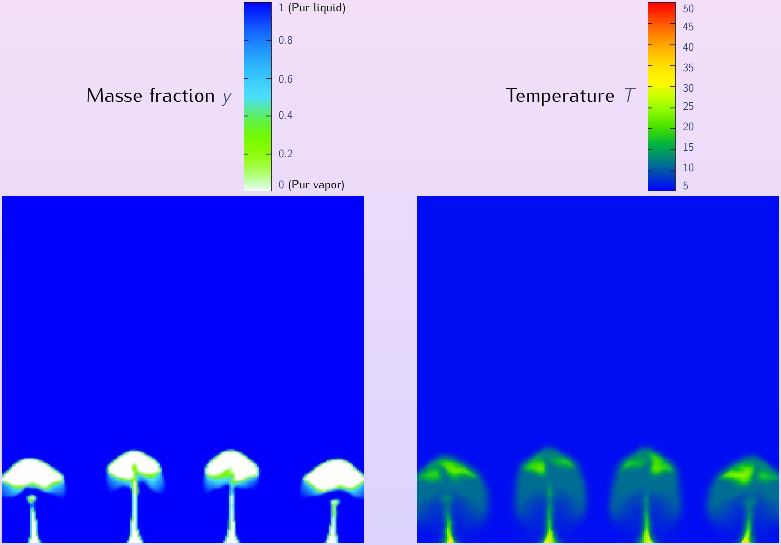

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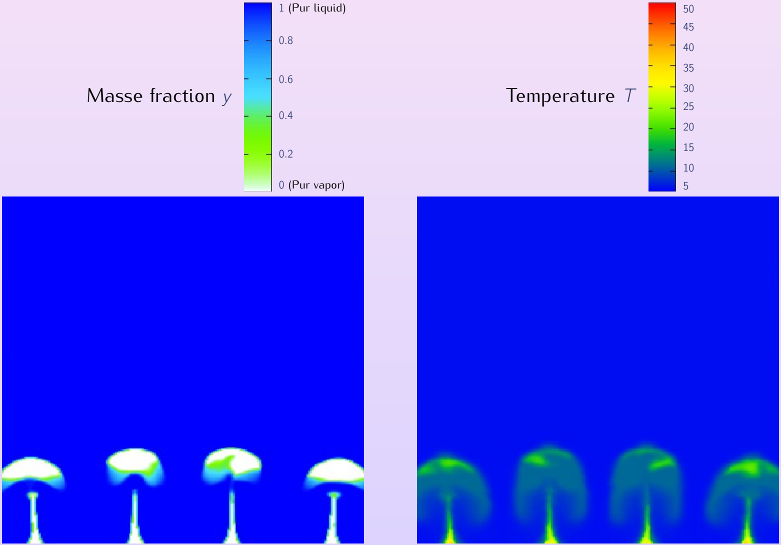

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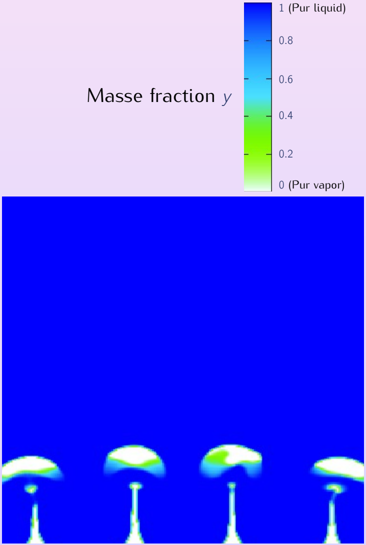

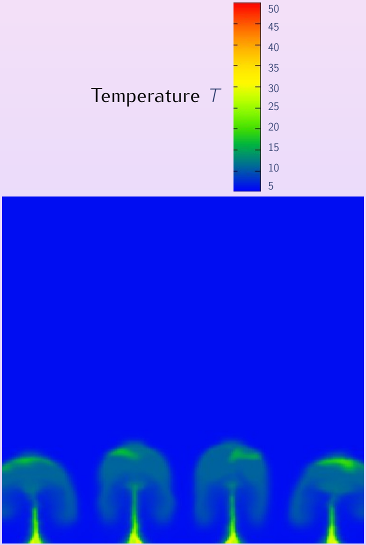

◀ Geometry ▶ Play ⏩ Skip

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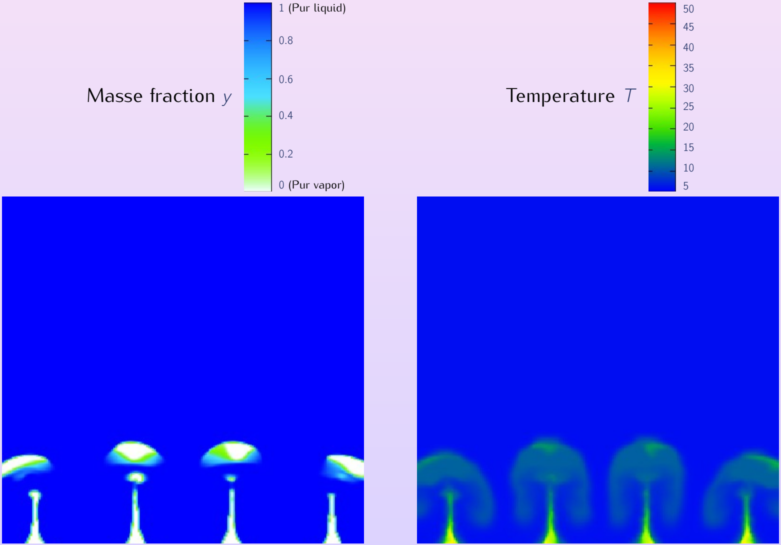

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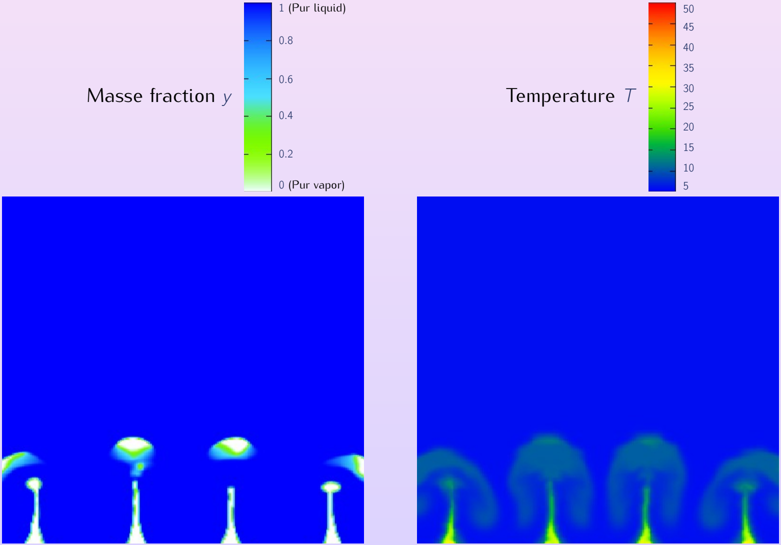

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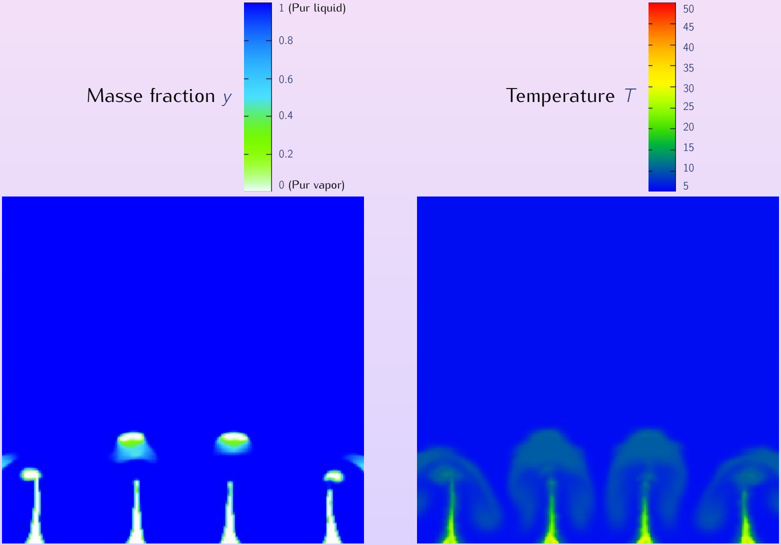

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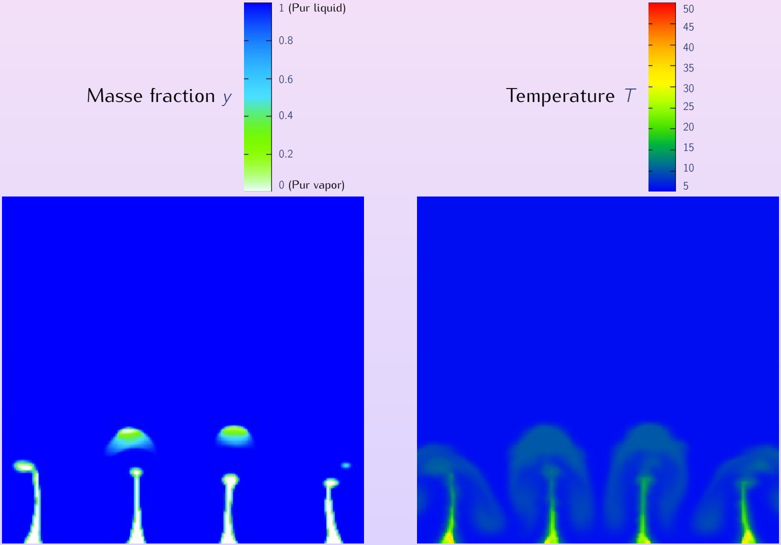

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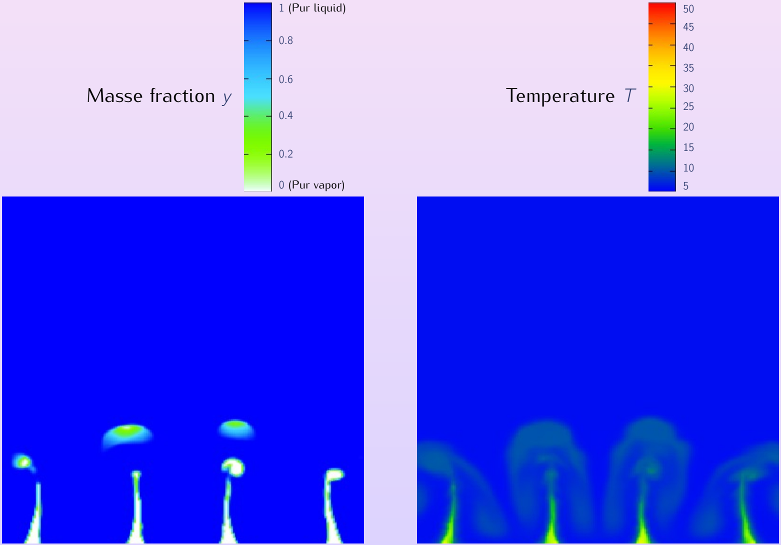

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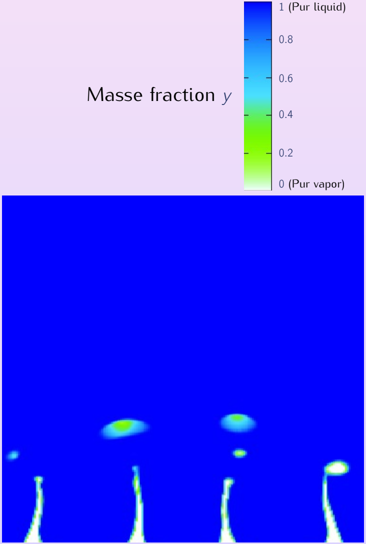

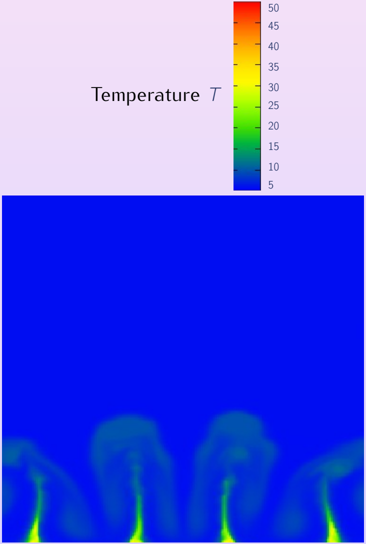

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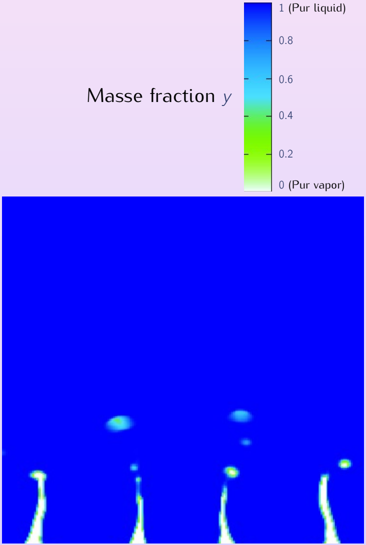

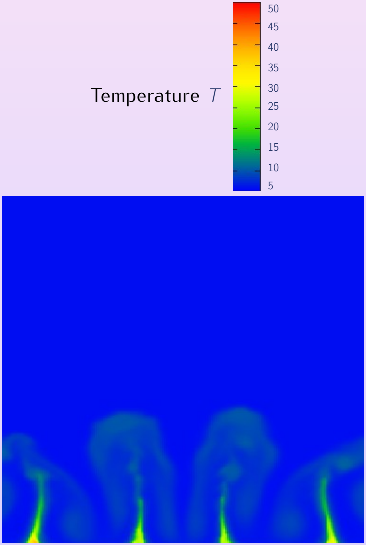

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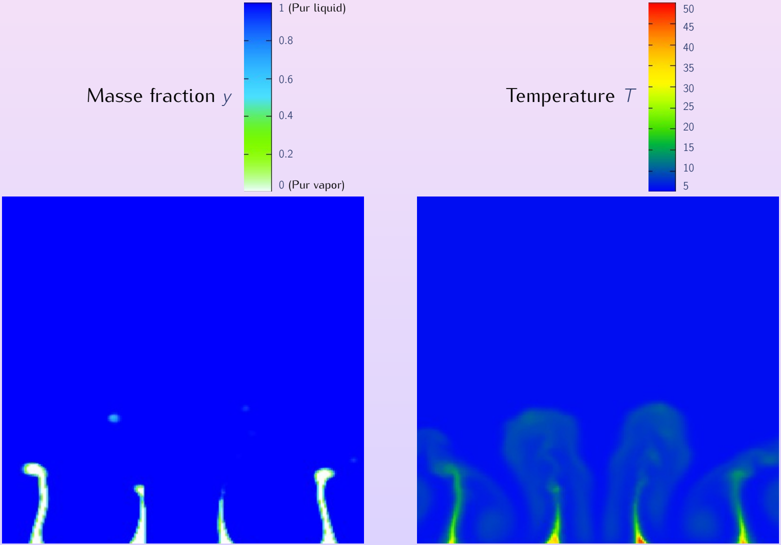
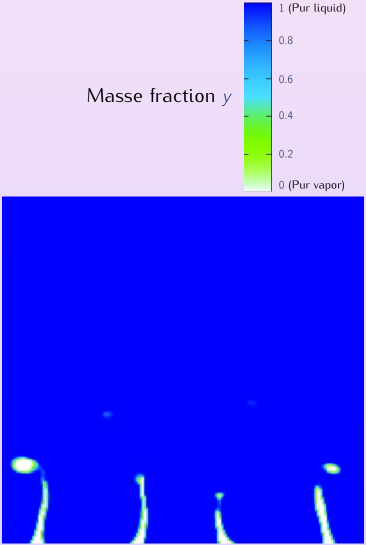


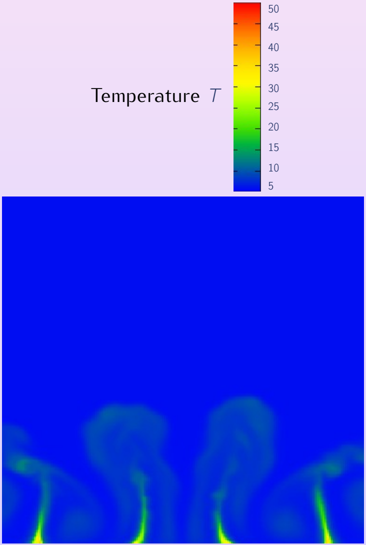
◂ Geometry ▸ Play ▸▸ Skip

Transition to a Film Boiling

Masse fraction y



Temperature T



Geometry Play Skip

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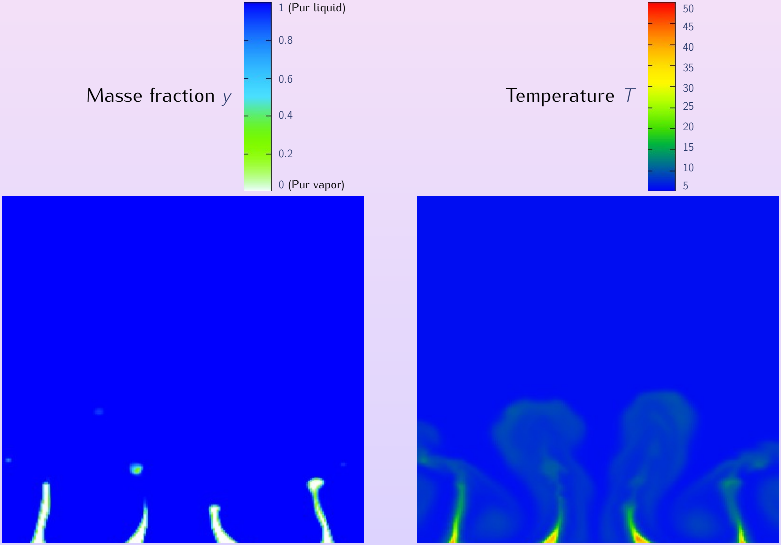

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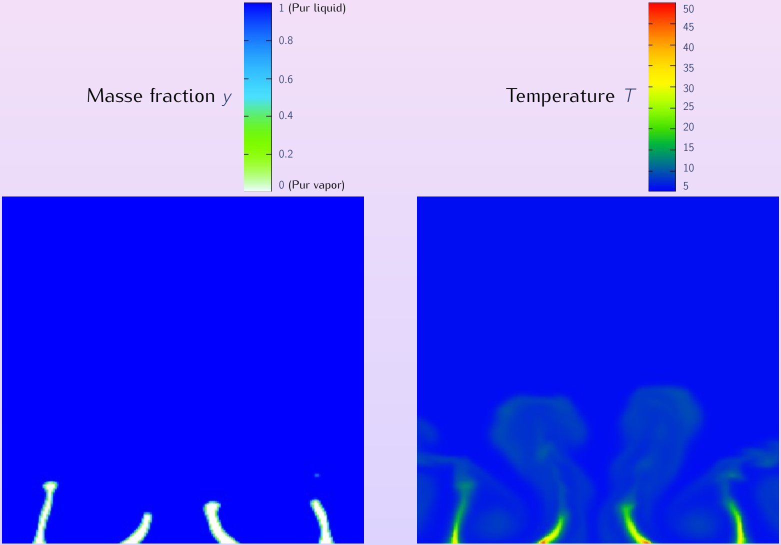

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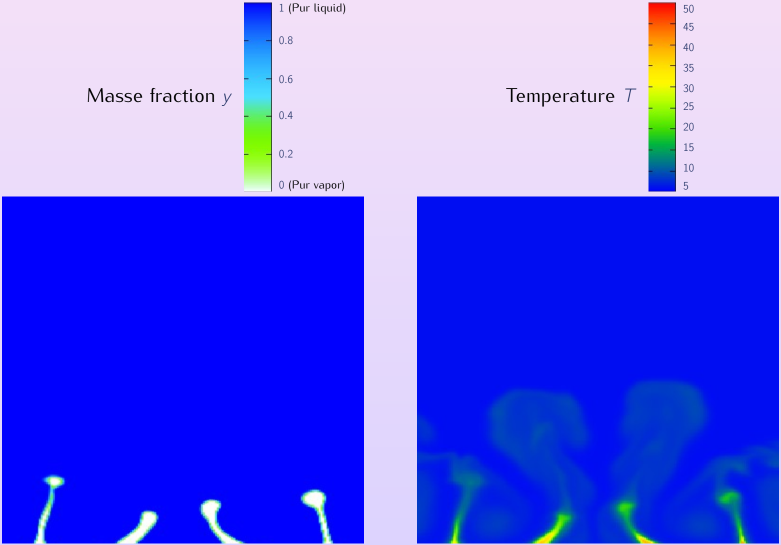

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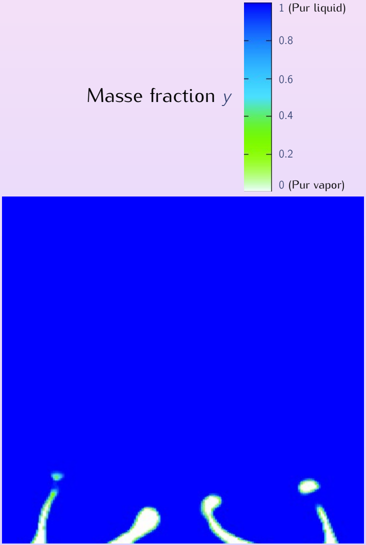
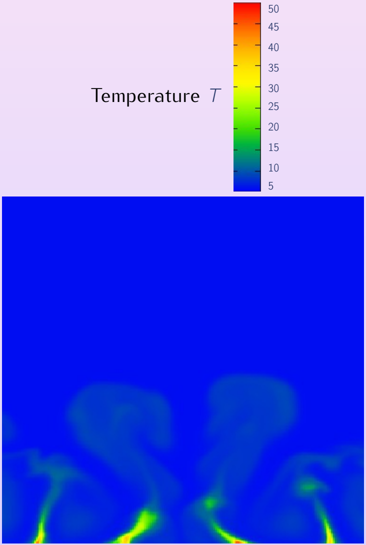
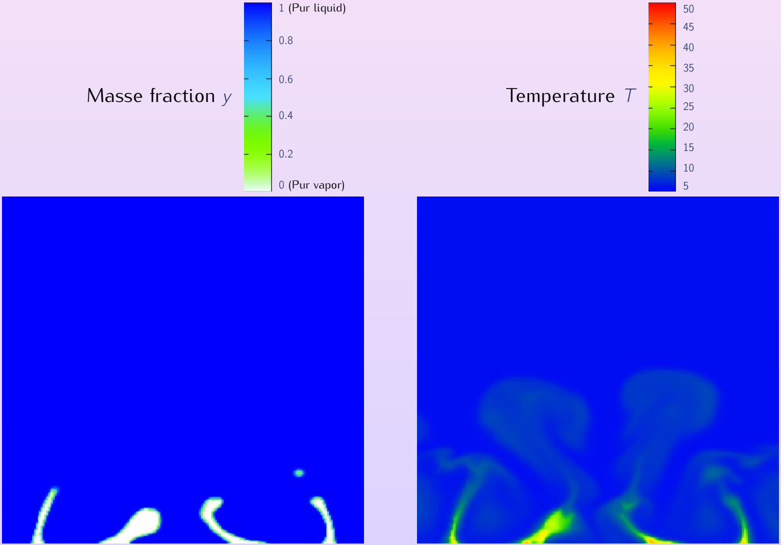




◀ Geometry ▶ Play ⏩ Skip

Transition to a Film Boiling



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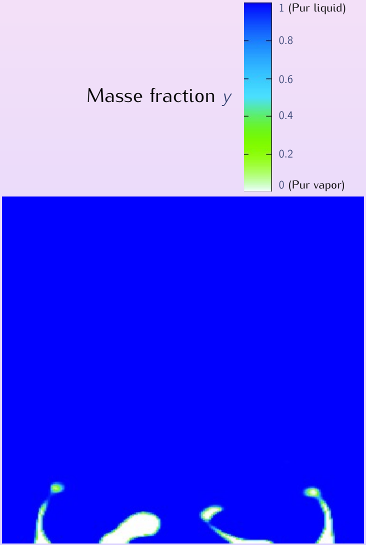

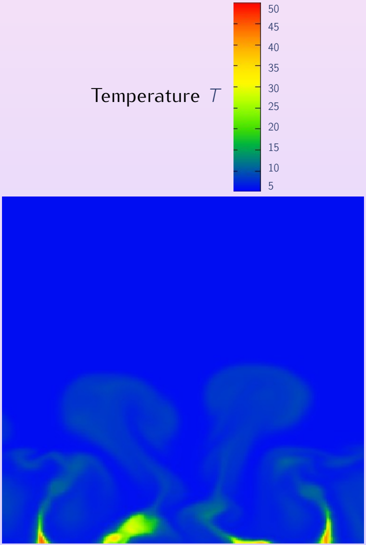

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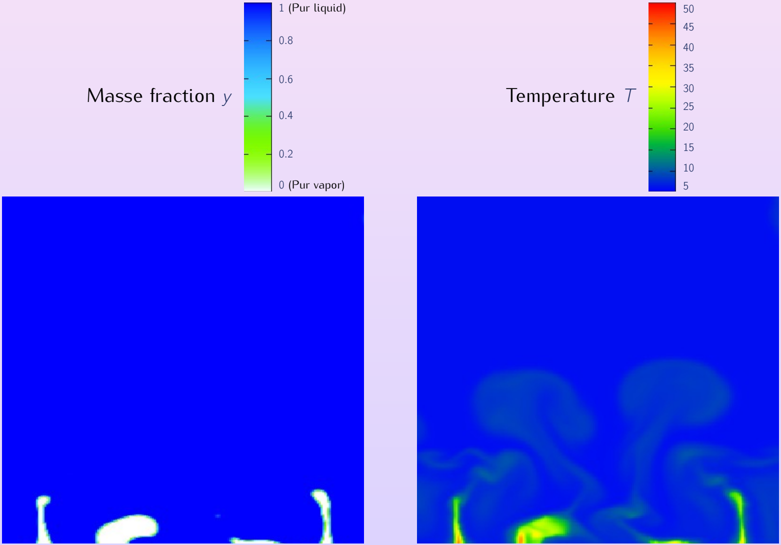

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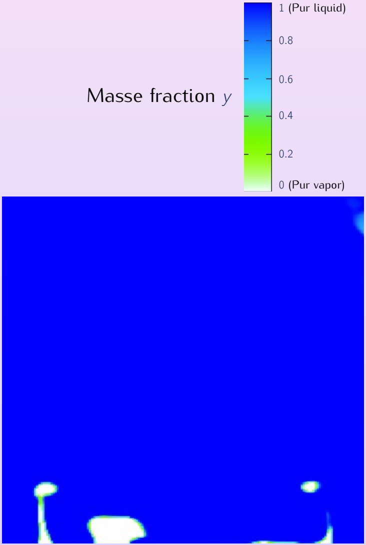

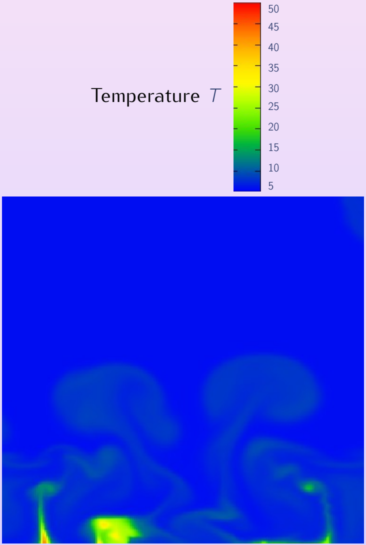

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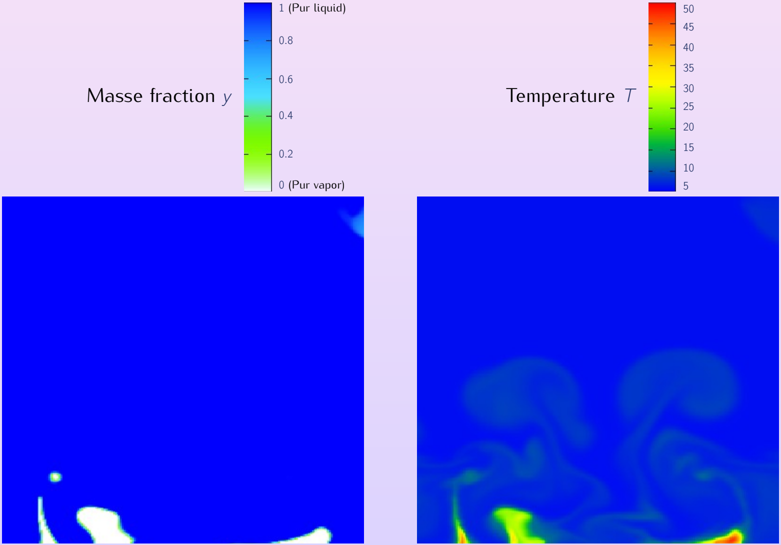

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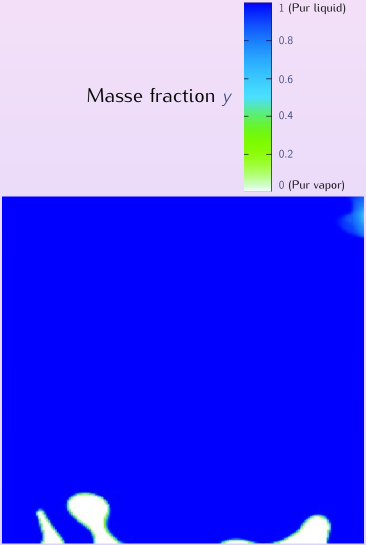

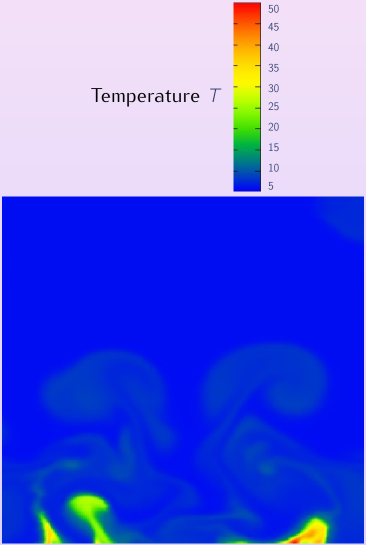

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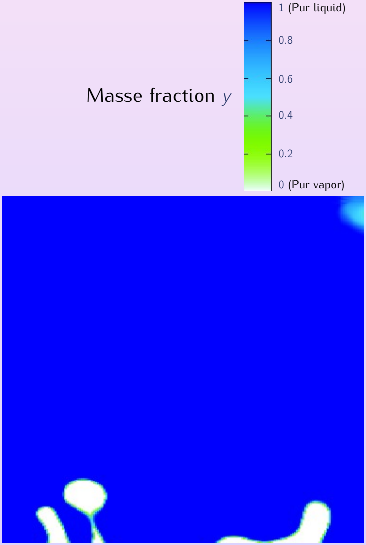

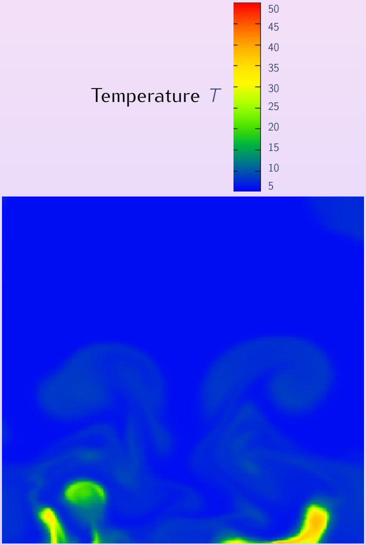

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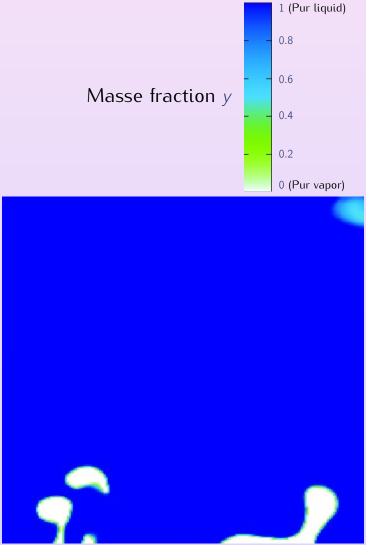

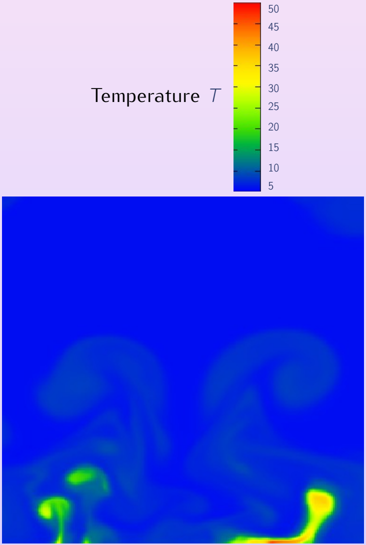

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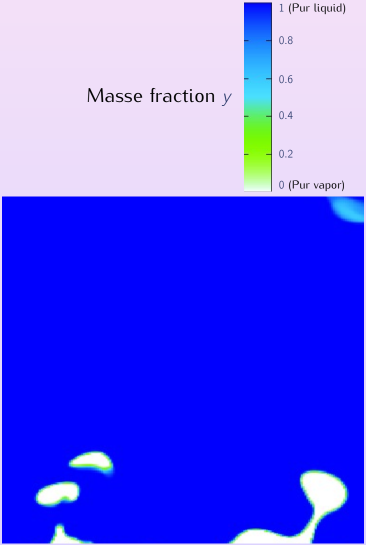

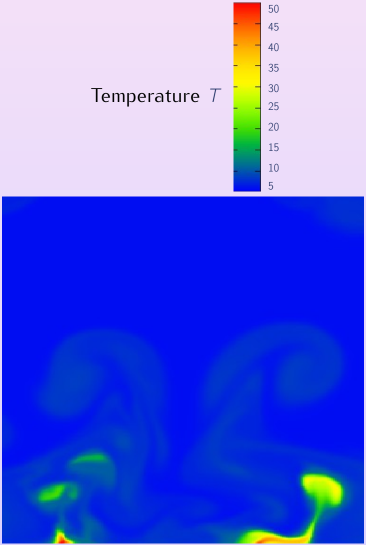

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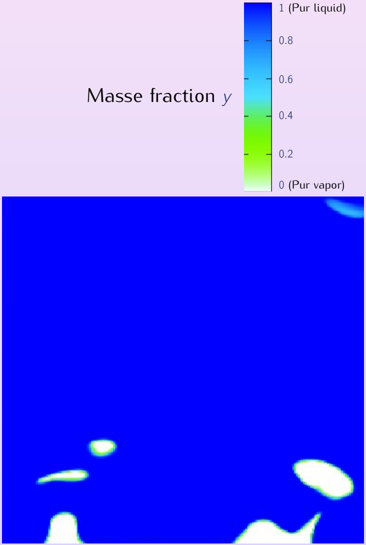

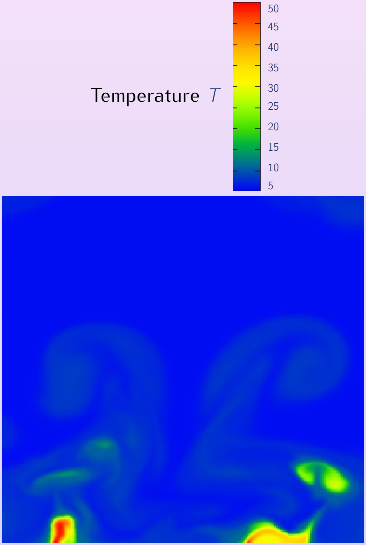

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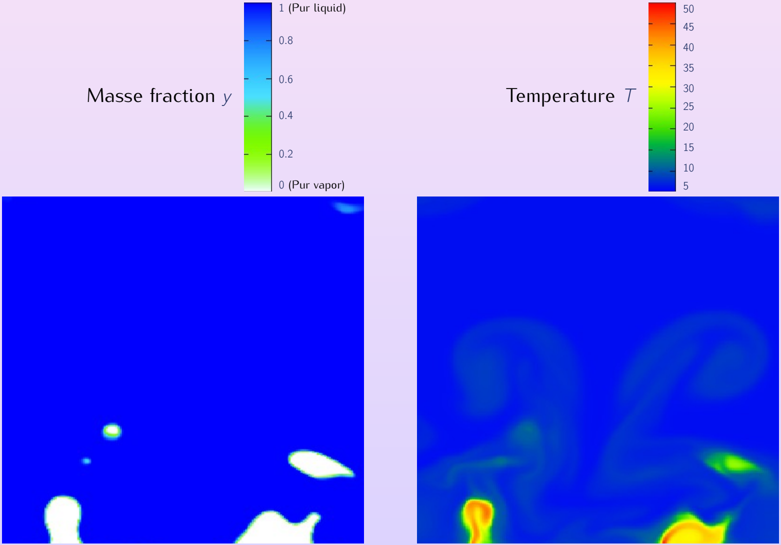

Geometry Play Skip

Outline

1. Context
2. Model
   - Equation of State
   - Conservation Laws
3. Numerical Approximation and Example
   - The Phase Change Equation
   - Numerical Scheme and Example
4. **Conclusion**

Summary & Perspectives

- Model
  - ✓ based on a general construction of the Equilibrium EOS (also for tabulated data),
- Numerical Method based on the relaxation approach: off-equilibrium system with relaxation terms
  - ✓ preliminary results: dynamic generation of a phase in a 2D-flow in a pure phase with surface tension, gravity and heat diffusion,
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  - ✗ quantitative simulations: tabulated EOS for pure phases, implicit transport step (Low Mach) and 3D (parallelization).

Appendix

- Stiffened Gas for Water
- Tabulated EOS for Water
- Speed of Sound
- Isentropic Curves
- Surface Tension
- Metastability
- Critical Point
- Summary & To Do

Stiffened Gas for Water

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
Steam	1040.14	1.43	0	2030.255×10^3	-33265.65947

Table: Parameters proposed by [O. Le Metayer] for water.

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

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

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

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Water Tabulated EOS

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

$\widehat{\varepsilon}_\alpha^{\text{sat}}$ 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

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

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

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

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

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

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

Speed of sound

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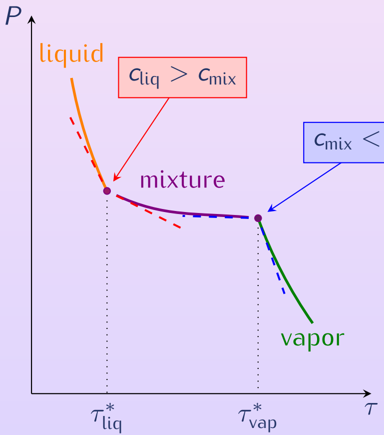
$$\forall \mathbf{w} \text{ equilibrium mixture state, } \mathbf{v}(\mathbf{w}) \overset{?}{\not\asymp} [P^{eq}(\mathbf{w}), -1]$$

Isentropic curves



$$\gamma \stackrel{\text{def}}{=} -\frac{\tau}{P}\left.\frac{\partial P}{\partial \tau}\right|_s$$

$$\Gamma \stackrel{\text{def}}{=} \tau\left.\frac{\partial P}{\partial \varepsilon}\right|_\tau$$

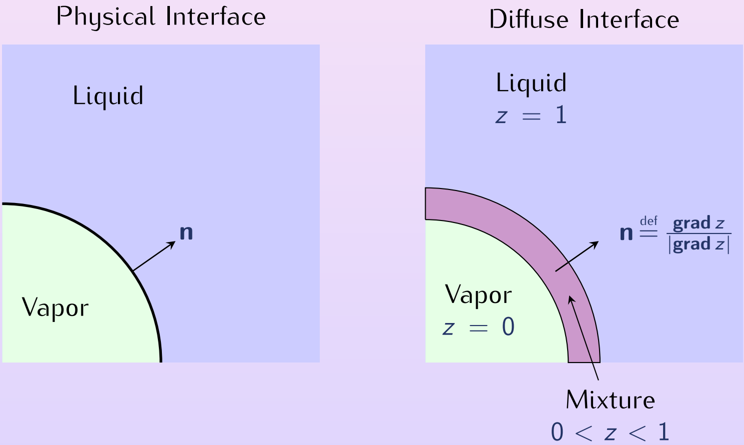
$$\mathfrak{G} \stackrel{\text{def}}{=} \frac{\tau^2}{2\gamma P}\left.\frac{\partial^2 P}{\partial \tau^2}\right|_s$$

- Pure Phases
  - (H) $\gamma > 0$
  - (H) $\Gamma > 0$
  - (H) $\mathfrak{G} > 0$
- Mixture
  - (P) $\gamma > 0$
  - (P) $\Gamma > 0$
  - (H) $\mathfrak{G} > 0$

- Regularity: [J. Correia, P.G. LeFloch, M.D. Thanh]
- Loss of convexity: [A. Voss]

Return

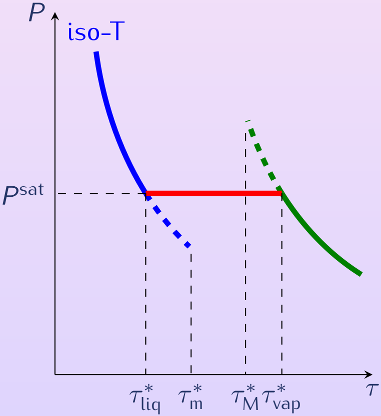
Continuum Surface Force (CSF) Approach



$$\Pi_{\text{tension}} = -\sigma\, \text{div}(\mathbf{n})\mathbf{n}$$

[J.U. Brackbill, D.B. Kothe, C. Zemach]

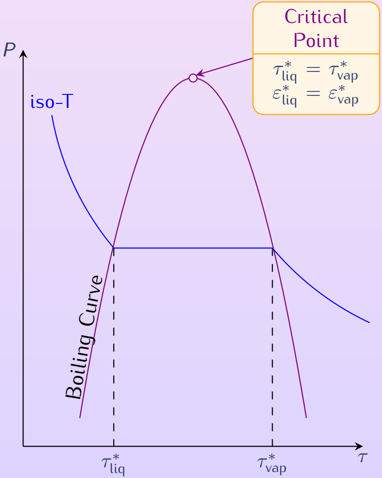
Metastability



$$P^{\text{eq}} = \begin{cases} P_{\text{liq}}, & \text{if } \tau < \tau^*_{\text{liq}}, \\ P^{\text{sat}}, & \text{if } \tau^*_{\text{liq}} < \tau < \tau^*_{\text{vap}}, \\ P_{\text{vap}}, & \text{if } \tau^*_{\text{vap}} < \tau. \end{cases}$$

$$P^{\text{met}} = \begin{cases} P_{\text{liq}}, & \text{if } \tau < \tau^*_{\text{liq}}, \\ [P^{\text{sat}} \text{ or } P_{\text{liq}}], & \text{if } \tau^*_{\text{liq}} < \tau < \tau^*_{\text{m}}, \\ P^{\text{sat}}, & \text{if } \tau^*_{\text{m}} < \tau < \tau^*_{\text{M}}, \\ [P^{\text{sat}} \text{ or } P_{\text{vap}}], & \text{if } \tau^*_{\text{M}} < \tau < \tau^*_{\text{vap}}, \\ P_{\text{vap}}, & \text{if } \tau^*_{\text{vap}} < \tau, \end{cases}$$

Critical Point



Physic

- 2 Pure Phases EOS $(\tau, \varepsilon) \mapsto P_\alpha$
- 1 Saturation EOS $\tau \mapsto P^{sat}$

Eq

EOS

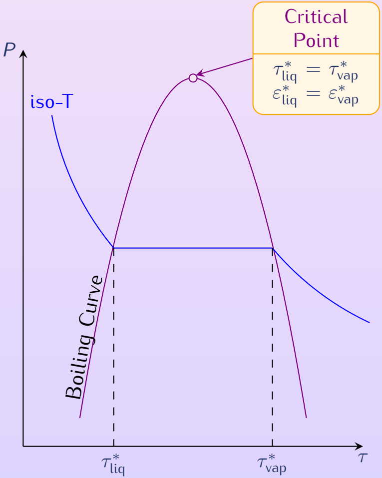
PG $\varepsilon^*_{liq} = \varepsilon^*_{vap} \Leftrightarrow c_{v_{liq}} = c_{v_{vap}}$ (indip. of T)

SG $\left\{\tau_i, P_i^{sat,e}\right\}_i \rightsquigarrow (\tau, \varepsilon) \mapsto P_\alpha \rightsquigarrow \tau \mapsto P^{sat}$

$\tau^*_{liq} = \tau^*_{vap}$ but $\varepsilon^*_{liq} \neq \varepsilon^*_{vap}$

TAB

Critical Point



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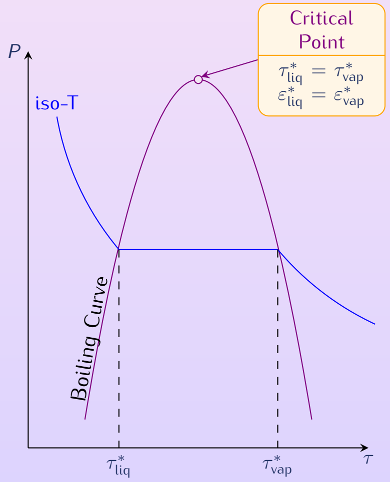

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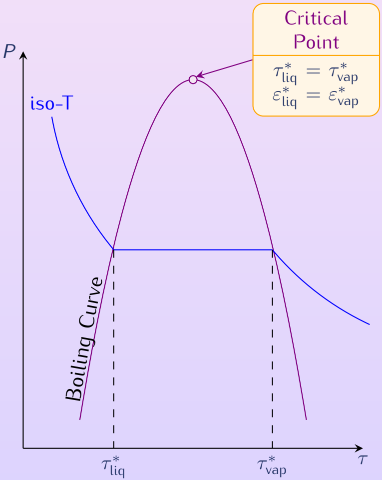
$\{(\tau_i, \varepsilon_i), (P_\alpha^{\text{e}})_i\}_i \rightsquigarrow (\tau, \varepsilon) \mapsto P_\alpha$

Critical Point



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$\{(\tau_i, \varepsilon_i), (P^e_\alpha)_i\}_i \rightsquigarrow (\tau, \varepsilon) \mapsto P_\alpha$

Summary

Phase Change Equation

$$\frac{\tau - \tau_{\text{vap}}^{\text{sat}}}{\tau_{\text{liq}}^{\text{sat}} - \tau_{\text{vap}}^{\text{sat}}} = \frac{\varepsilon - \varepsilon_{\text{vap}}^{\text{sat}}}{\varepsilon_{\text{liq}}^{\text{sat}} - \varepsilon_{\text{vap}}^{\text{sat}}}$$

with

$$T \mapsto \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha^{\text{sat}} (T) = \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha (T, P^{\text{sat}}(T))$$

or

$$P \mapsto \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha^{\text{sat}} (P) = \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha (T^{\text{sat}}(P), P)$$

Summary

How to compute saturation functions τ_α^{sat} and $\varepsilon_\alpha^{\text{sat}}$

- Analytical EOS: we compute the saturation functions τ_α^{sat} and $\varepsilon_\alpha^{\text{sat}}$ by the Coexistence Curve:
  - Exact: $T \mapsto P^{\text{sat}}(T)$ or $P \mapsto T^{\text{sat}}(P)$

$$\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(P) = \begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha (T^{\text{sat}}(P), P) \qquad \text{e.g. Simplified Stiffened Gases}$$

  - Approximated: $T \mapsto \widehat{P}^{\text{sat}}(T) \approx P^{\text{sat}}(T)$

$$\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T) \approx \begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha (T, \widehat{P}^{\text{sat}}(T)) \qquad \text{e.g. General Stiffened Gases}$$

- Tabulated EOS: the saturation functions τ_α^{sat} and $\varepsilon_\alpha^{\text{sat}}$ are given by experiments and we set

$$\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T \text{ or } P) \approx \begin{pmatrix}\widehat{\tau}\\ \widehat{\varepsilon}\end{pmatrix}_\alpha^{\text{sat}}(T \text{ or } P)$$

To Do

	EOS		Simulation		
	Pure Phases	Equilibrium	Cavitation	Boiling	Film
Virtual Fluid (SG)	✓	✓	✓	✓	①
Real Fluid (SG)	✓	✓	✓	②	③
Tabulated	④	✓	⑤	⑥	⑦