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MODELLING AND SIMULATION OF LIQUID-VAPOR PHASE TRANSITION

A CONTRIBUTION TO THE STUDY OF THE BOILING CRISIS

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Outline

- 1 **Context**
- 2 **Model**
- 3 **Numerical Approximation**
- 4 **Numerical Examples**
- 5 **Conclusion**

Outline

1 Context

2 Model

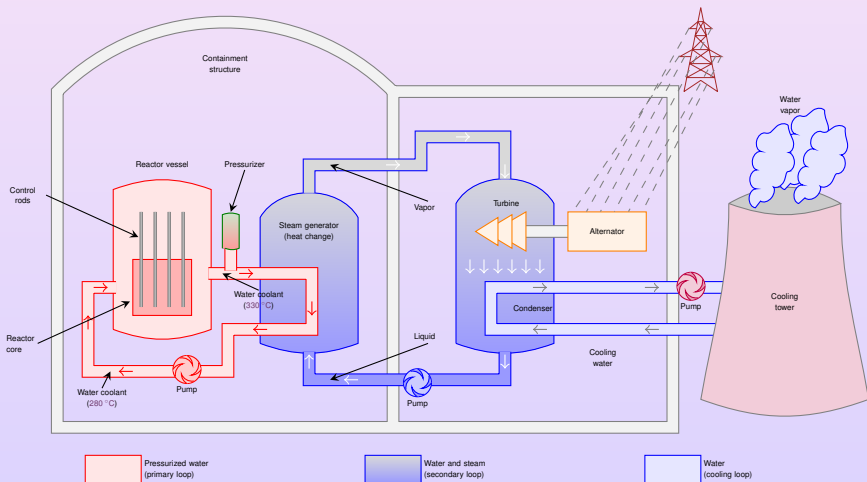
- Equation of State WITHOUT Phase Change
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- The Phase Change Equation
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3 Numerical Approximation

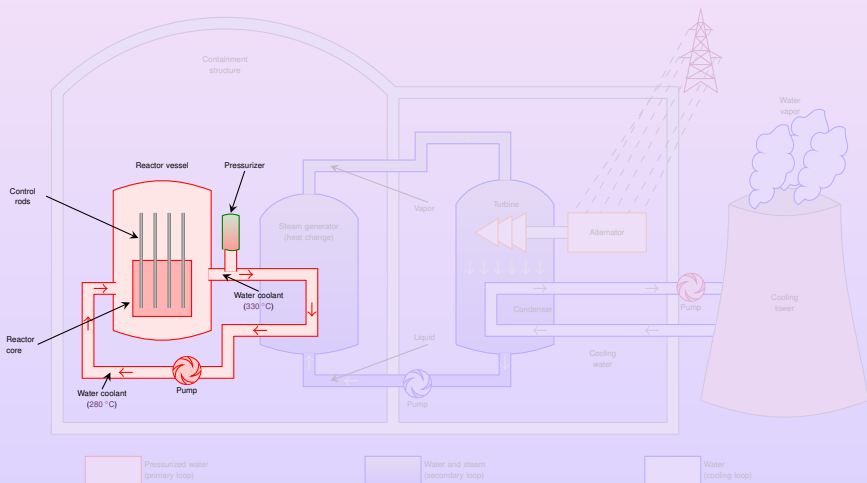
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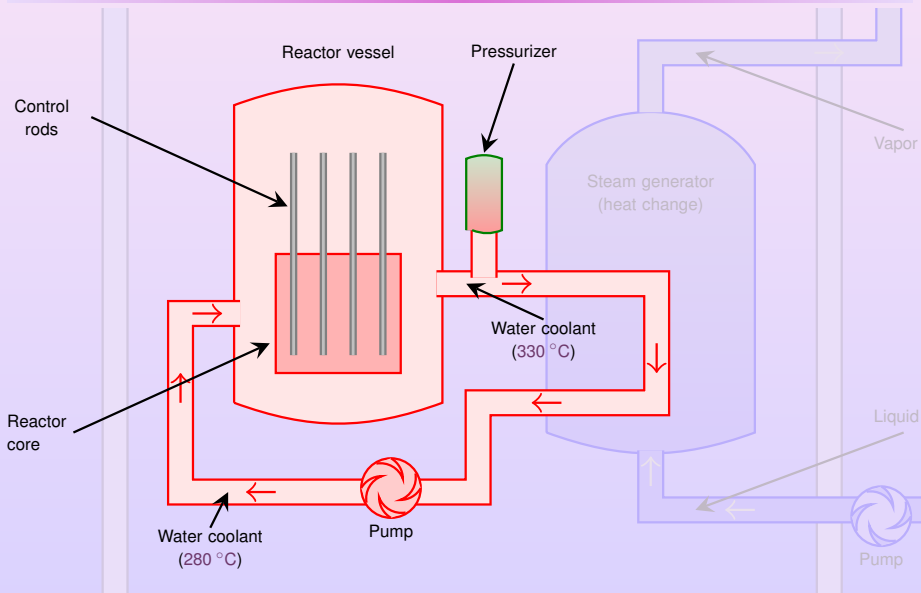
Pressurized Water Reactor



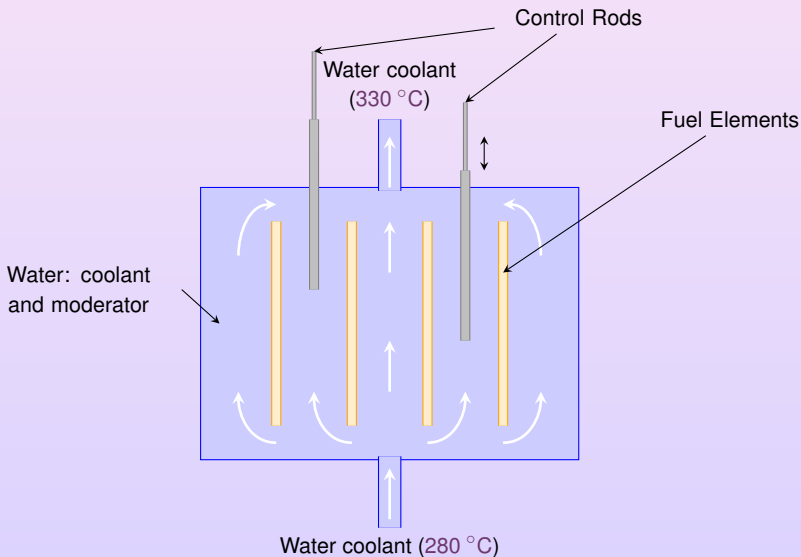
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Pressurized Water Reactor



Core of a Pressurized Water Reactor

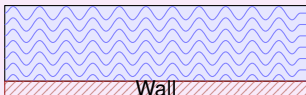


Boiling Crisis

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**.

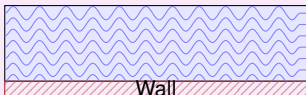


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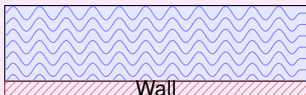
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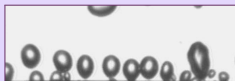
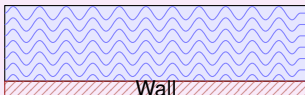
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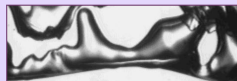
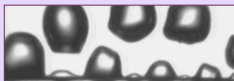
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OMEGA - CEA Grenoble



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- Equation of State WITHOUT Phase Change
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“Ingredients” of the Model

✓ Simulating all bubbles,

- System of PDEs for the fluid flow (monophasic or diphasic),
- Phase transition (pressure and/or temperature variations),
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Euler System

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

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

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

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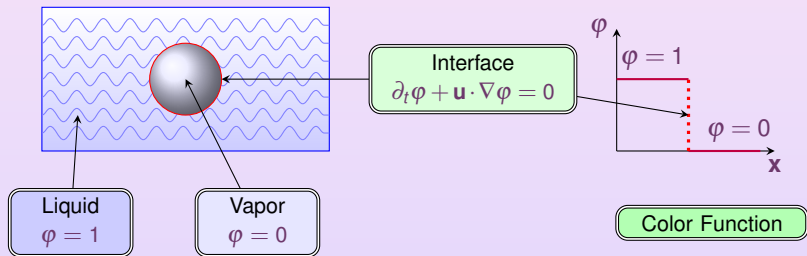
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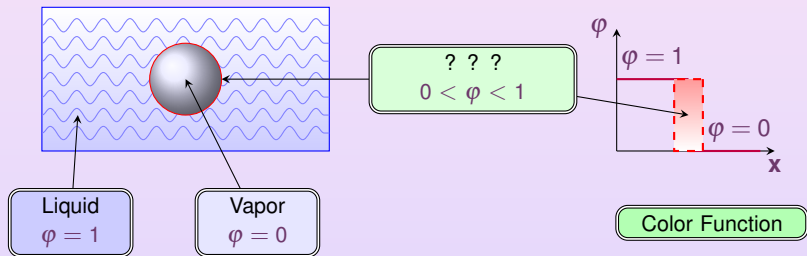
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Liquid-Vapor Interface



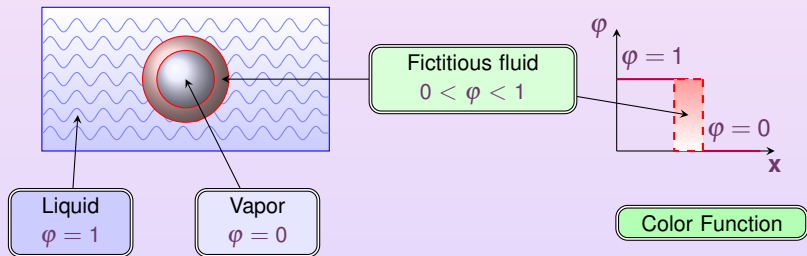
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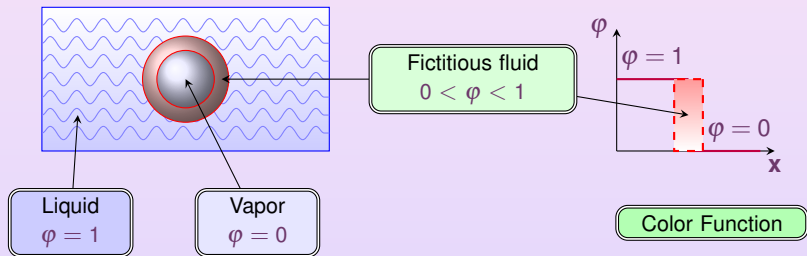
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Liquid-Vapor Interface



➡ Goal: define a global pressure law such that

- $(\rho, \varepsilon, \mathbf{u}, P)$ are continuous (3 zones)
- the interface position and the phase change are implicit (i.e. $\nabla \phi$)
- coherence with classical thermodynamics [H. CALLEN]

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

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

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

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- $\mathbf{w} \stackrel{\text{def}}{=} y\mathbf{w}_1 + (1 - y)\mathbf{w}_2$;
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EOS with Phase Change

ENTROPY WITHOUT PH.CH.

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



ENTROPY AT EQUILIBRIUM

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

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

Solution: (z^*, y^*, ψ^*)

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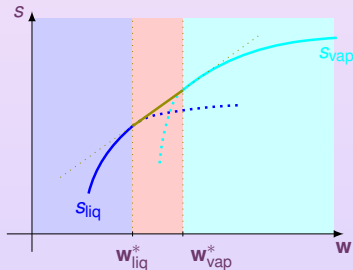
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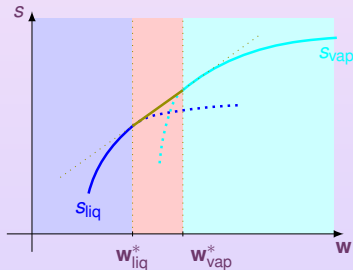
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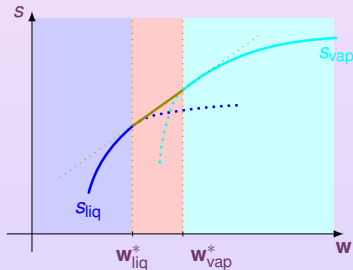
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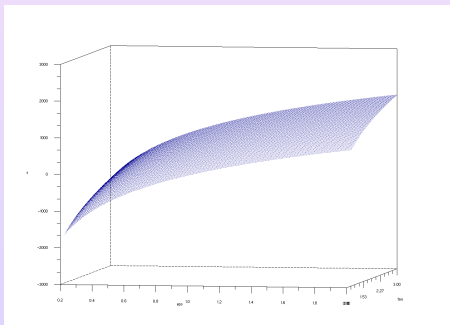
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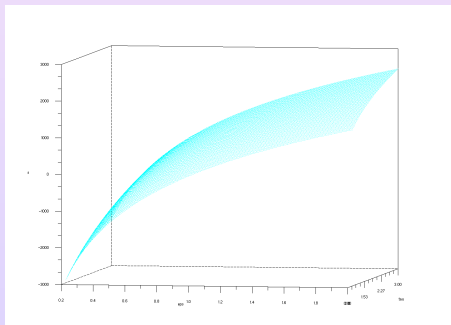
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Concave Hull with two Perfect Gases

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

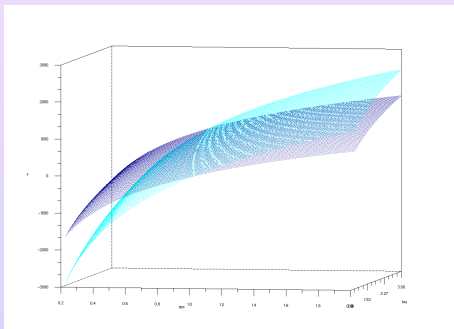


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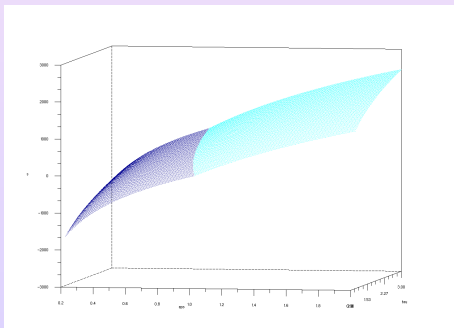
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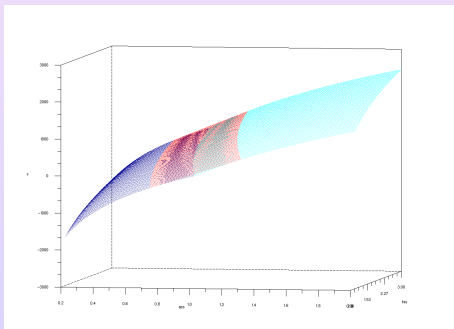
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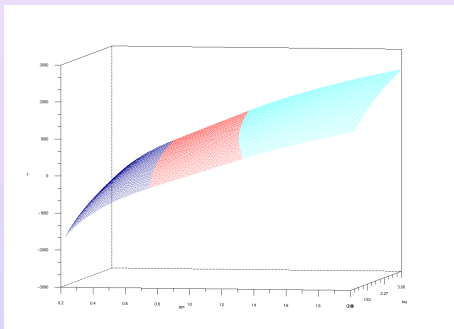
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From $\mathbf{w} \mapsto \mathbf{s}^{\text{eq}}$ to $\mathbf{w} \mapsto P^{\text{eq}}$

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

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

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

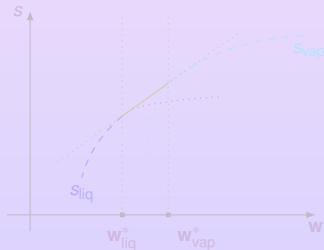
$$\mathbf{s}^{\text{eq}}(\tilde{\mathbf{w}}) = y^* \mathbf{s}_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1-y^*) \mathbf{s}_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

$$P^{\text{eq}}(\tilde{\mathbf{w}}) = P_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}^*);$$

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

$$\mathbf{s}^{\text{eq}}(\tilde{\mathbf{w}}) = \max\{\mathbf{s}_{\text{liq}}(\tilde{\mathbf{w}}), \mathbf{s}_{\text{vap}}(\tilde{\mathbf{w}})\},$$

$$P^{\text{eq}}(\tilde{\mathbf{w}}) = P_{\text{liq}}(\tilde{\mathbf{w}})$$



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

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

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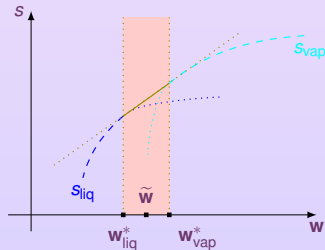
$$s^{\text{eq}}(\tilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1-y^*) s_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

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

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

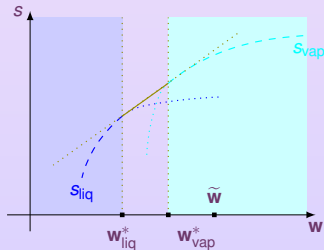
$$\mathbf{s}^{\text{eq}}(\tilde{\mathbf{w}}) = y^* \mathbf{s}_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1-y^*) \mathbf{s}_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

$$P^{\text{eq}}(\tilde{\mathbf{w}}) = P_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}^*);$$

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

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

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

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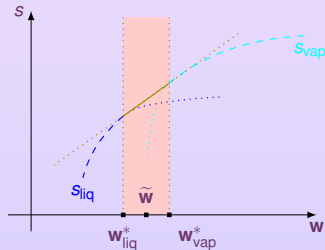
$$s^{\text{eq}}(\tilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1-y^*) s_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

$$P^{\text{eq}}(\tilde{\mathbf{w}}) = P_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}^*);$$

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

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

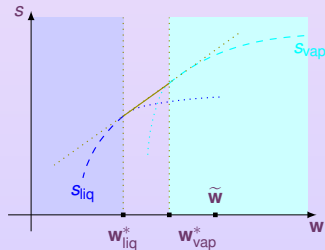
$$s^{\text{eq}}(\tilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1-y^*) s_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

$$P^{\text{eq}}(\tilde{\mathbf{w}}) = P_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}^*);$$

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Summary of the Model

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

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

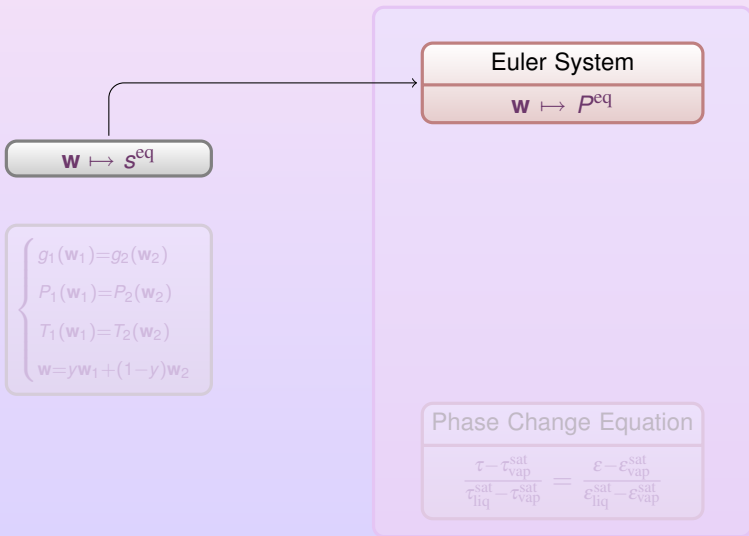
Euler System

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

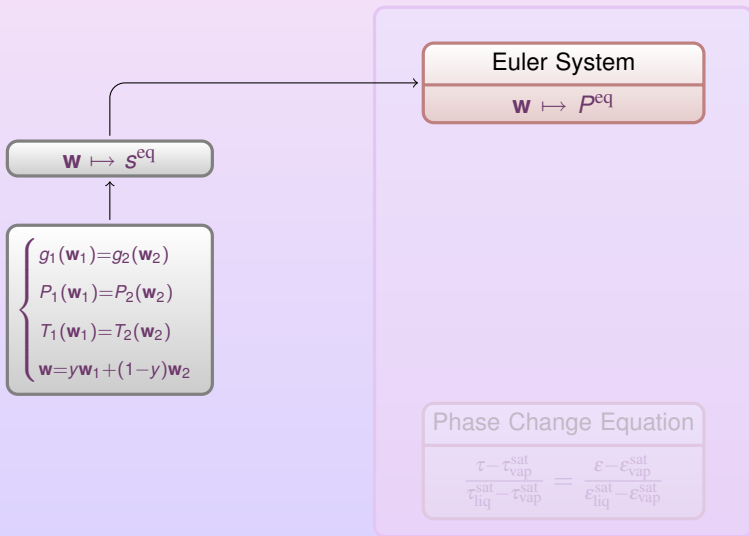
Phase Change Equation

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

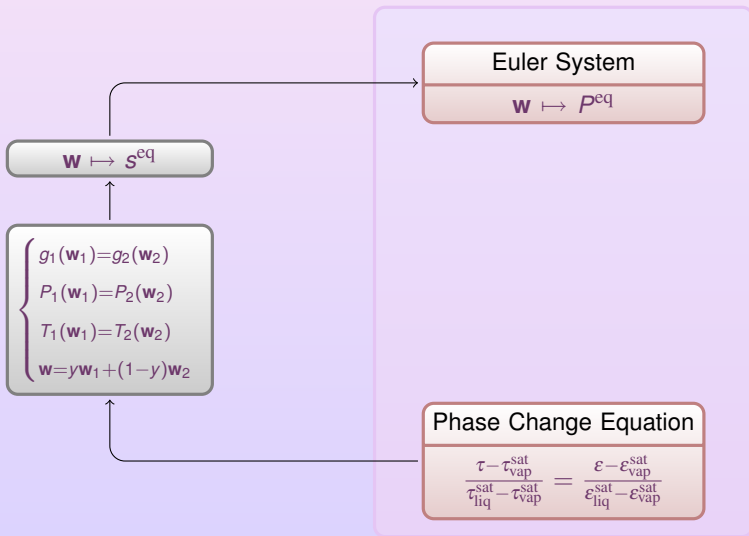
Summary of the Model



Summary of the Model



Summary of the Model



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

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

Outline

1 Context

2 Model

- Equation of State WITHOUT Phase Change
- Equation of State WITH Phase Change
- **The Phase Change Equation**
- Conservation Laws

3 Numerical Approximation

4 Numerical Examples

5 Conclusion

Analytical EOS

(τ, ε) fixed

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

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

(P, T) SOLUTION OF

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

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

T SOLUTION OF

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

→ more examples

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

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

→ More Examples

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

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

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

→ next example

Analytical EOS

(τ, ε) fixed

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

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

(P, T) SOLUTION OF

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

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

T SOLUTION OF

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

→ next lecture

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

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

least square approximation

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

T SOLUTION OF

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

► Water Example

Tabulated EOS

T (K)	P^{sat} (MPa)	Volume (m^3/kg)		Internal Energy (kJ/kg)	
		$\tau_{\text{liq}}^{\text{sat}}$	$\tau_{\text{vap}}^{\text{sat}}$	$\epsilon_{\text{liq}}^{\text{sat}}$	$\epsilon_{\text{vap}}^{\text{sat}}$
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

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

\rightsquigarrow

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

★ Water Examples

Tabulated EOS

(τ, ε) fixed

T SOLUTION OF

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

$\}} \leftarrow$

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

least square approximations

★ Water Examples

Tabulated EOS

(τ, ε) fixed

T SOLUTION OF

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

$\}} \leftarrow$

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

least square approximations

▶▶ Water Examples

Phase Change Equation: 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

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

Phase Change Equation: 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 $P \mapsto T^{\text{sat}}(P)$

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

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

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

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

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

Outline

1 Context

2 Model

- Equation of State WITHOUT Phase Change
- Equation of State WITH Phase Change
- The Phase Change Equation
- **Conservation Laws**

3 Numerical Approximation

4 Numerical Examples

5 Conclusion

Dynamic Liquid-Vapor Phase Change

EULER SYSTEM

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

PROPERTIES

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

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

- ① Euler system: strict hyperbolicity (\neq p-system),
- ② Riemann problem: multitude of entropy (Lax) solutions [R. MENIKOFF, B. J. PLOHR], uniqueness of Liu solution.

Dynamic Liquid-Vapor Phase Change

EULER SYSTEM

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Outline

1 Context

2 Model

- Equation of State WITHOUT Phase Change
- Equation of State WITH Phase Change
- The Phase Change Equation
- Conservation Laws

3 Numerical Approximation

4 Numerical Examples

5 Conclusion

How to simulate the “Liu solution”

- Exact Riemann Solver
like [A. VOSS] for Van der Waals EOS
- Viscous Solver (the Liu solution is the only solution that has a viscous profile)
like [S. JAOUEN] for Perfect Gas EOS with $c_{V_{liq}} = c_{V_{vap}}$
- 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],
[R. ABGRALL, R. SAUREL],
[V. GUILLEMAUD, J.-M. HÉRARD, S. KOKH],
...

Relaxation Approach

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

Relaxation Approach

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

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HOW TO BUILD THE AUGMENTED SYSTEM

1 Lagrangian:

$$\mathcal{L}(\rho, \mathbf{u}, \sigma, y, z, \psi) \stackrel{\text{def}}{=} \rho \left(\frac{|\mathbf{u}|^2}{2} - \varepsilon(\rho, \sigma, y, z, \psi) \right)$$

Action:

$$\mathcal{A}(\mathbf{v}) \stackrel{\text{def}}{=} \int_{t_1}^{t_2} \int_{\hat{\Omega}(t; \mathbf{v})} \mathcal{L}(\hat{\rho}, \hat{\rho} \mathbf{u}, \hat{s}, \hat{y}, \hat{z}, \hat{\psi})(\hat{\mathbf{x}}, t; \mathbf{v}) d\hat{\mathbf{x}} dt$$

Minimization of the Action: $\frac{d\mathcal{A}}{d\mathbf{v}}(\mathbf{v} = 0) = 0$

2 Energy: $\varepsilon \stackrel{\text{def}}{=} \sum_{\alpha} y_{\alpha} \varepsilon_{\alpha} \left(\frac{z_{\alpha}}{y_{\alpha}} \frac{1}{\rho}, \frac{\psi_{\alpha}}{y_{\alpha}} \sigma \right)$

3 Positive Entropy Production: $D_t \sigma \geq 0$

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

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In the interface

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

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Formally
 $\mu_j \rightarrow 0$

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NOTE: we can replace an EDP by an algebraic closure, for example

~~$$\partial_t \psi + \mathbf{u} \cdot \operatorname{grad} \psi = \frac{1}{\mu_\psi} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \varepsilon \rightsquigarrow T_1 = T_2.$$~~

Numerical Scheme

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

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

$$\textcircled{1} \mu_j \rightarrow +\infty$$



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

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

Aug. System: 5-eq. iso-T
 Num. Scheme: op. splitting
 $\partial_t \mathbf{V} + \operatorname{div} \mathbf{G}(\mathbf{V}) = 0$ [G. ALLAIRE and all.]
 $\mathbf{S}(\mathbf{V}) = \mathbf{S}_{\text{at}}(\mathbf{V}) + \mathbf{S}_{\text{trans}}(\mathbf{V}) + \mathbf{S}_{\text{p}}(\mathbf{V})$
 $\partial_t \mathbf{V} - \mathbf{S}_{\text{at}}(\mathbf{V})$ [J. U. BRACKBILL and all.]
 $\partial_t \mathbf{V} - \mathbf{S}_{\text{trans}}(\mathbf{V})$ 2D implicit
 $\partial_t \mathbf{V} - \mathbf{S}_{\text{p}}(\mathbf{V})$ Euler

update fractions
 (y, z, ψ)
 solving the
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 Equation

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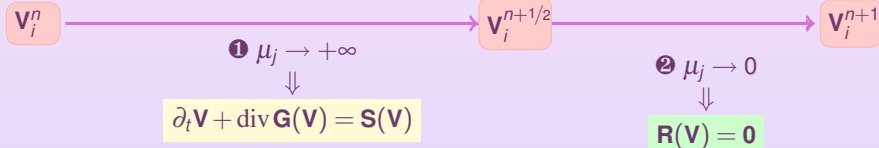
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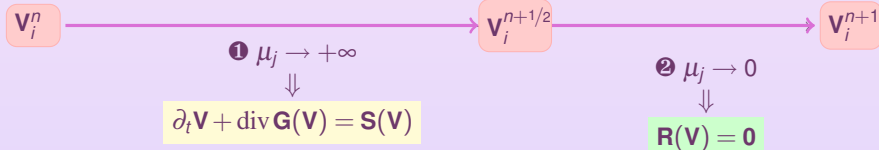
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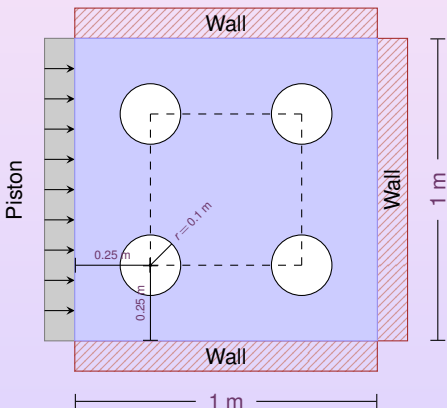
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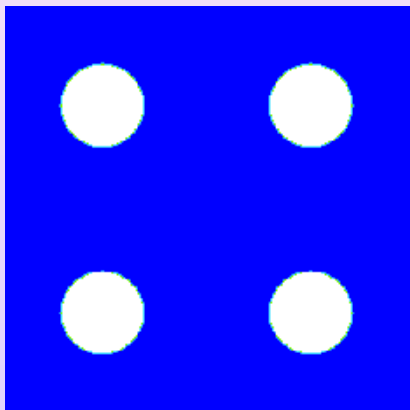
Compression of Vapor Bubbles



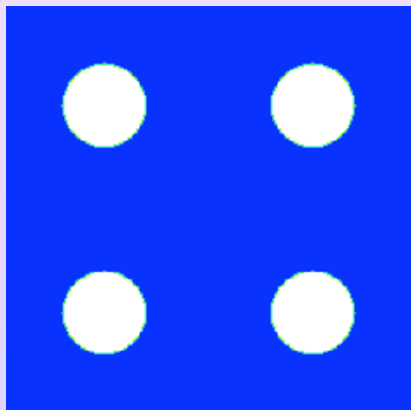
Compression of 4 Vapor Bubbles involving two Stiffened Gases for water and steam. The piston moves towards right at constant speed $u_p = 30 \text{ m/s}$.

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



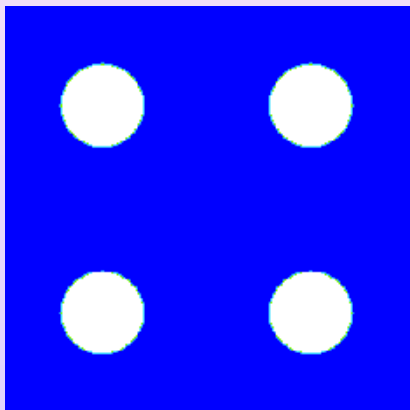
◀ Geometry

▶ Play

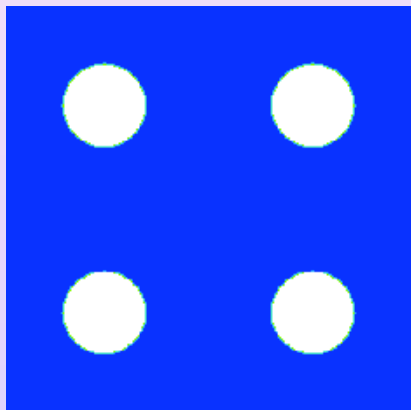
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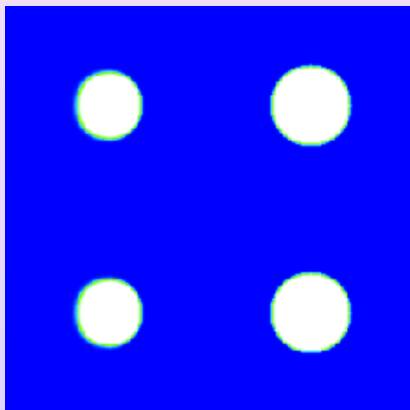
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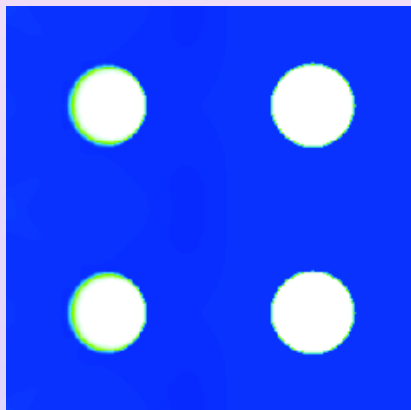
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Compression of Vapor Bubbles

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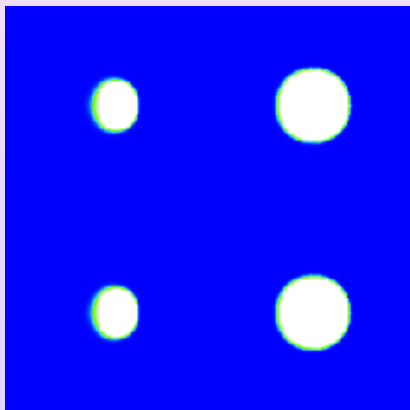
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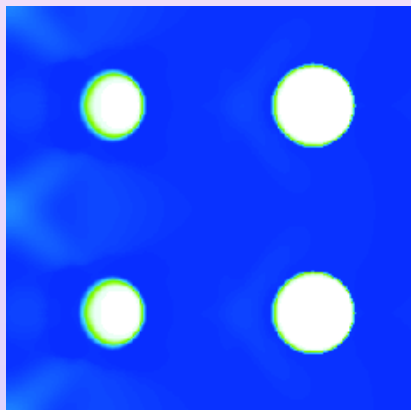
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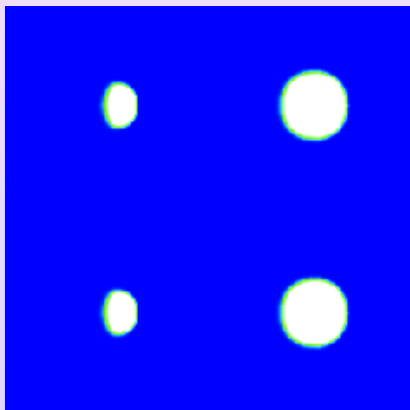
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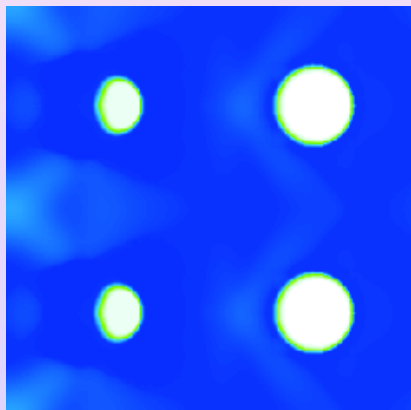
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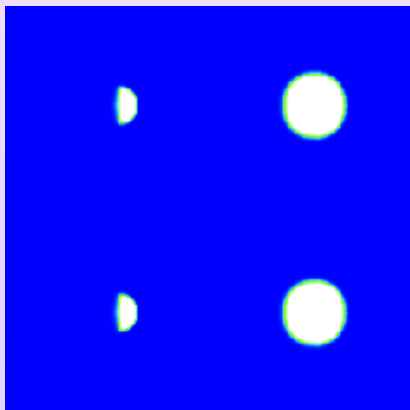
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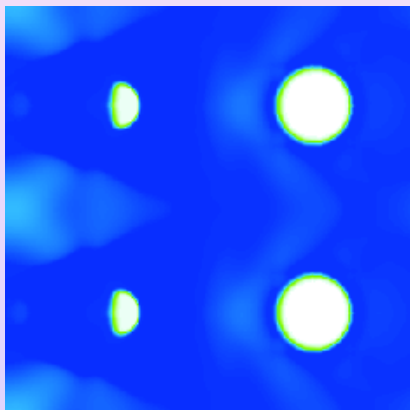
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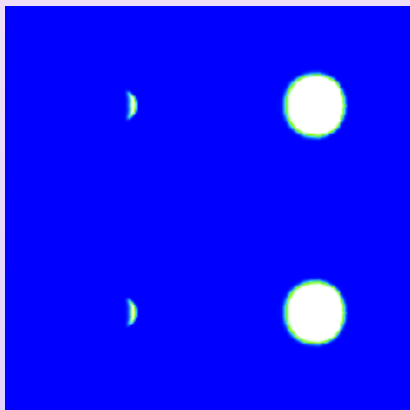
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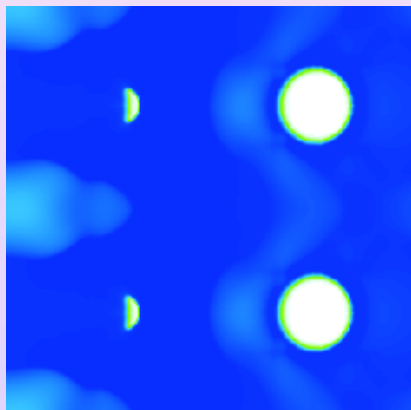
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Mass Fraction y



Density ρ



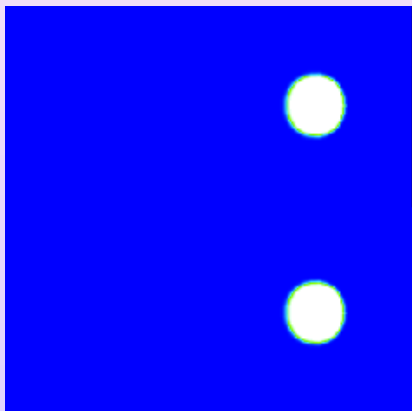
◀ Geometry

▶ Play

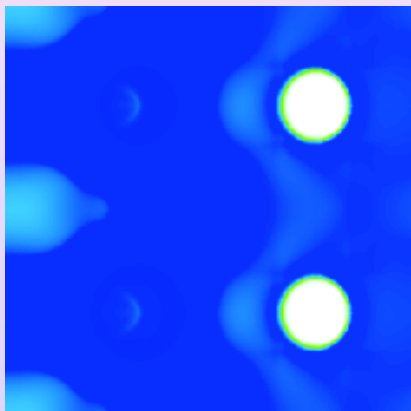
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



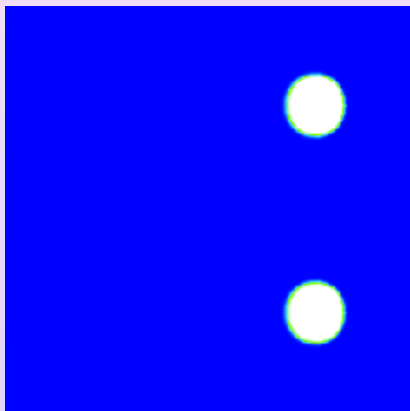
◀ Geometry

▶ Play

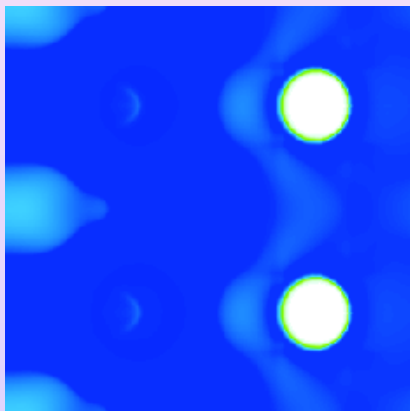
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



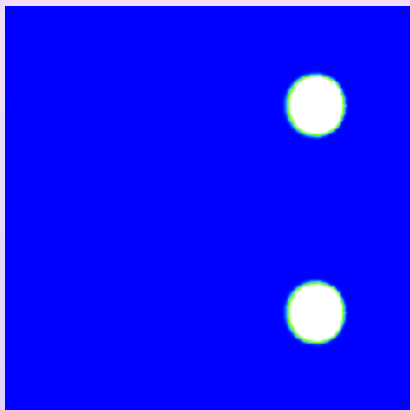
◀ Geometry

▶ Play

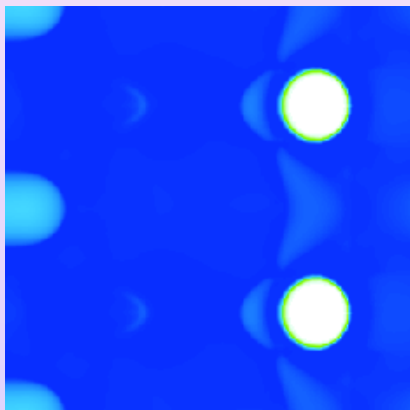
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



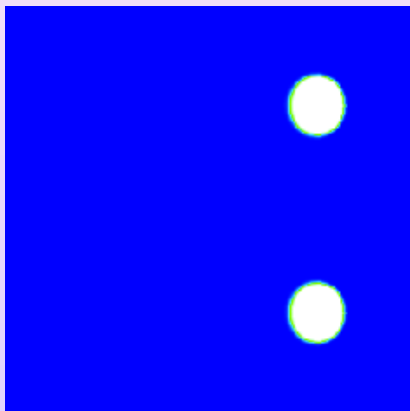
◀ Geometry

▶ Play

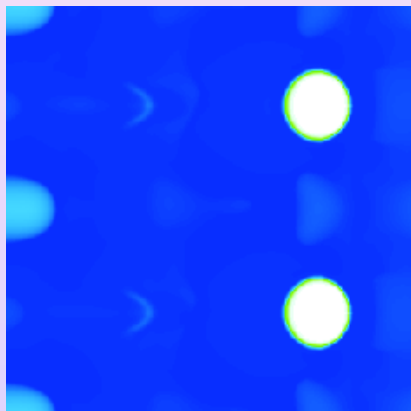
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



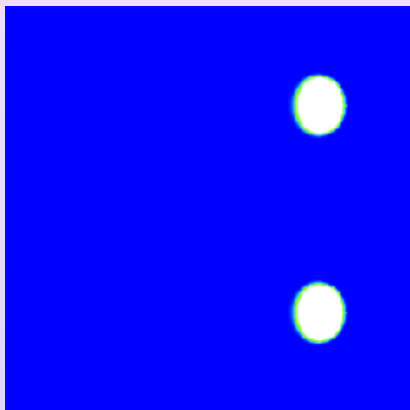
◀ Geometry

▶ Play

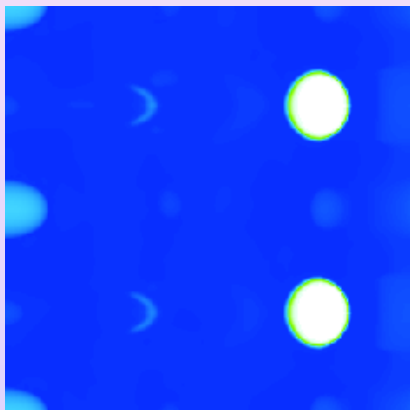
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



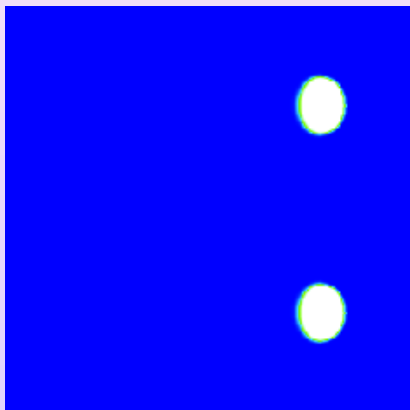
◀ Geometry

▶ Play

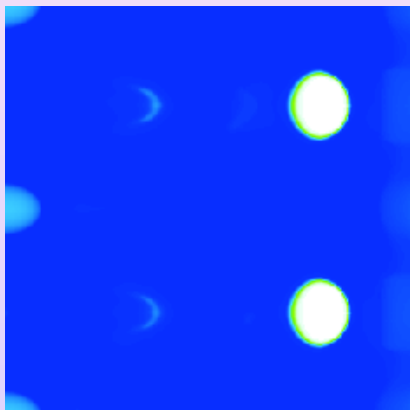
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



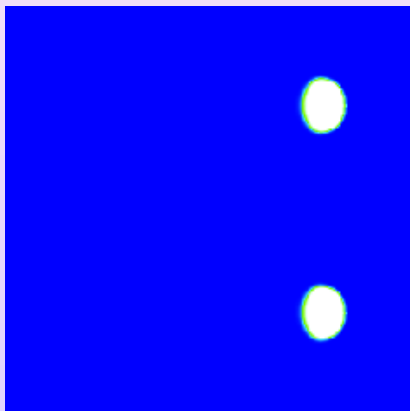
◀ Geometry

▶ Play

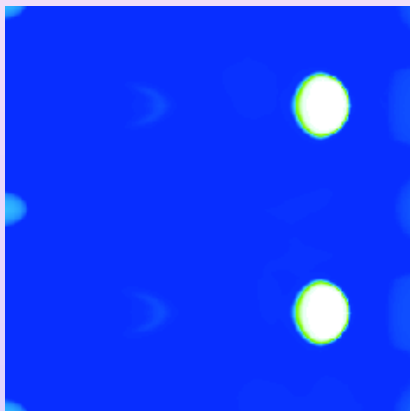
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



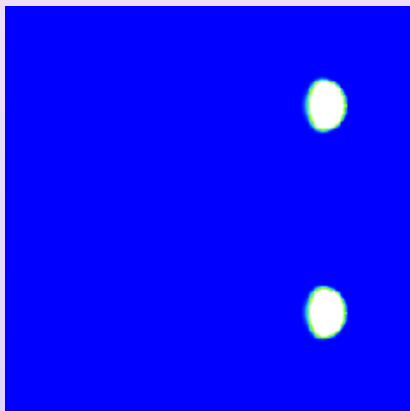
◀ Geometry

▶ Play

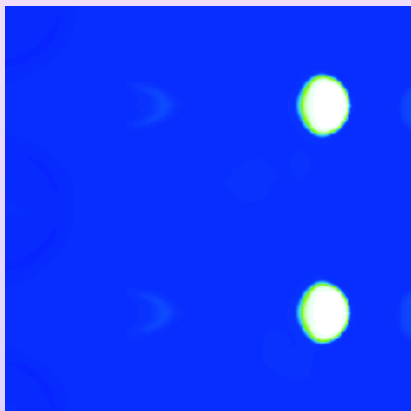
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



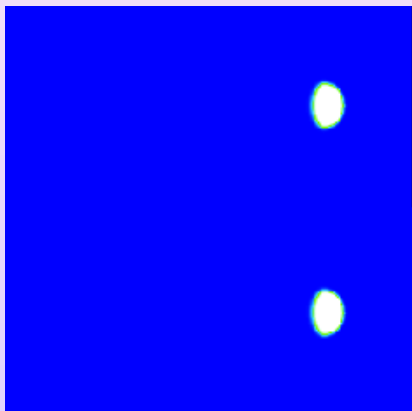
◀ Geometry

▶ Play

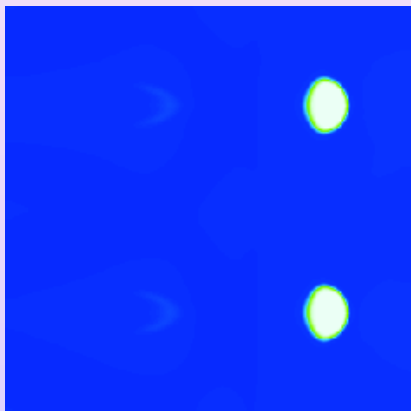
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



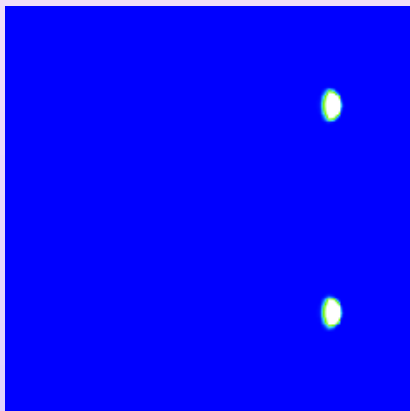
◀ Geometry

▶ Play

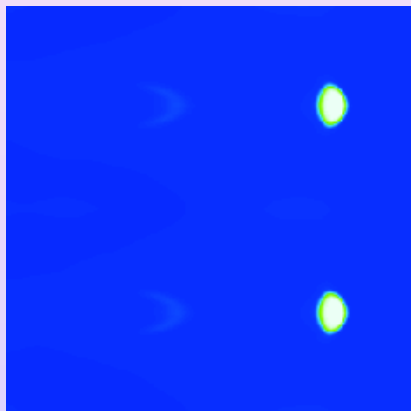
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



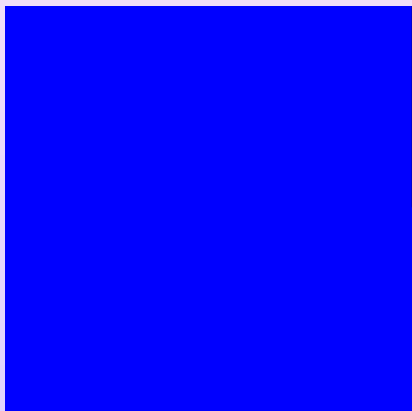
◀ Geometry

▶ Play

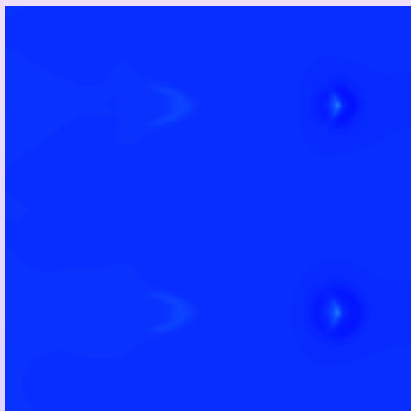
▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



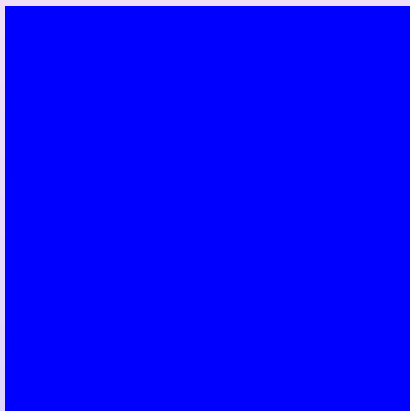
◀ Geometry

▶ Play

▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



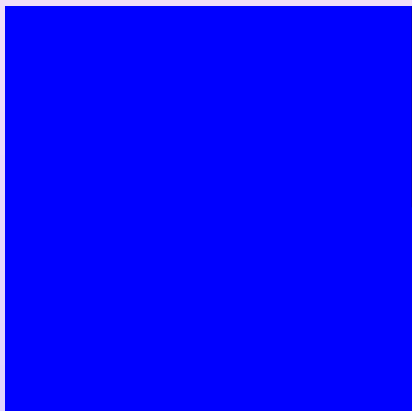
◀ Geometry

▶ Play

▶▶ Skip

Compression of Vapor Bubbles

Mass Fraction y



Density ρ



◀ Geometry

▶ Play

▶▶ Skip

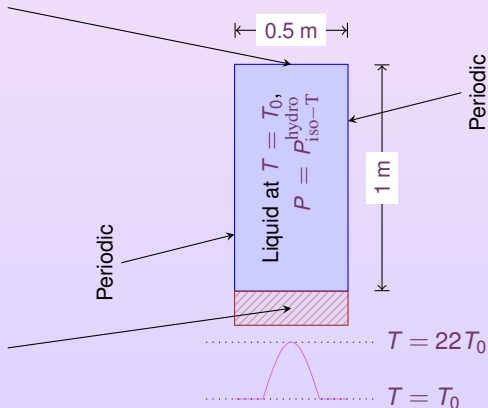
Nucleating Bubble

Pressure and
temperature
imposed

$$P = P^{\text{ref}} > P^{\text{sat}}(T_0),$$

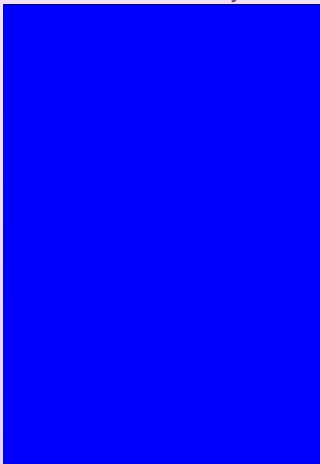
$$T = T_0$$

Wall,
temperature imposed

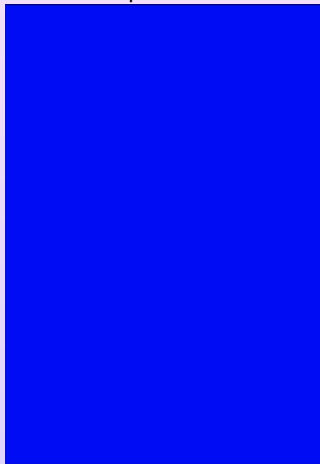


Nucleating Bubble

Mass Fraction y



Temperature T



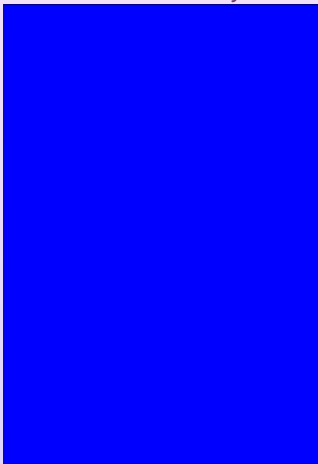
◀ Geometry

▶ Play

▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



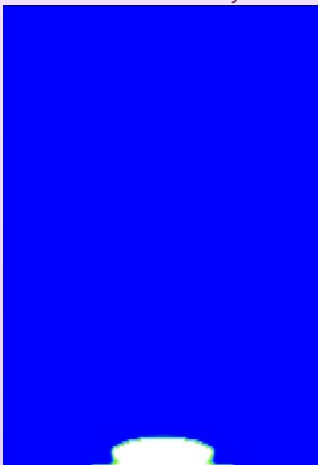
◀ Geometry

▶ Play

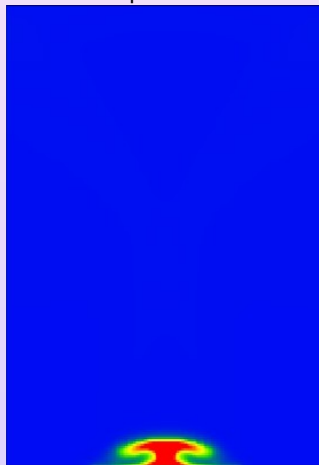
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



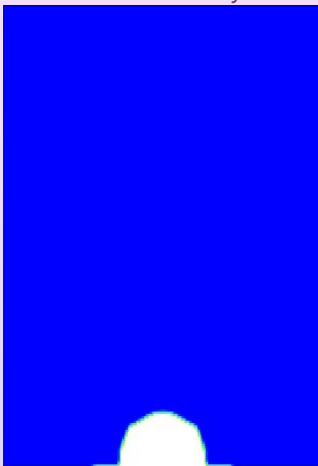
◀ Geometry

▶ Play

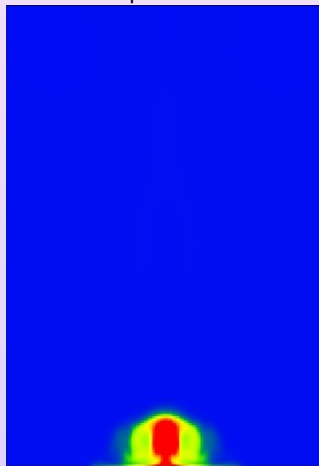
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



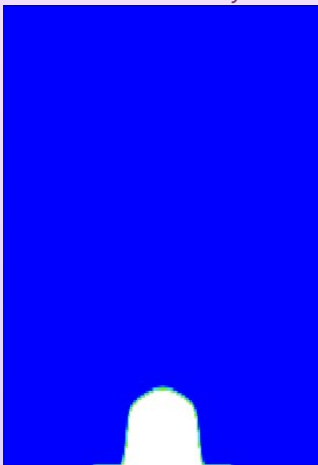
◀ Geometry

▶ Play

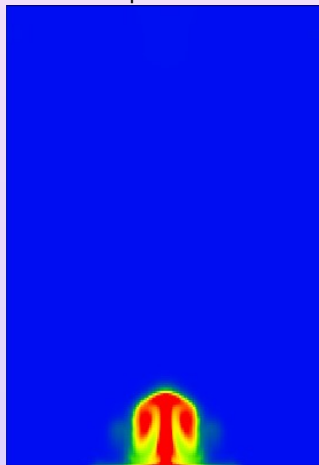
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



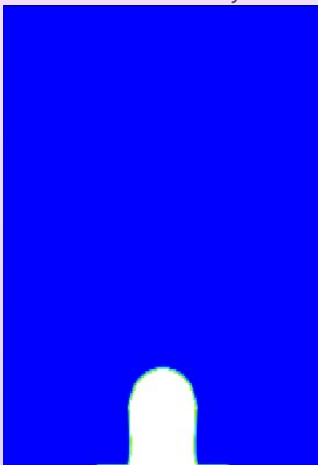
◀ Geometry

▶ Play

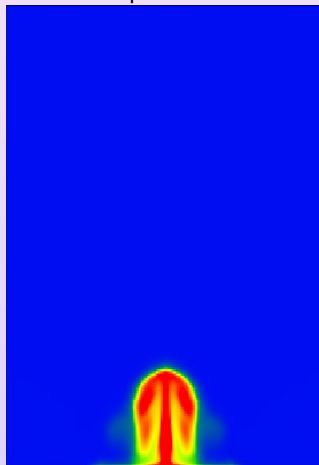
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



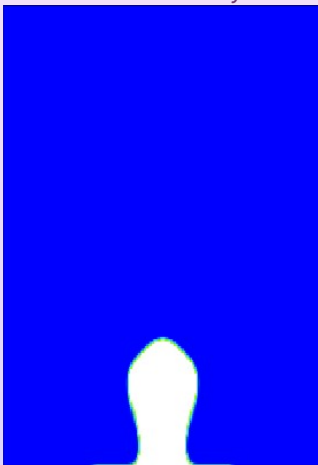
◀ Geometry

▶ Play

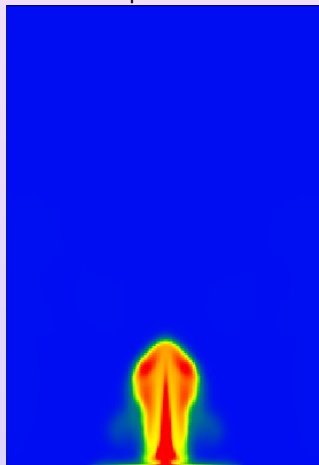
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



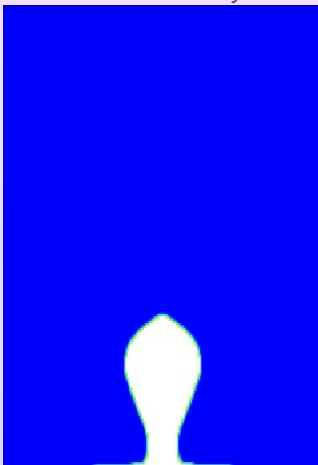
◀ Geometry

▶ Play

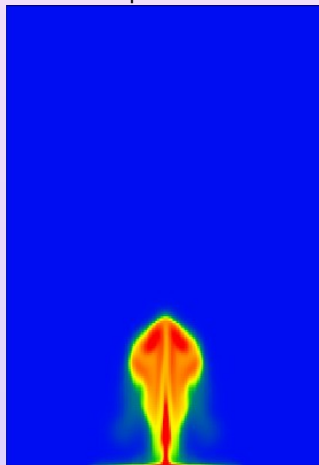
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



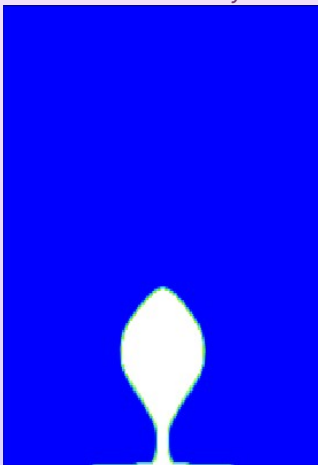
◀ Geometry

▶ Play

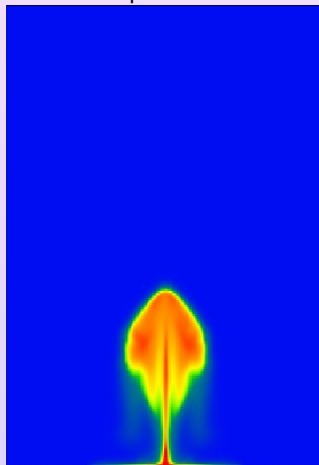
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



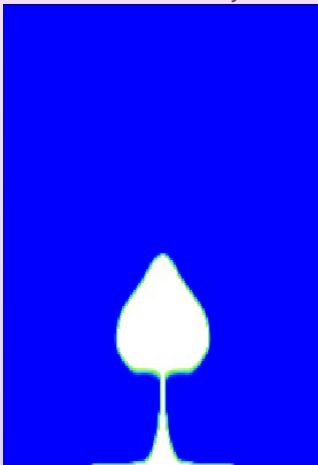
◀ Geometry

▶ Play

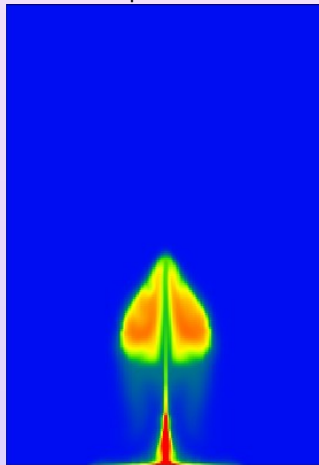
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



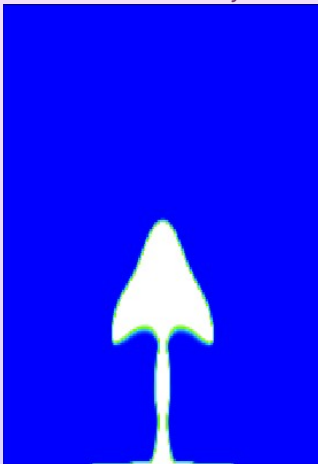
◀ Geometry

▶ Play

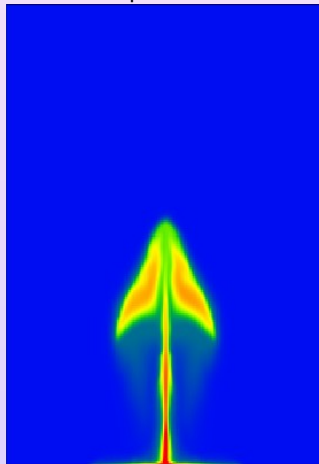
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



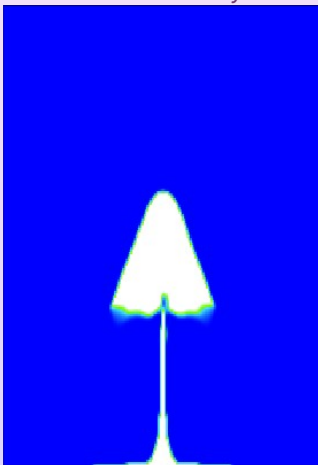
◀ Geometry

▶ Play

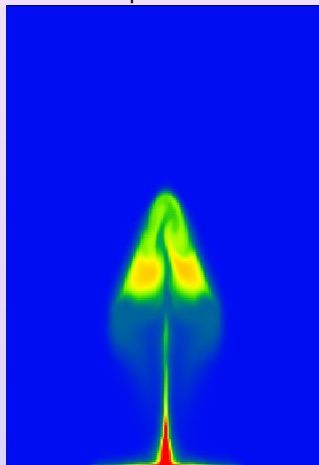
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



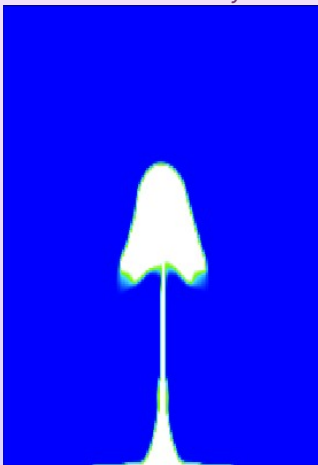
◀ Geometry

▶ Play

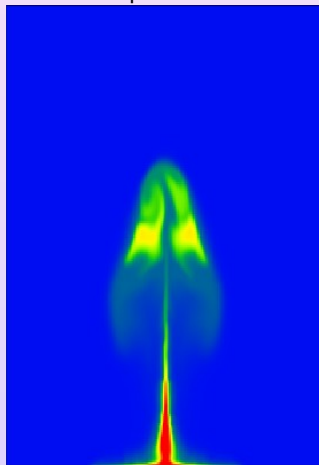
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



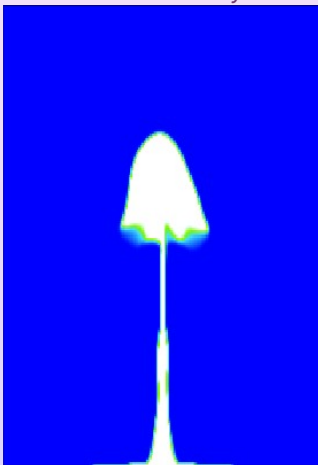
◀ Geometry

▶ Play

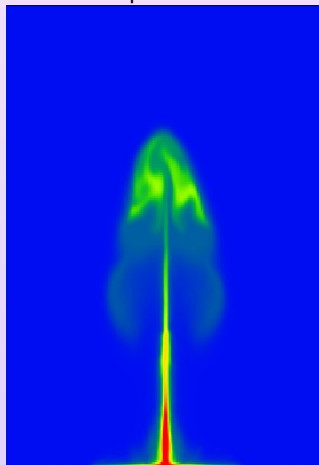
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



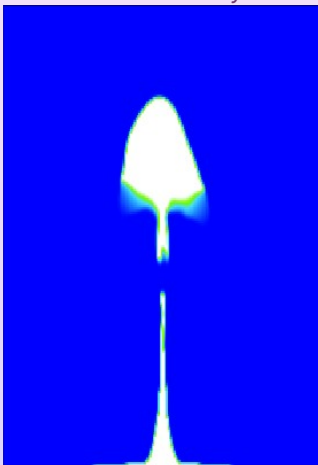
◀ Geometry

▶ Play

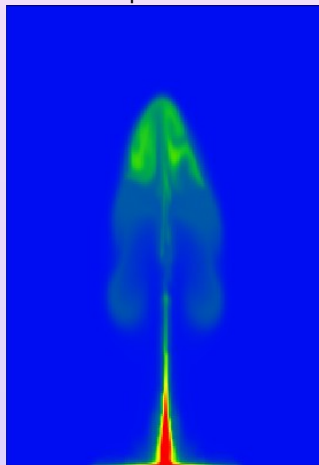
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



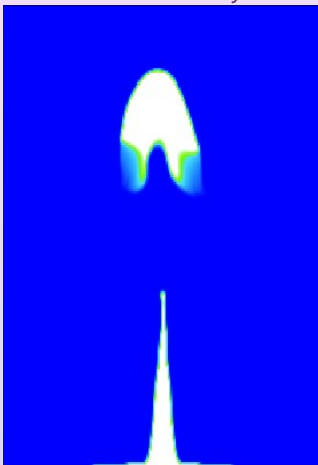
◀ Geometry

▶ Play

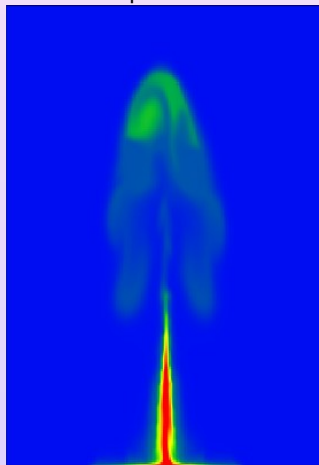
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



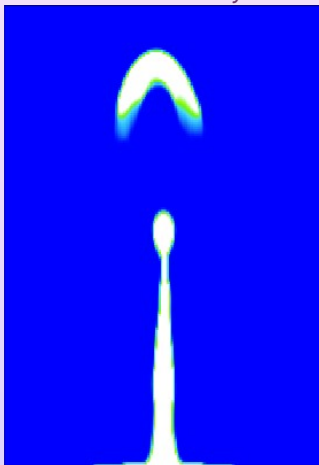
◀ Geometry

▶ Play

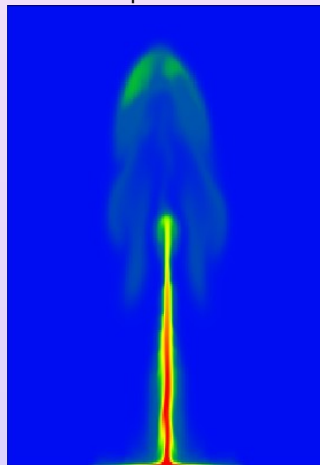
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



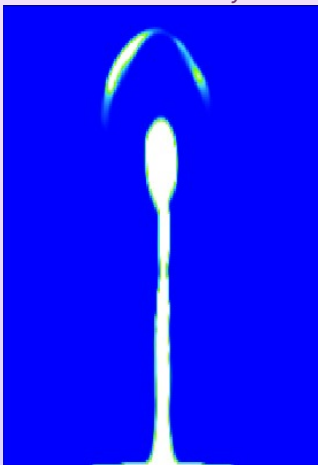
◀ Geometry

▶ Play

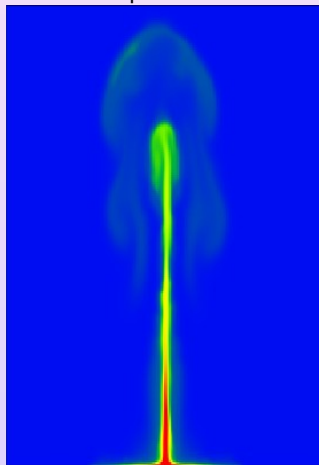
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



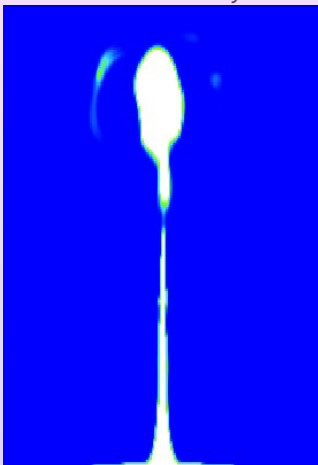
◀ Geometry

▶ Play

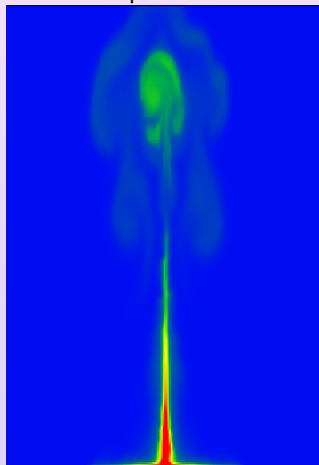
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



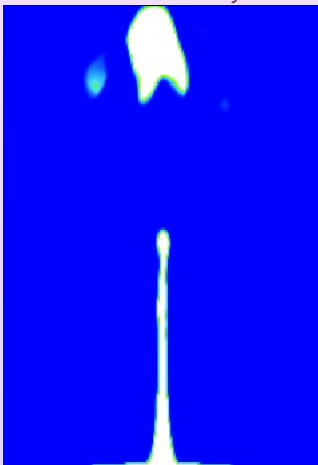
◀ Geometry

▶ Play

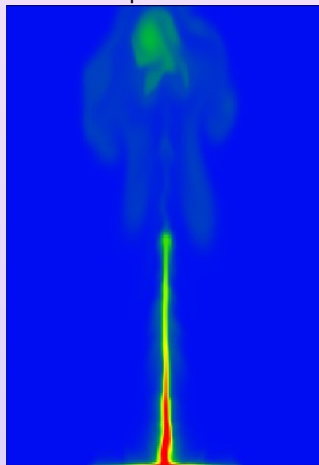
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



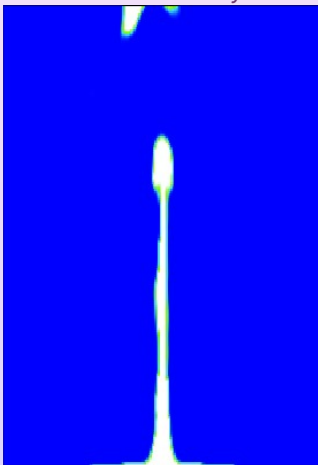
◀ Geometry

▶ Play

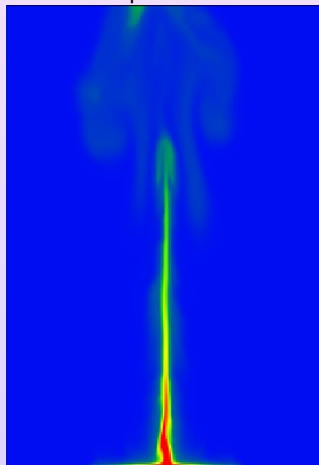
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



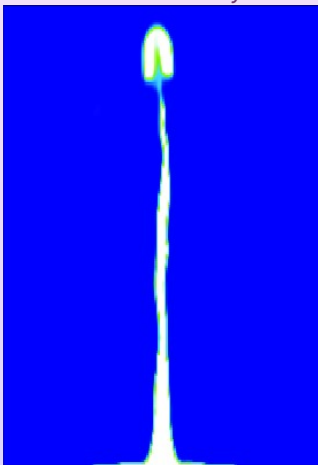
◀ Geometry

▶ Play

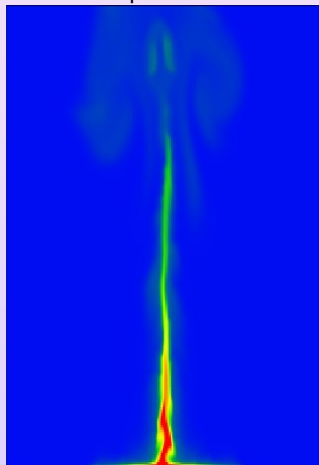
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



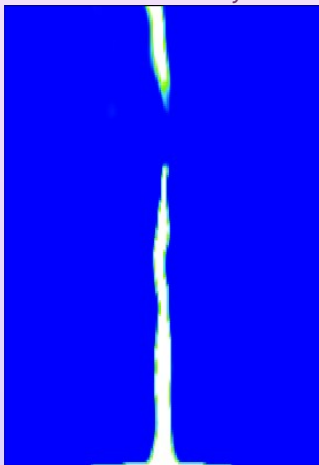
◀ Geometry

▶ Play

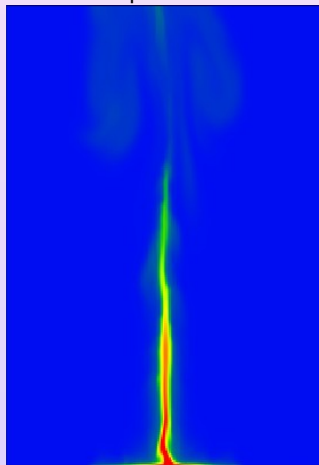
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



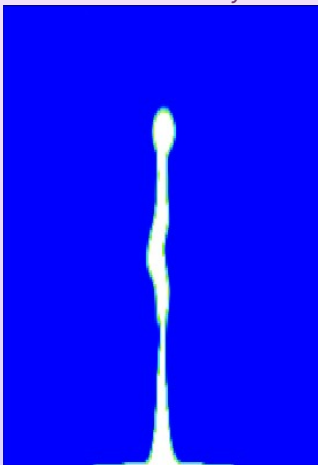
◀ Geometry

▶ Play

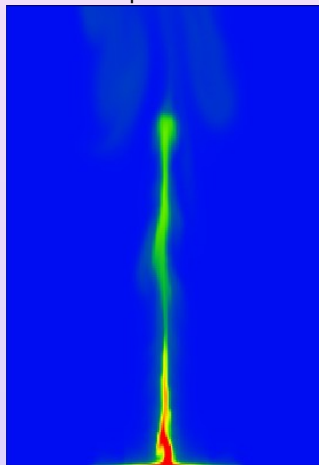
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



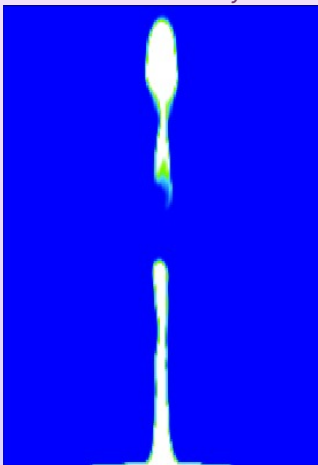
◀ Geometry

▶ Play

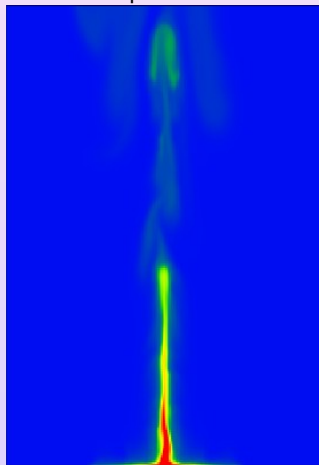
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



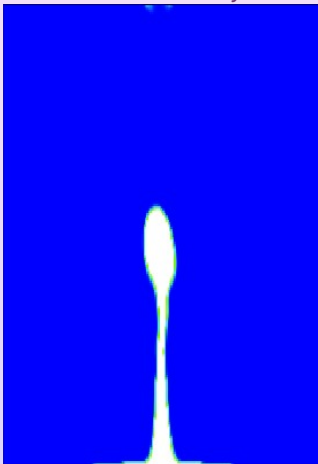
◀ Geometry

▶ Play

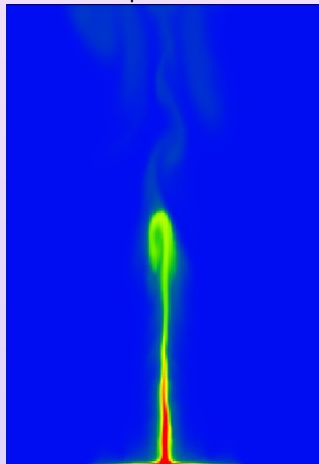
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



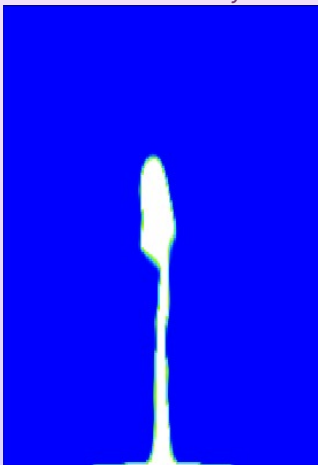
◀ Geometry

▶ Play

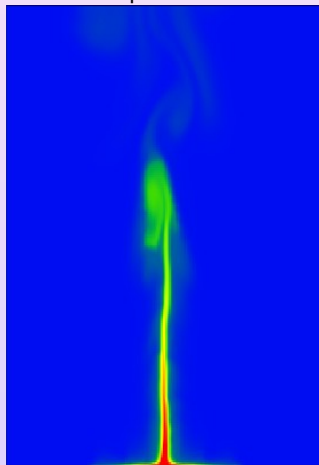
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



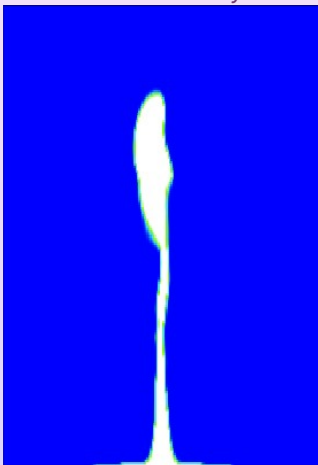
◀ Geometry

▶ Play

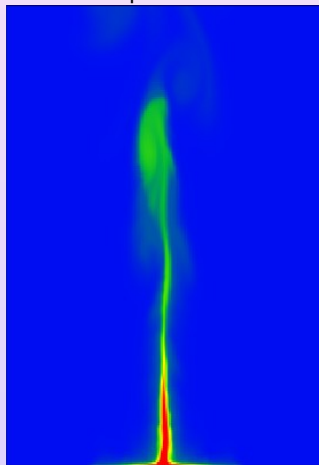
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



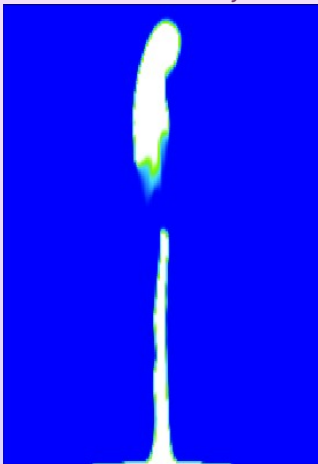
◀ Geometry

▶ Play

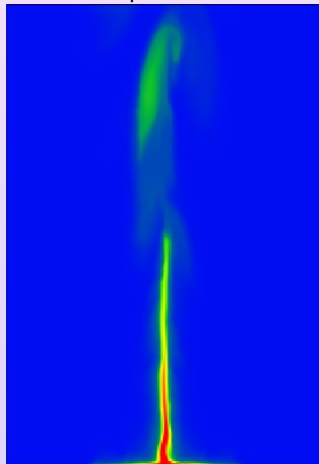
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Nucleating Bubble

Mass Fraction y



Temperature T



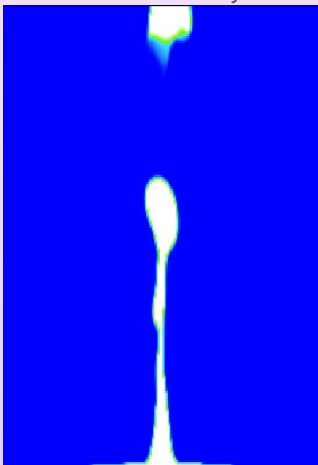
◀ Geometry

▶ Play

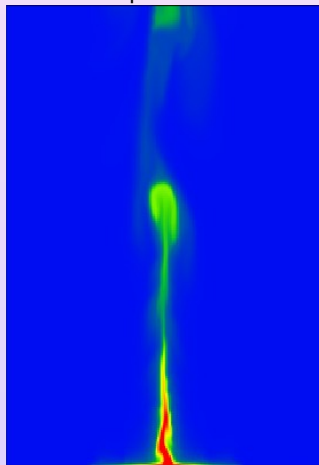
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Nucleating Bubble

Mass Fraction y



Temperature T



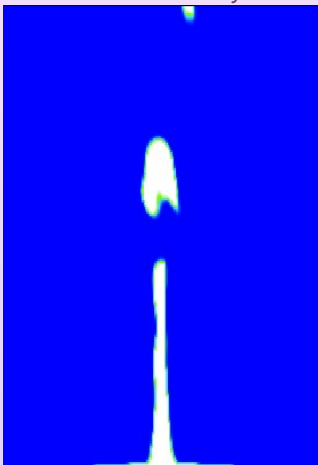
◀ Geometry

▶ Play

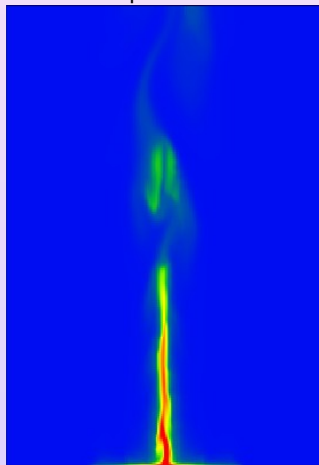
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Nucleating Bubble

Mass Fraction y



Temperature T



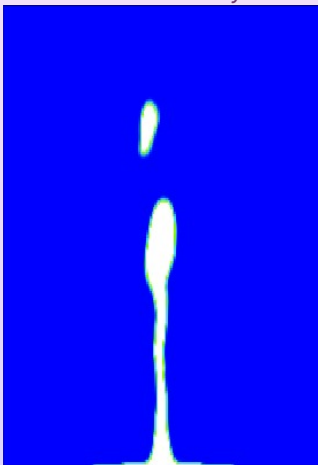
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▶ Play

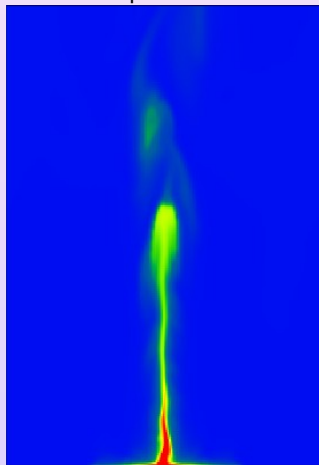
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Nucleating Bubble

Mass Fraction y



Temperature T



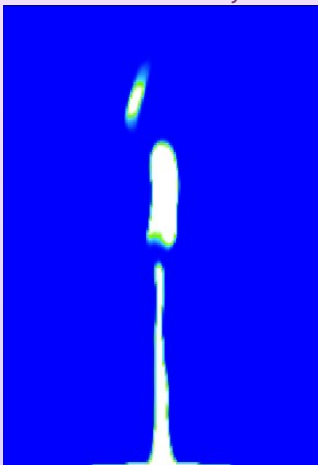
◀ Geometry

▶ Play

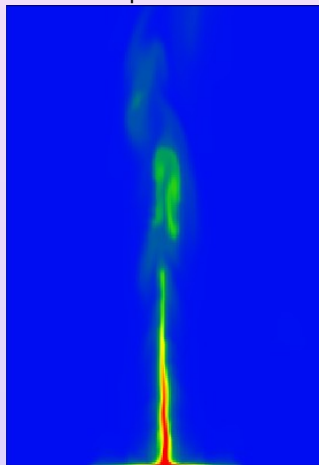
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Nucleating Bubble

Mass Fraction y



Temperature T



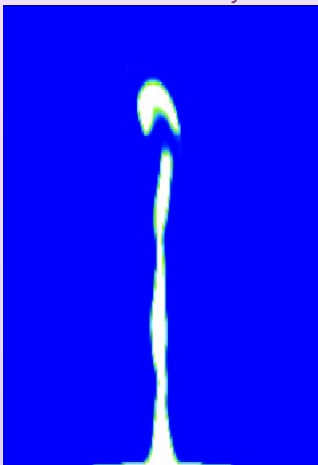
◀ Geometry

▶ Play

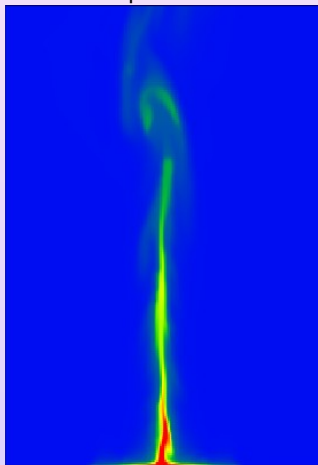
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Nucleating Bubble

Mass Fraction y



Temperature T



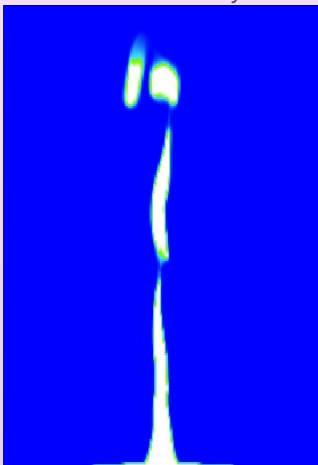
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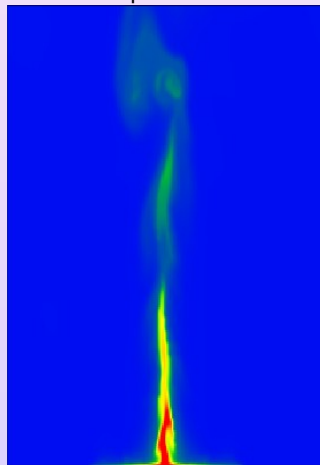
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Nucleating Bubble

Mass Fraction y



Temperature T



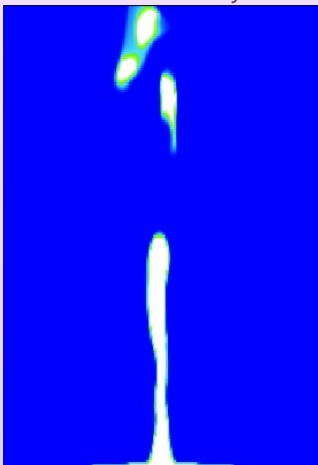
◀ Geometry

▶ Play

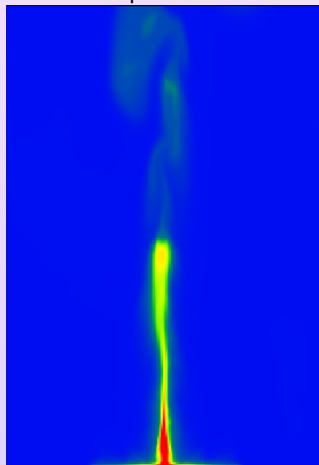
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Nucleating Bubble

Mass Fraction y



Temperature T



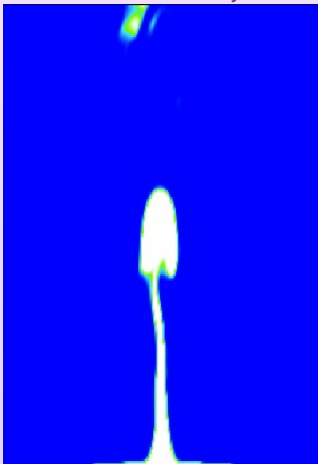
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▶ Play

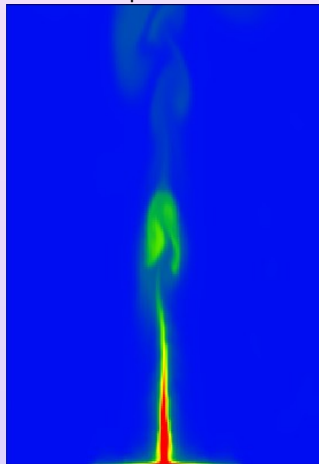
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Nucleating Bubble

Mass Fraction y



Temperature T



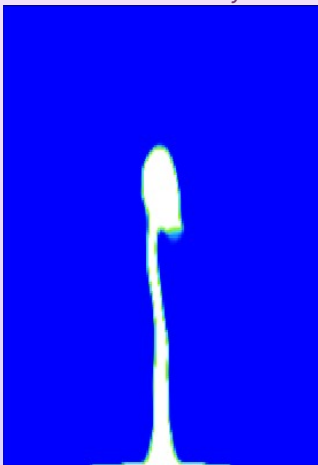
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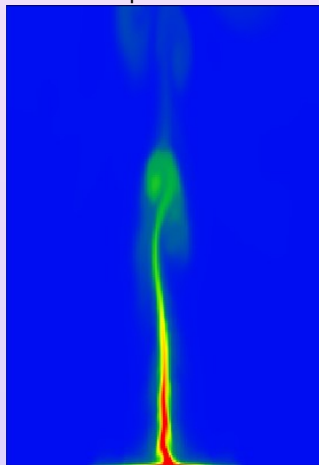
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Nucleating Bubble

Mass Fraction y



Temperature T



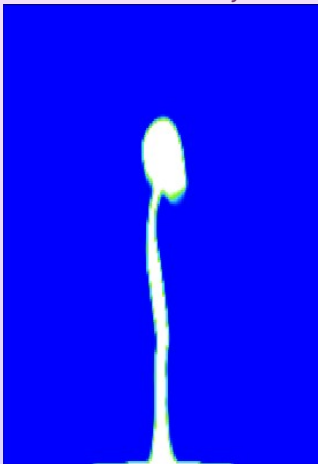
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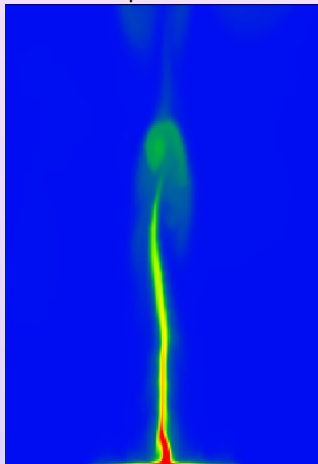
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Nucleating Bubble

Mass Fraction y



Temperature T



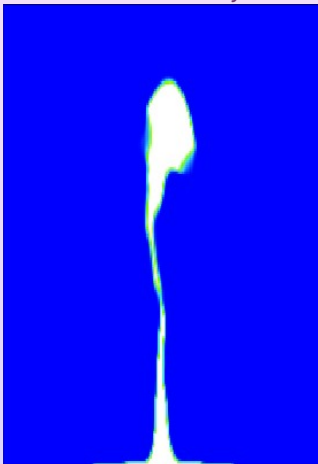
◀ Geometry

▶ Play

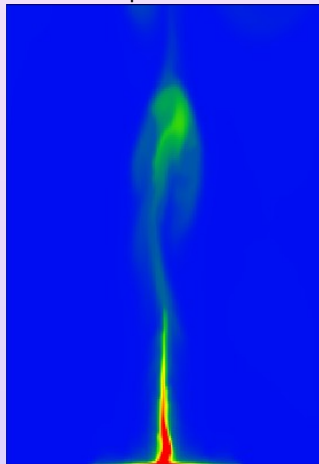
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Nucleating Bubble

Mass Fraction y



Temperature T



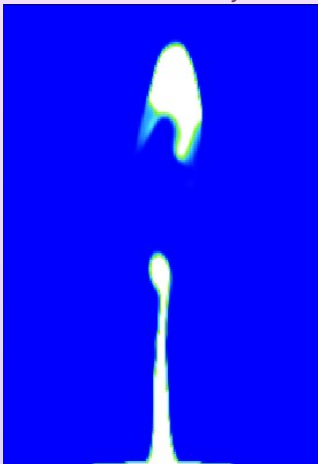
◀ Geometry

▶ Play

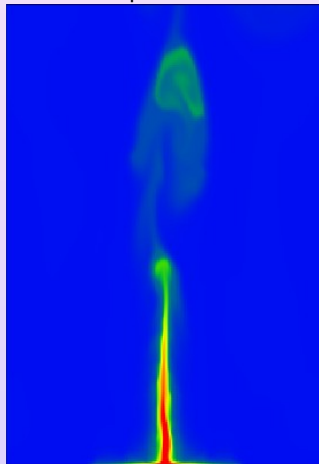
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Nucleating Bubble

Mass Fraction y



Temperature T



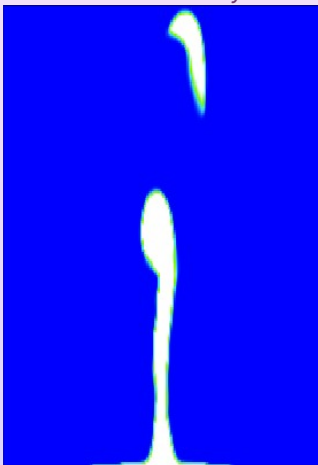
◀ Geometry

▶ Play

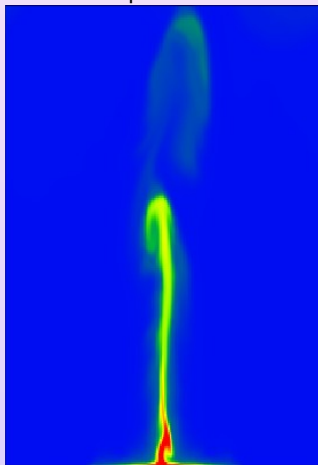
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Nucleating Bubble

Mass Fraction y



Temperature T



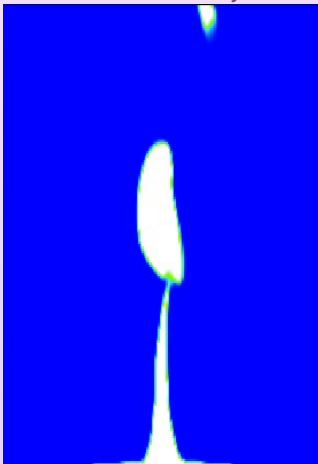
◀ Geometry

▶ Play

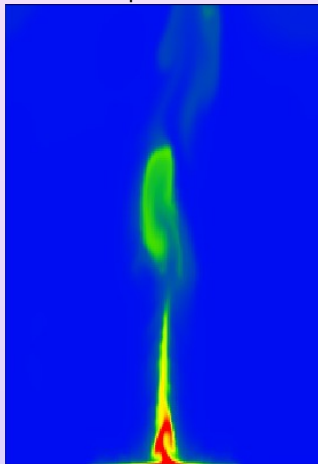
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Nucleating Bubble

Mass Fraction y



Temperature T



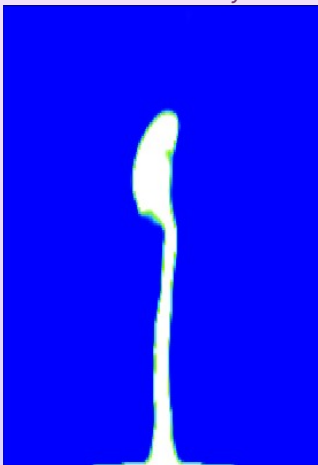
◀ Geometry

▶ Play

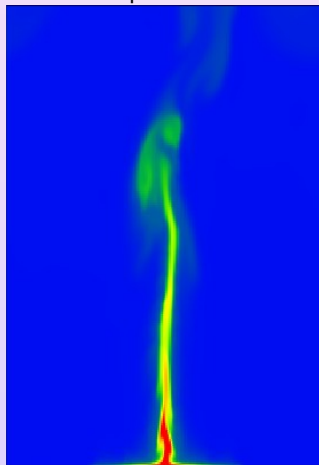
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



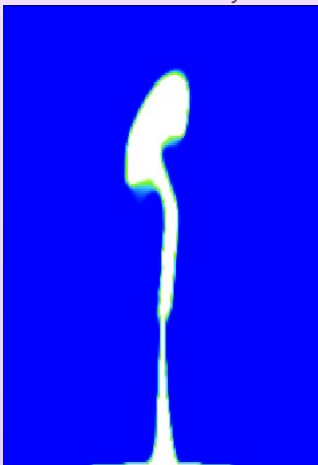
◀ Geometry

▶ Play

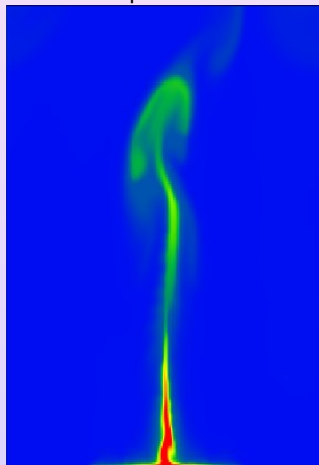
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Nucleating Bubble

Mass Fraction y



Temperature T



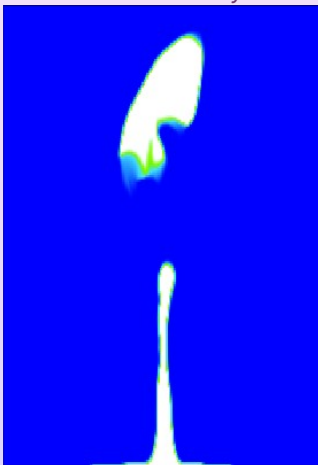
◀ Geometry

▶ Play

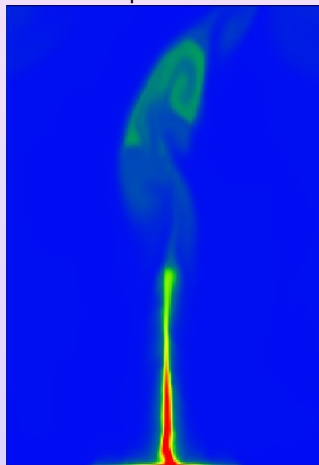
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Nucleating Bubble

Mass Fraction y



Temperature T



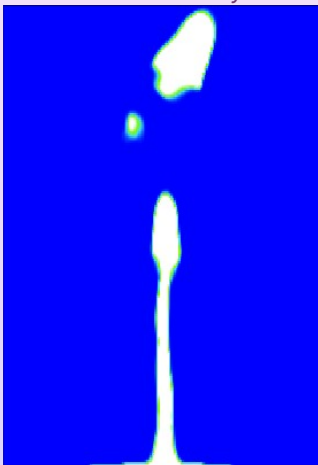
◀ Geometry

▶ Play

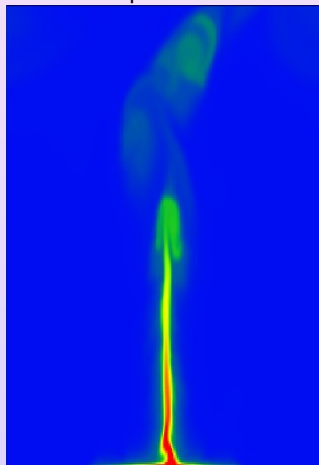
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Nucleating Bubble

Mass Fraction y



Temperature T



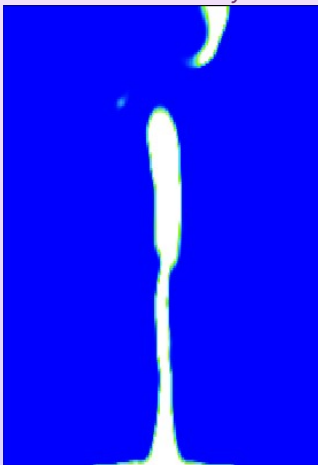
◀ Geometry

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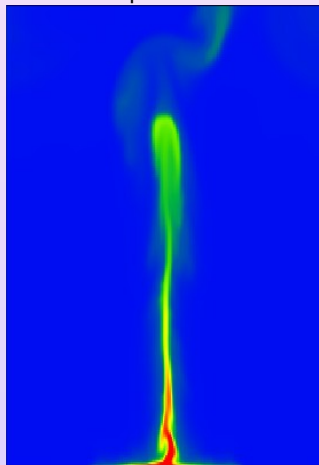
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Nucleating Bubble

Mass Fraction y



Temperature T



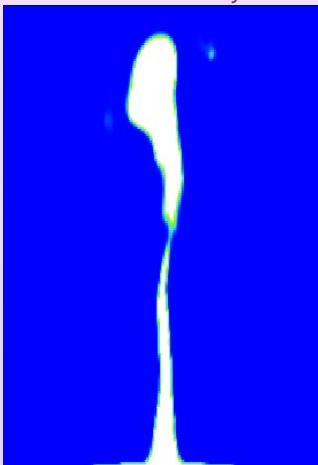
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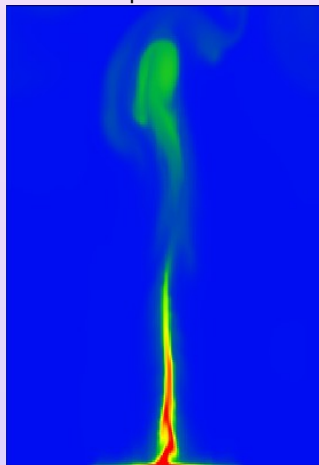
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Nucleating Bubble

Mass Fraction y



Temperature T



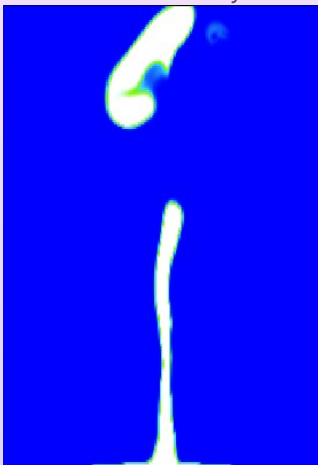
◀ Geometry

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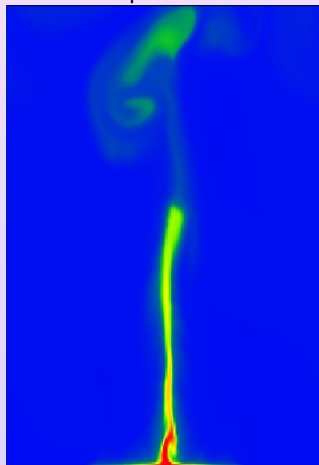
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Nucleating Bubble

Mass Fraction y



Temperature T



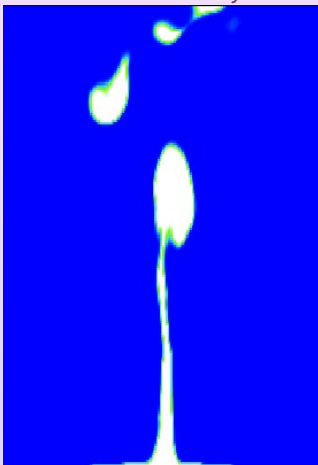
◀ Geometry

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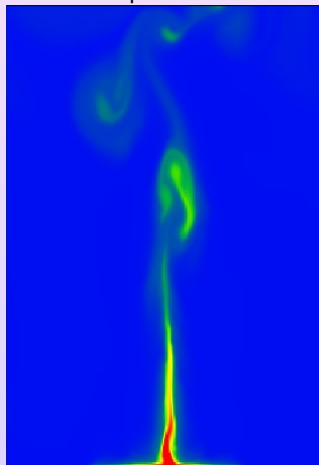
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Nucleating Bubble

Mass Fraction y



Temperature T



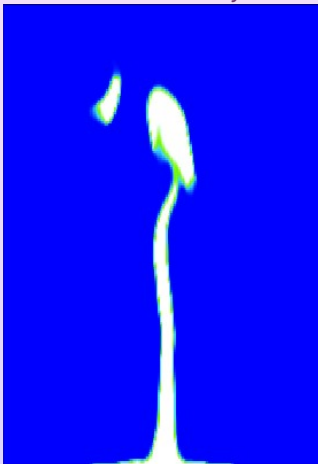
◀ Geometry

▶ Play

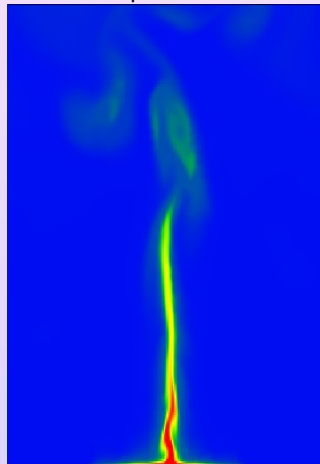
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Nucleating Bubble

Mass Fraction y



Temperature T



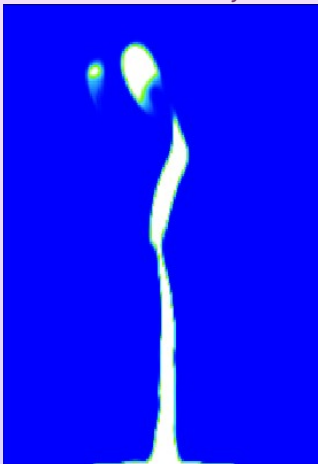
◀ Geometry

▶ Play

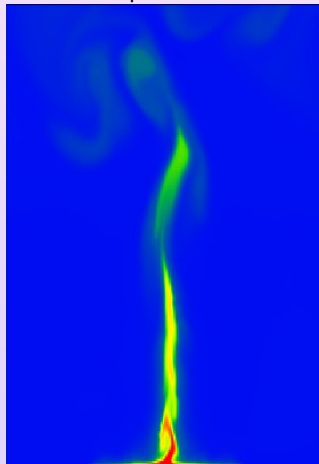
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Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

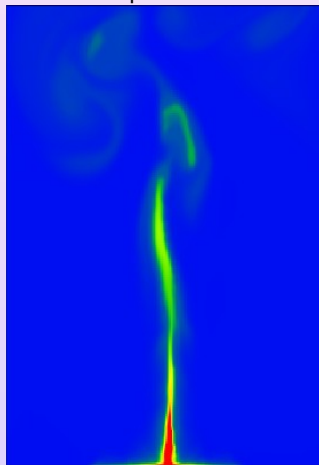
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Nucleating Bubble

Mass Fraction y



Temperature T



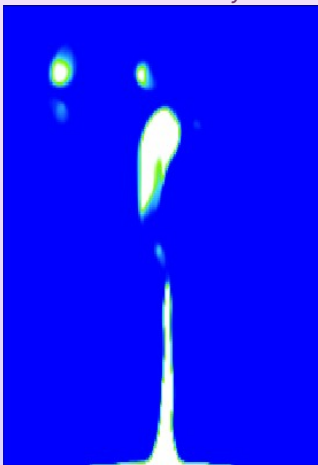
◀ Geometry

▶ Play

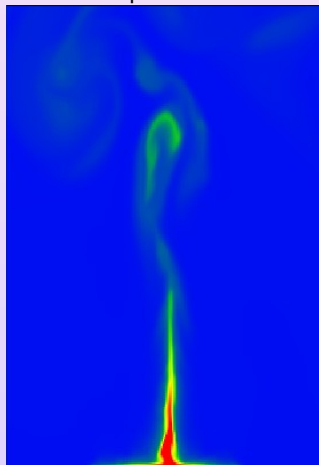
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Nucleating Bubble

Mass Fraction y



Temperature T



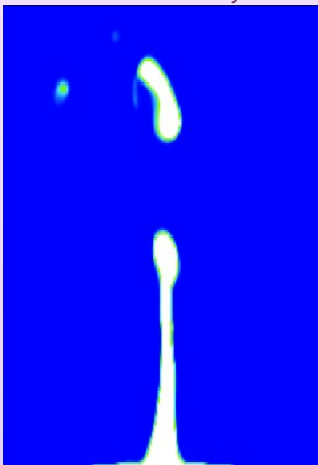
◀ Geometry

▶ Play

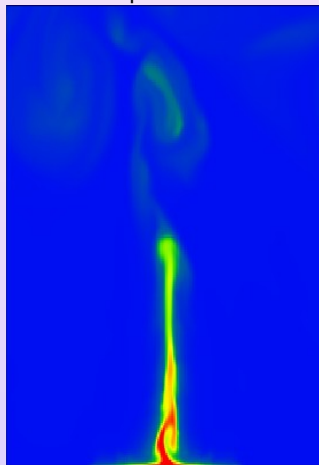
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Nucleating Bubble

Mass Fraction y



Temperature T



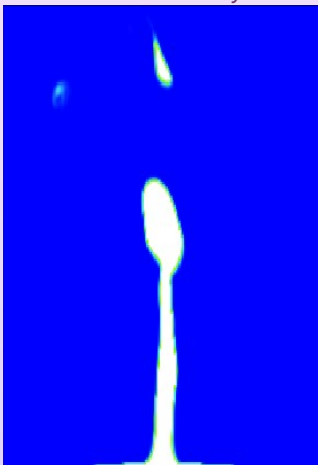
◀ Geometry

▶ Play

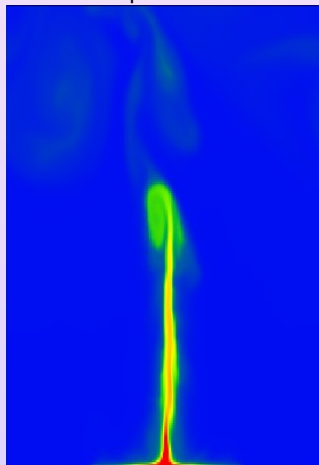
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Nucleating Bubble

Mass Fraction y



Temperature T



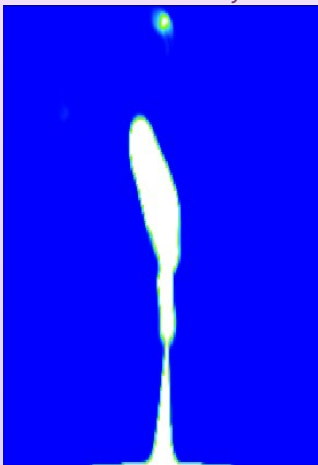
◀ Geometry

▶ Play

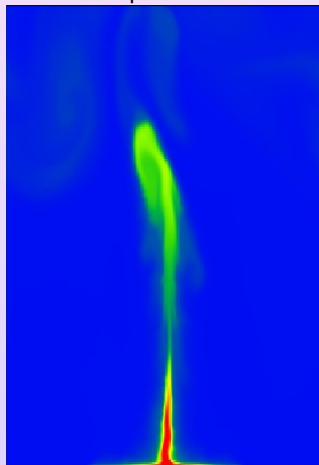
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Nucleating Bubble

Mass Fraction y



Temperature T



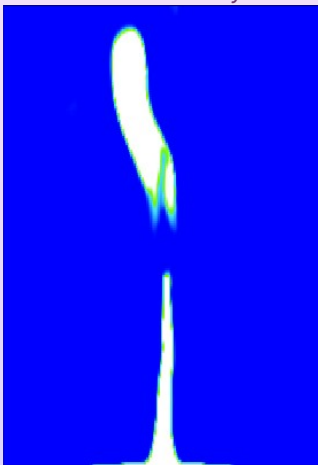
◀ Geometry

▶ Play

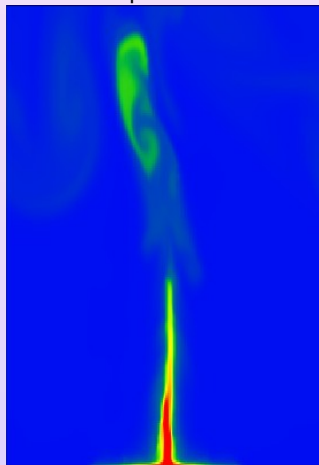
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Nucleating Bubble

Mass Fraction y



Temperature T



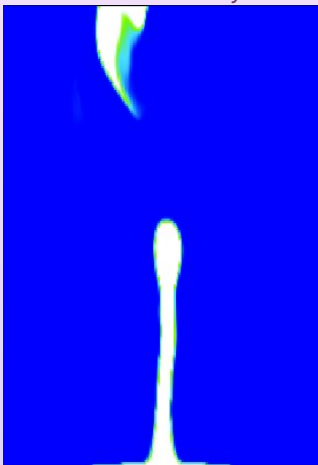
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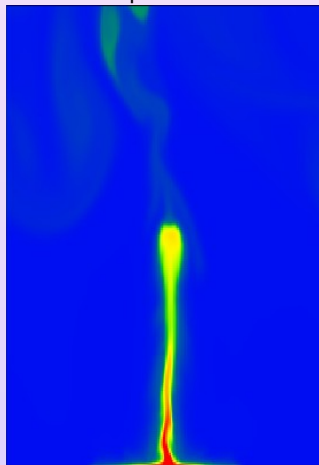
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Nucleating Bubble

Mass Fraction y



Temperature T



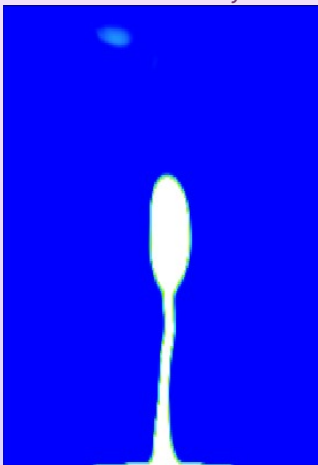
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▶ Play

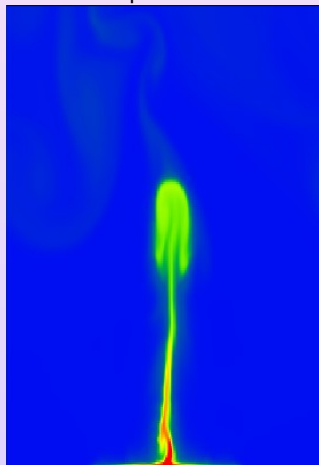
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Nucleating Bubble

Mass Fraction y



Temperature T



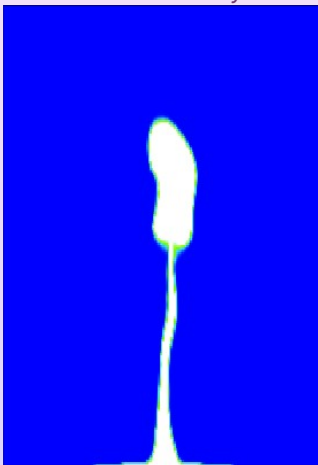
◀ Geometry

▶ Play

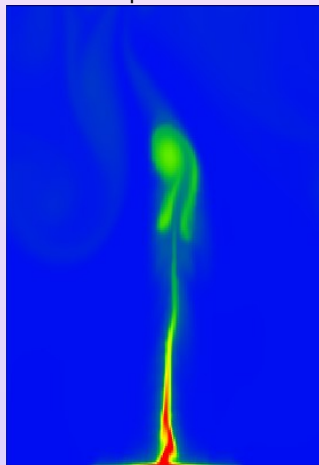
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Nucleating Bubble

Mass Fraction y



Temperature T



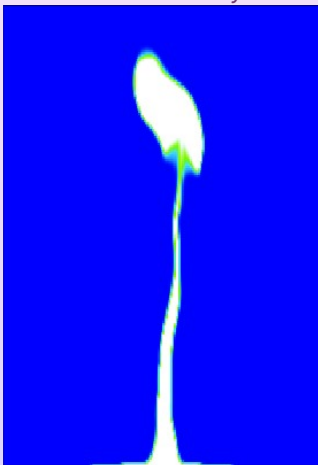
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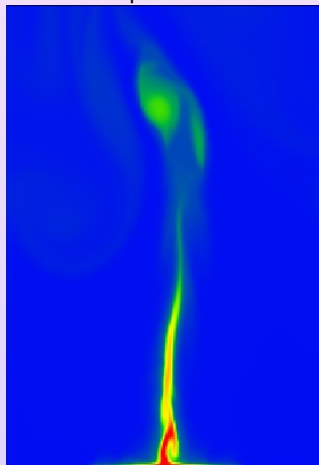
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Nucleating Bubble

Mass Fraction y



Temperature T



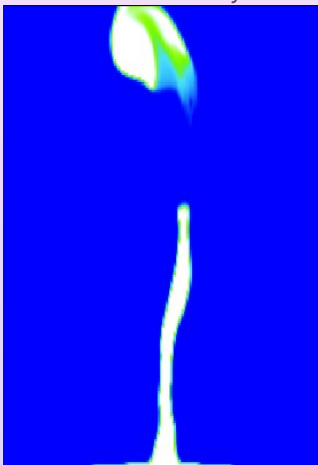
◀ Geometry

▶ Play

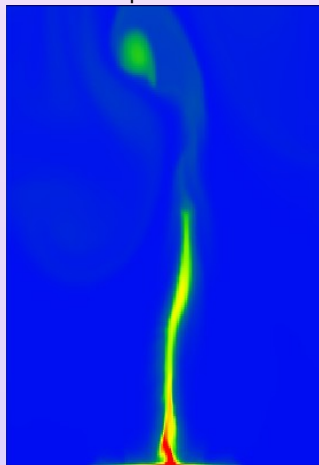
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Nucleating Bubble

Mass Fraction y



Temperature T



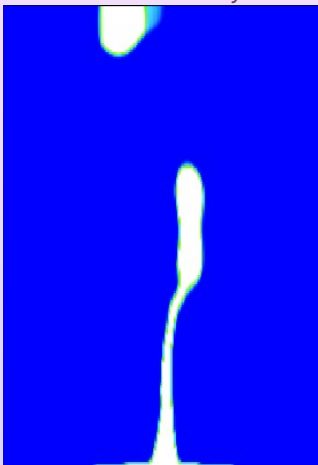
◀ Geometry

▶ Play

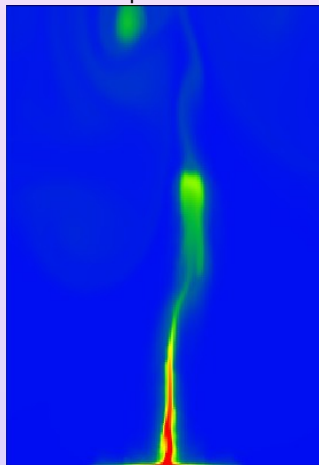
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



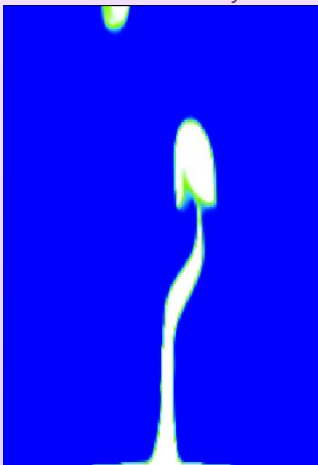
◀ Geometry

▶ Play

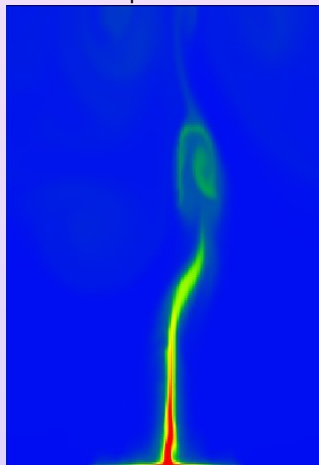
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Nucleating Bubble

Mass Fraction y



Temperature T



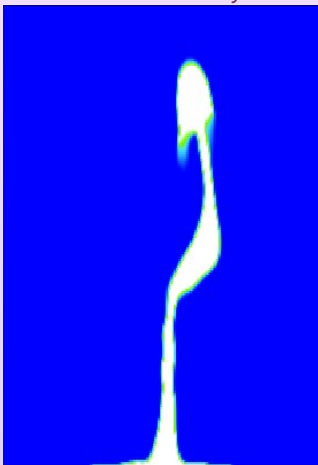
◀ Geometry

▶ Play

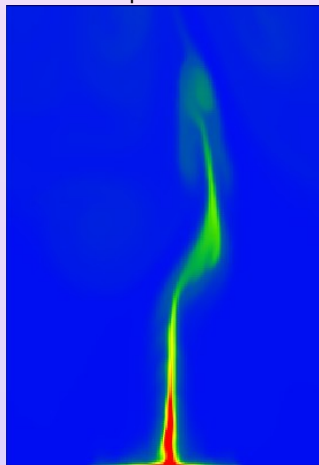
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Nucleating Bubble

Mass Fraction y



Temperature T



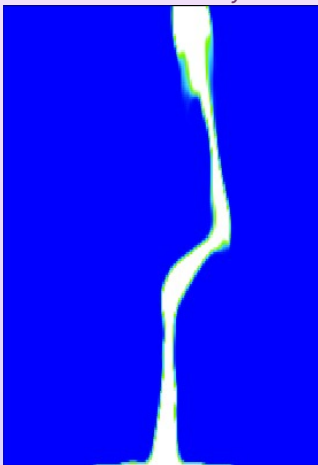
◀ Geometry

▶ Play

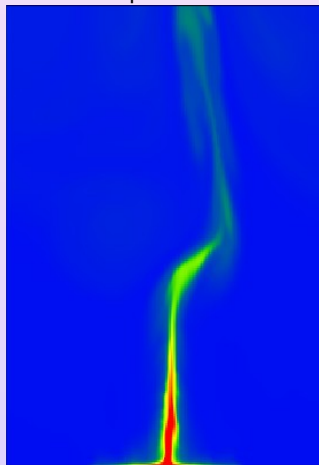
▶▶ Skip

Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

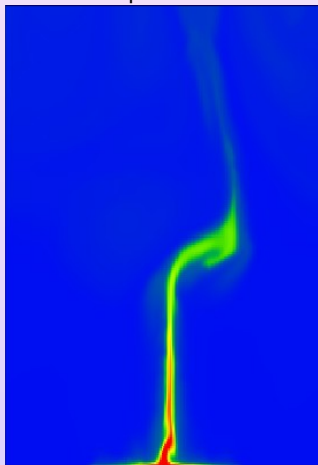
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Nucleating Bubble

Mass Fraction y



Temperature T



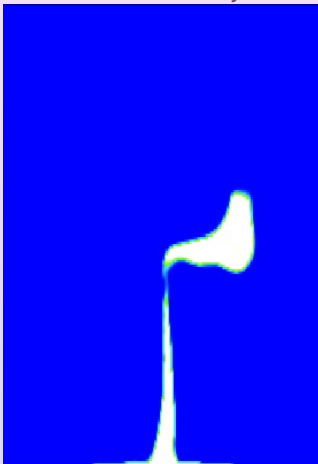
◀ Geometry

▶ Play

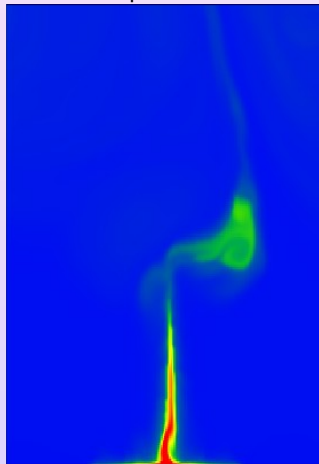
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Nucleating Bubble

Mass Fraction y



Temperature T



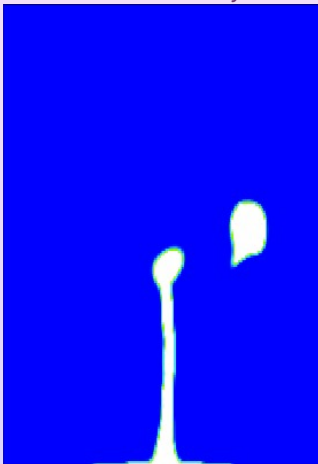
◀ Geometry

▶ Play

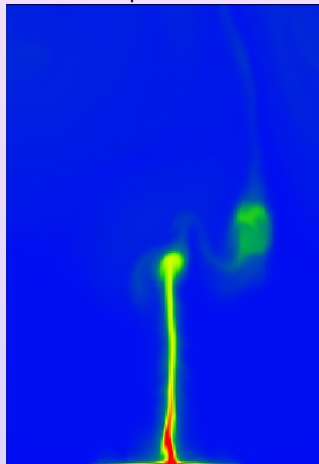
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Nucleating Bubble

Mass Fraction y



Temperature T



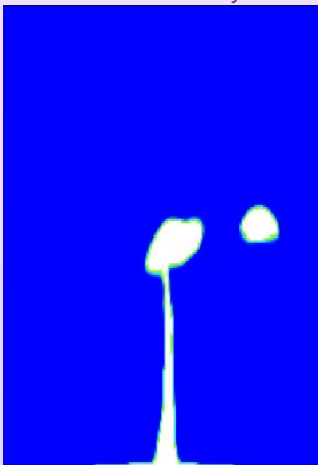
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▶ Play

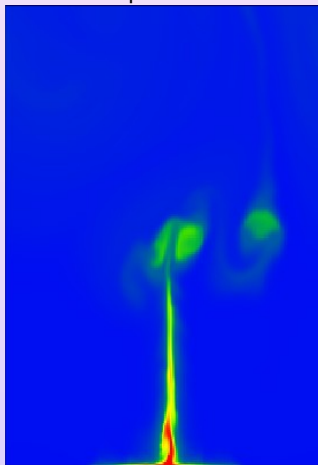
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Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

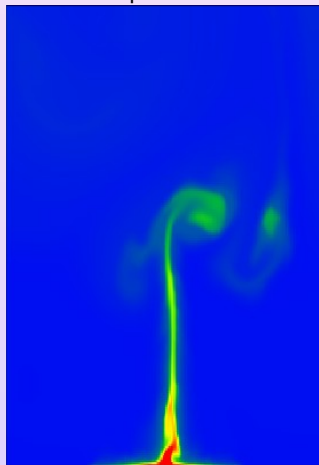
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Nucleating Bubble

Mass Fraction y



Temperature T



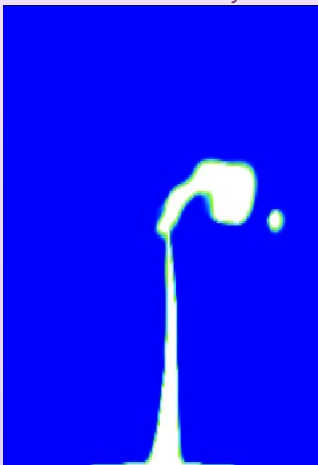
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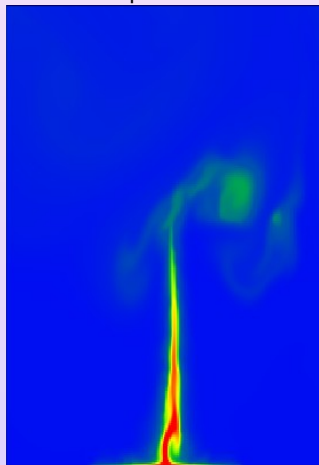
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Nucleating Bubble

Mass Fraction y



Temperature T



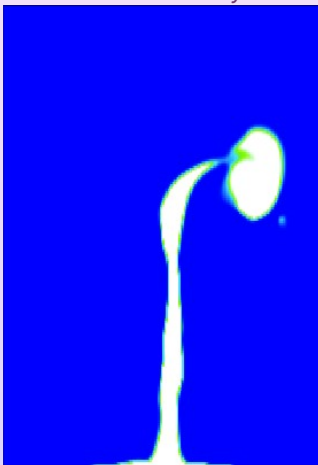
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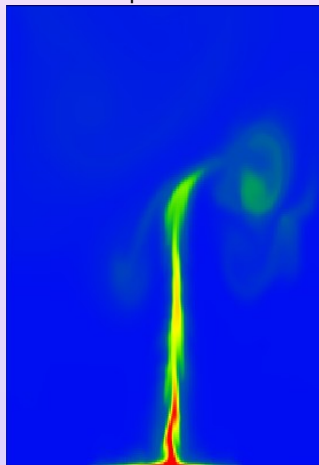
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Nucleating Bubble

Mass Fraction y



Temperature T



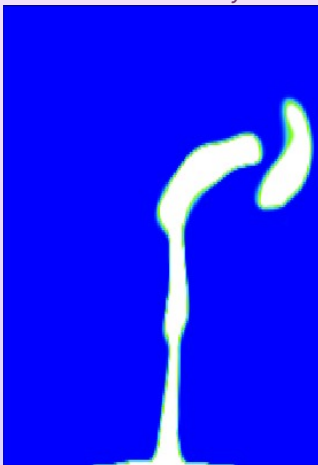
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▶ Play

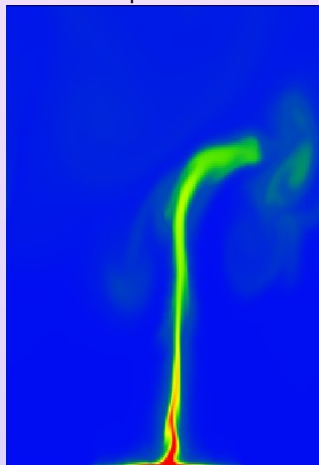
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Nucleating Bubble

Mass Fraction y



Temperature T



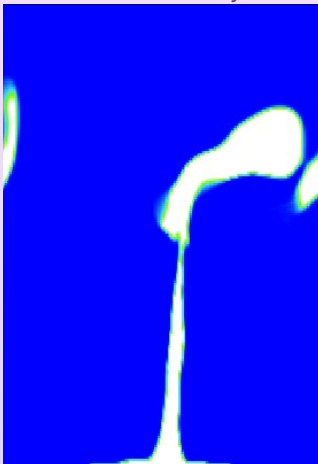
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▶ Play

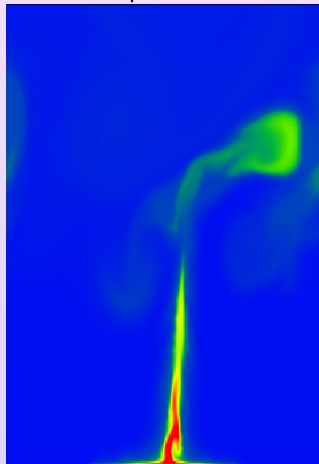
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Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

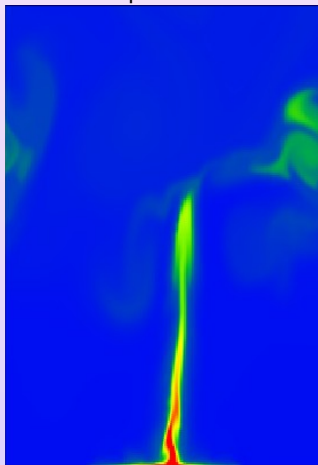
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Nucleating Bubble

Mass Fraction y



Temperature T



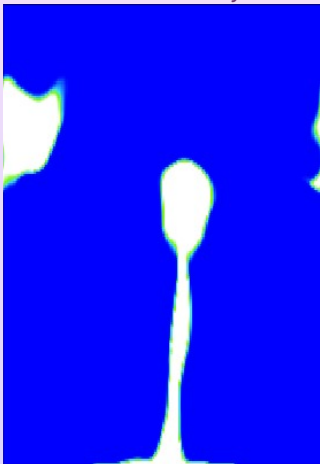
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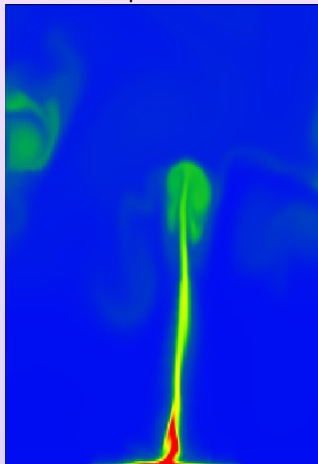
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Nucleating Bubble

Mass Fraction y



Temperature T



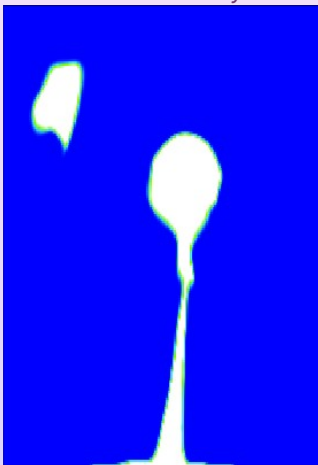
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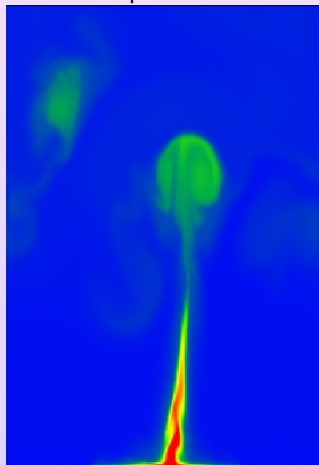
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Nucleating Bubble

Mass Fraction y



Temperature T



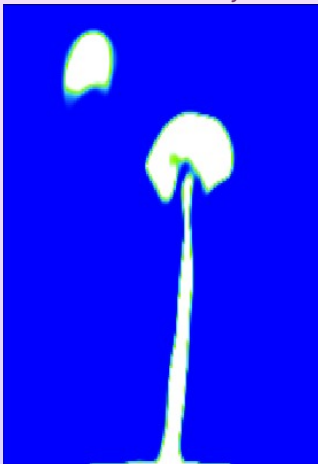
◀ Geometry

▶ Play

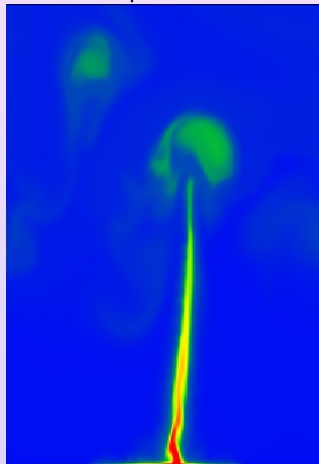
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Nucleating Bubble

Mass Fraction y



Temperature T



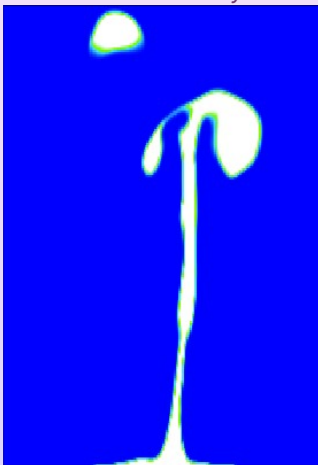
◀ Geometry

▶ Play

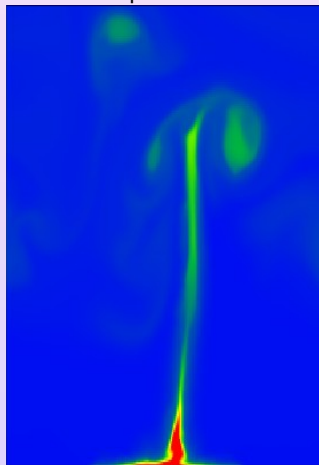
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Nucleating Bubble

Mass Fraction y



Temperature T



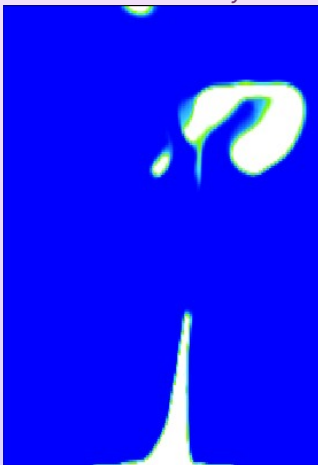
◀ Geometry

▶ Play

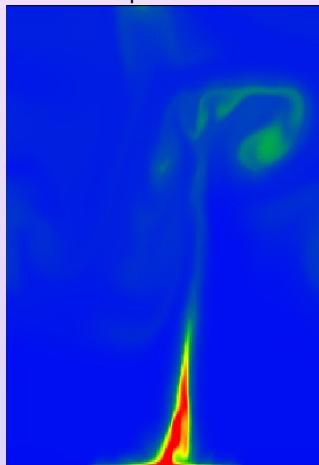
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Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

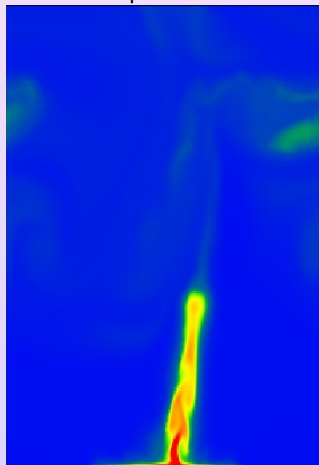
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Nucleating Bubble

Mass Fraction y



Temperature T



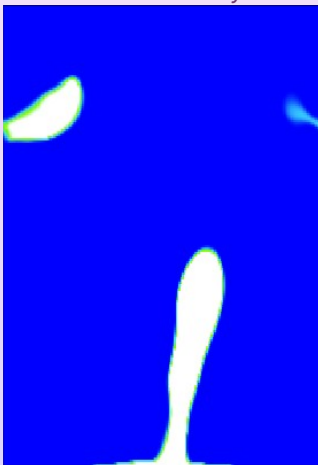
◀ Geometry

▶ Play

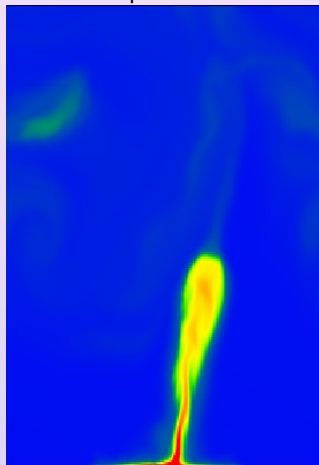
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Nucleating Bubble

Mass Fraction y



Temperature T



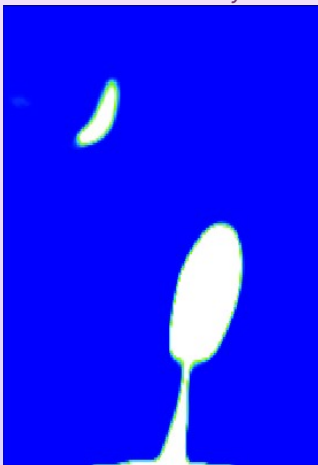
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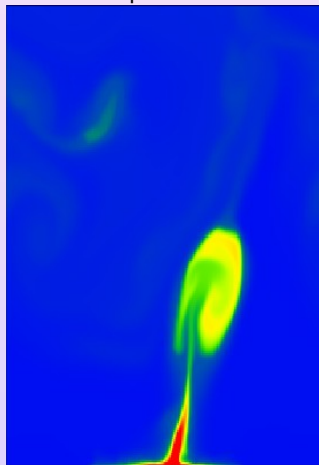
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Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

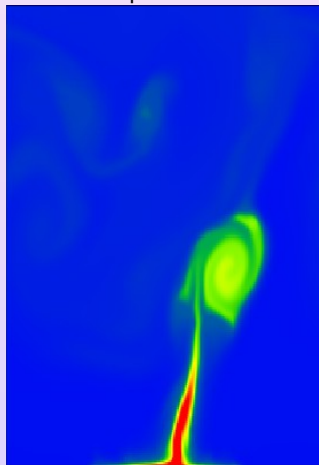
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Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

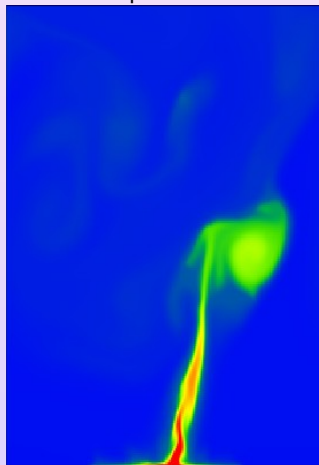
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Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

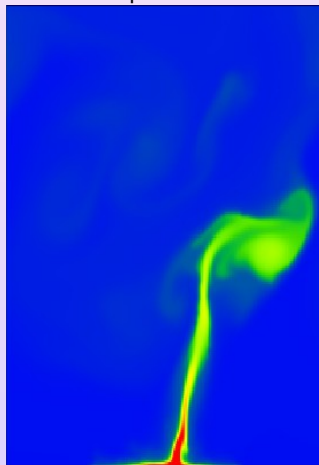
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Nucleating Bubble

Mass Fraction y



Temperature T



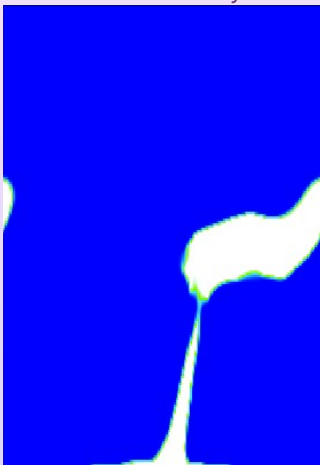
◀ Geometry

▶ Play

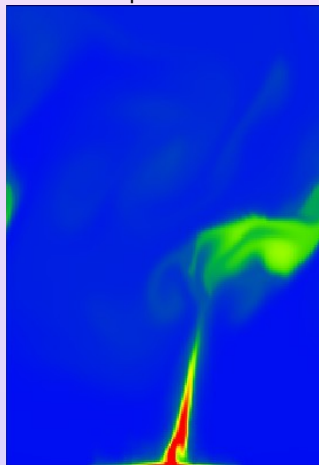
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Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

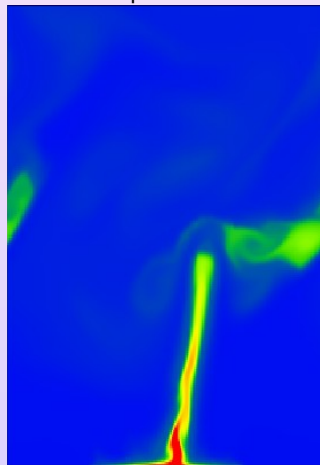
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Nucleating Bubble

Mass Fraction y



Temperature T



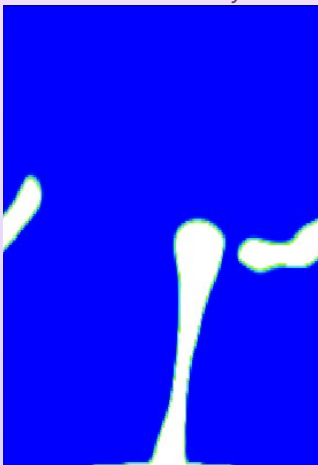
◀ Geometry

▶ Play

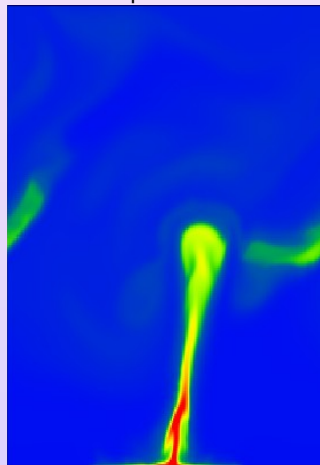
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Nucleating Bubble

Mass Fraction y



Temperature T



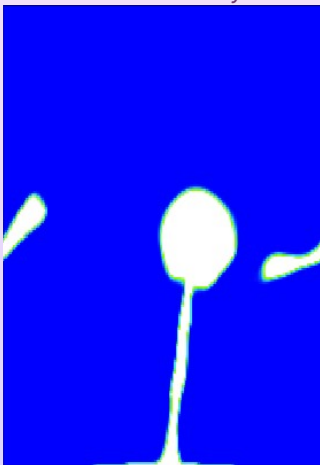
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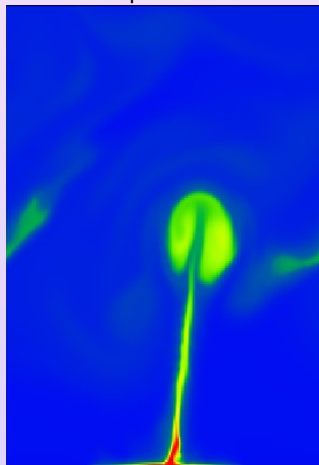
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Nucleating Bubble

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

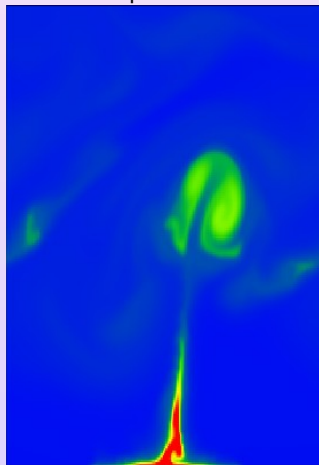
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Nucleating Bubble

Mass Fraction y



Temperature T



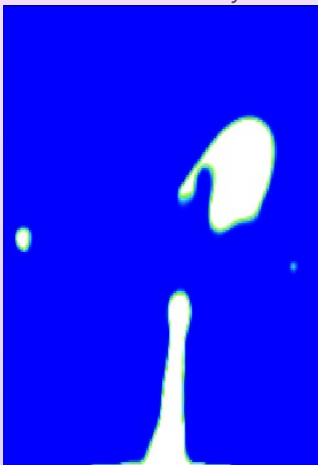
◀ Geometry

▶ Play

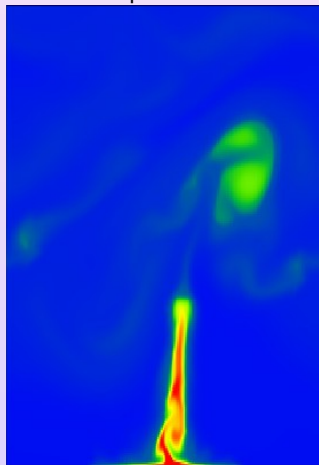
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Nucleating Bubble

Mass Fraction y



Temperature T



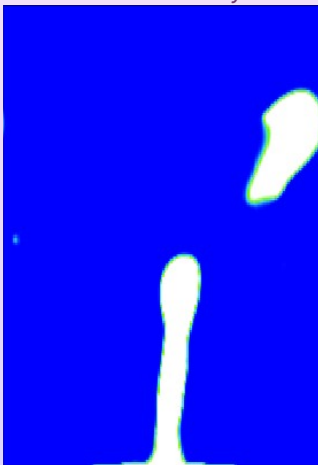
◀ Geometry

▶ Play

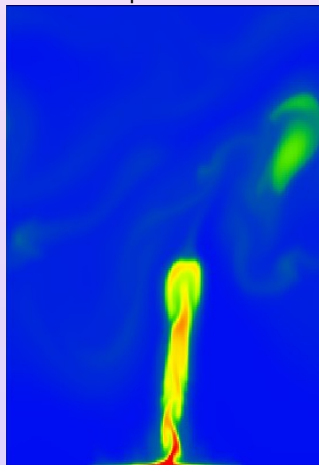
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Nucleating Bubble

Mass Fraction y



Temperature T



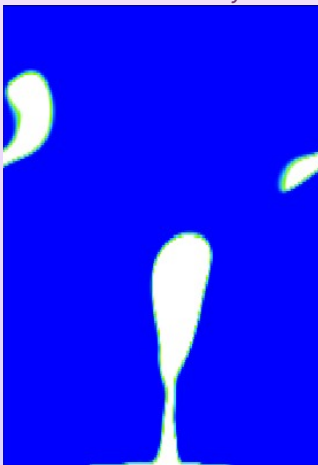
◀ Geometry

▶ Play

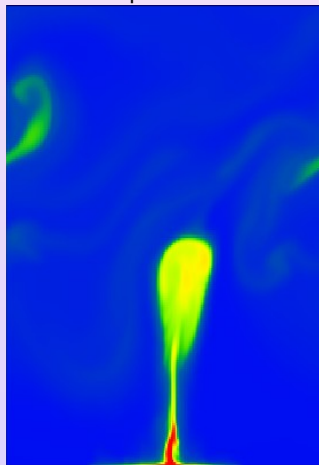
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Nucleating Bubble

Mass Fraction y



Temperature T



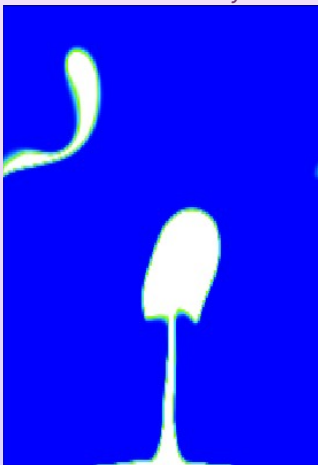
◀ Geometry

▶ Play

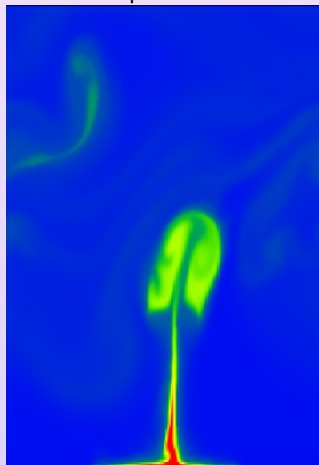
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Nucleating Bubble

Mass Fraction y



Temperature T



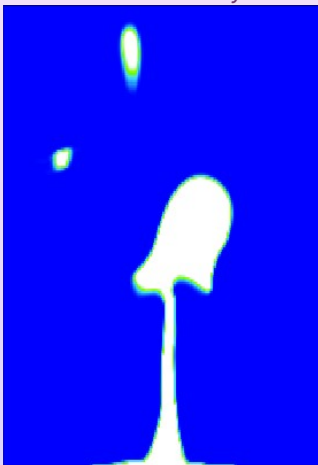
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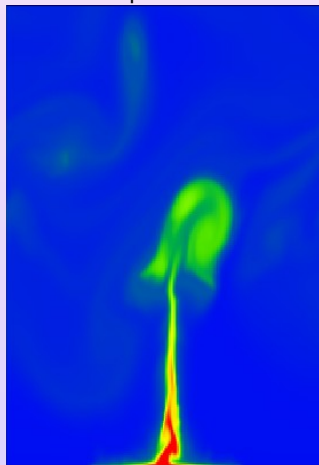
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Nucleating Bubble

Mass Fraction y



Temperature T



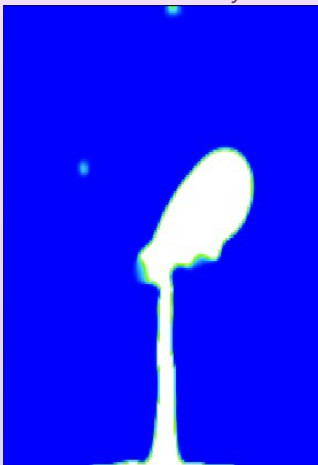
◀ Geometry

▶ Play

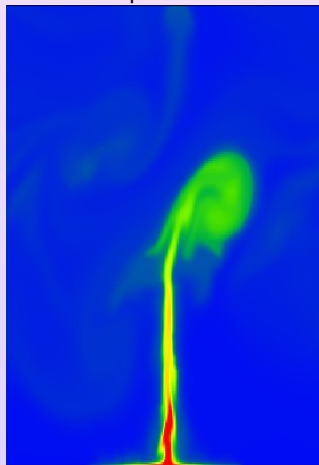
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Nucleating Bubble

Mass Fraction y



Temperature T



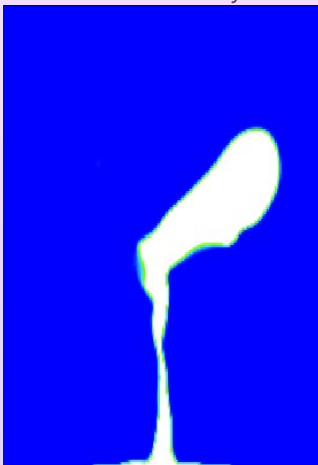
◀ Geometry

▶ Play

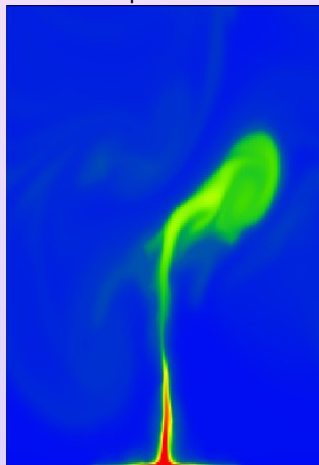
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Nucleating Bubble

Mass Fraction y



Temperature T



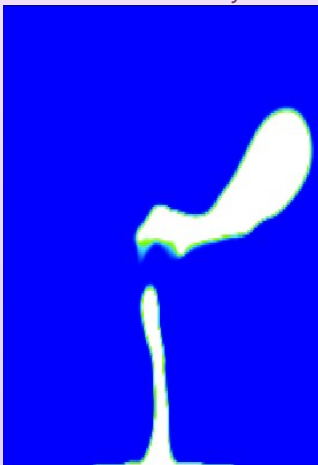
◀ Geometry

▶ Play

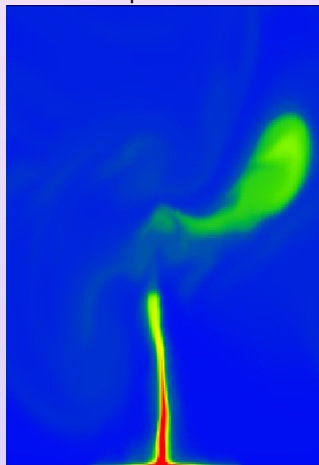
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Nucleating Bubble

Mass Fraction y



Temperature T



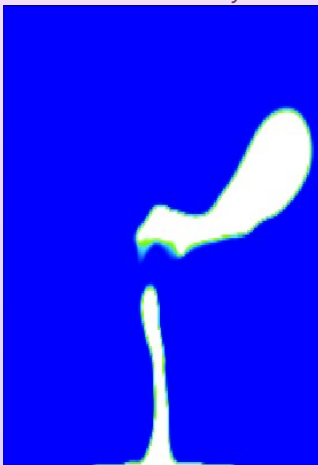
◀ Geometry

▶ Play

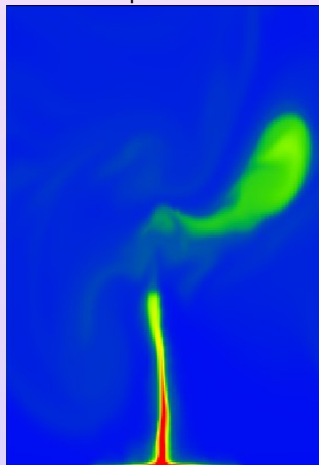
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Nucleating Bubble

Mass Fraction y



Temperature T

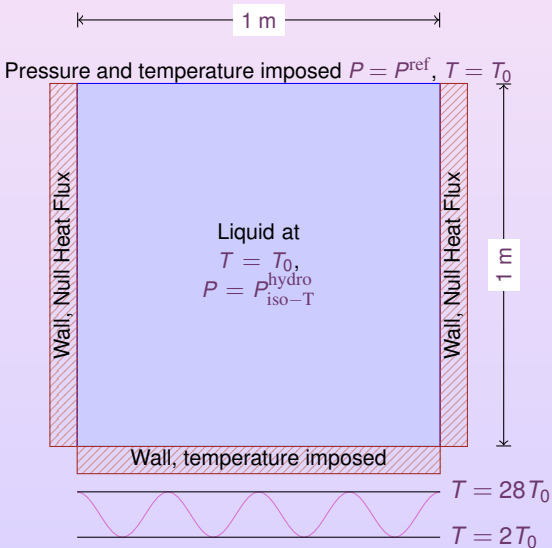


◀ Geometry

▶ Play

▶▶ Skip

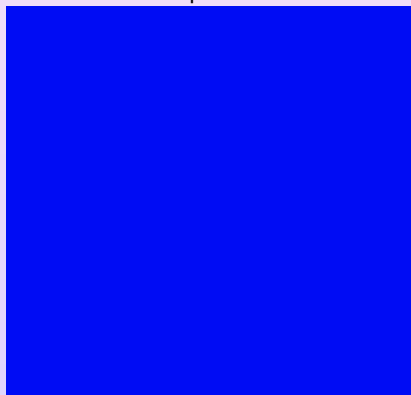
Film



Film

Mass Fraction y

Temperature T



◀ Geometry

▶ Play

▶▶ Skip

Film

Mass Fraction y



Temperature T



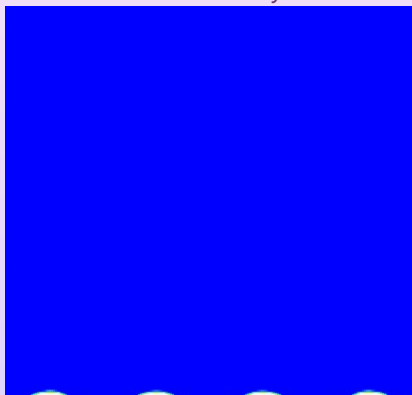
◀ Geometry

▶ Play

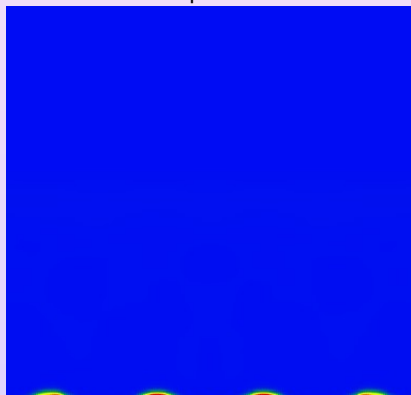
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Film

Mass Fraction y



Temperature T



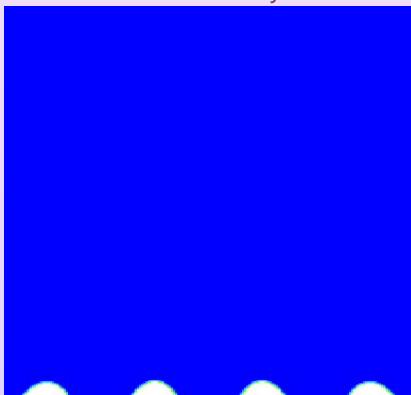
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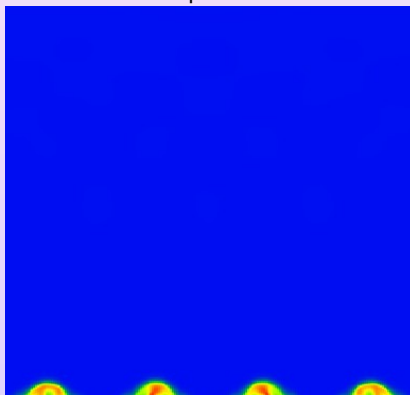
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Film

Mass Fraction y



Temperature T



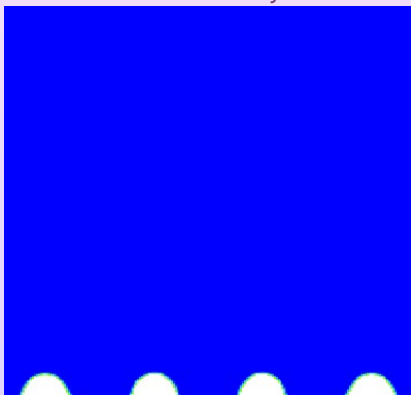
◀ Geometry

▶ Play

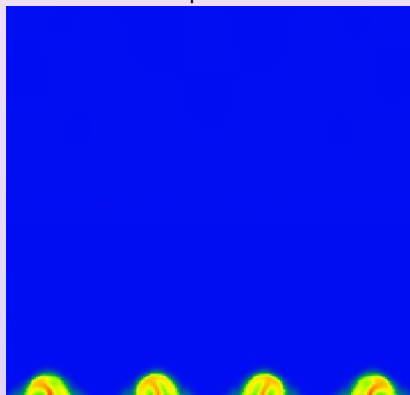
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Film

Mass Fraction y



Temperature T



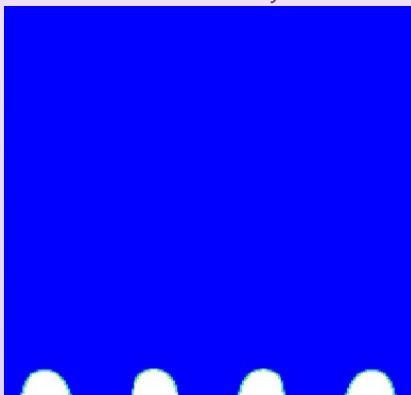
◀ Geometry

▶ Play

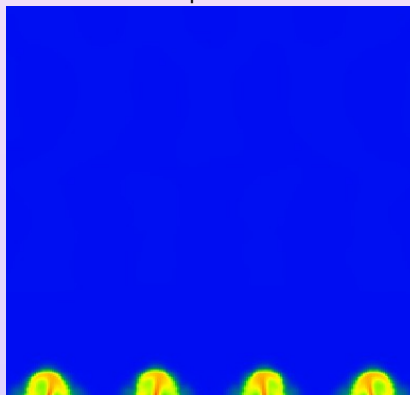
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Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

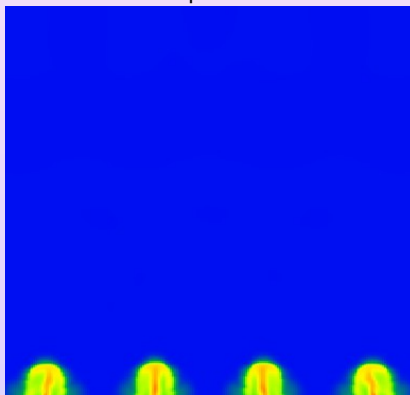
▶▶ Skip

Film

Mass Fraction y



Temperature T



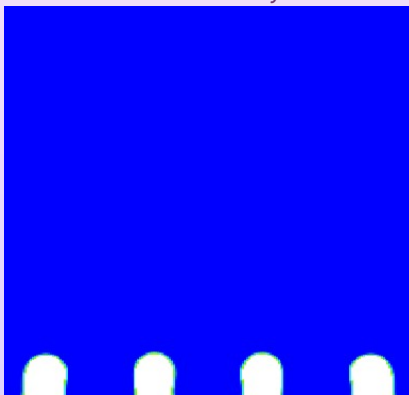
◀ Geometry

▶ Play

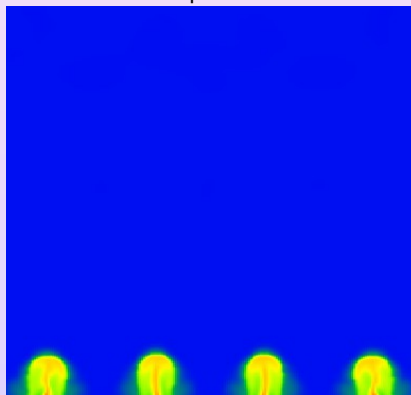
▶▶ Skip

Film

Mass Fraction y



Temperature T



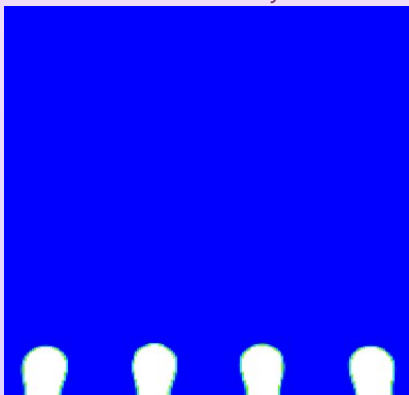
◀ Geometry

▶ Play

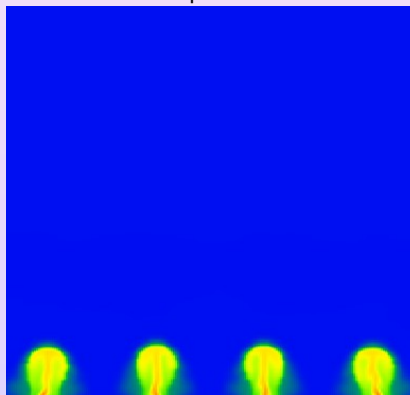
▶▶ Skip

Film

Mass Fraction y



Temperature T



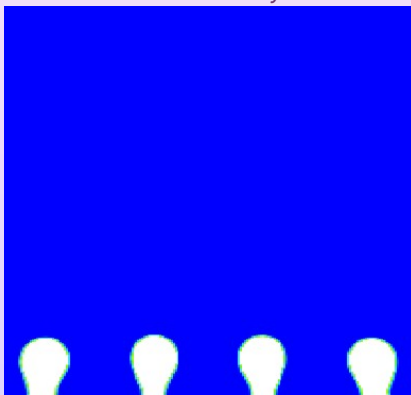
◀ Geometry

▶ Play

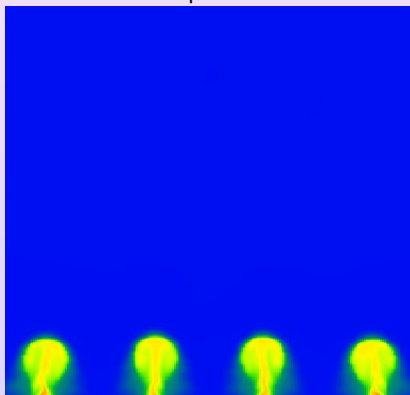
▶▶ Skip

Film

Mass Fraction y



Temperature T



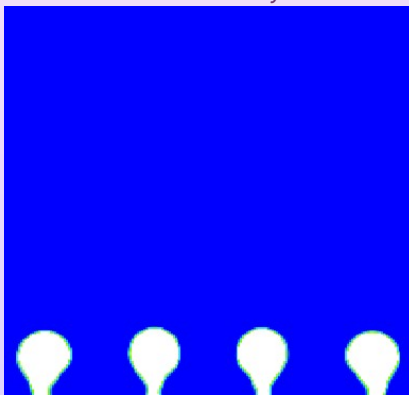
◀ Geometry

▶ Play

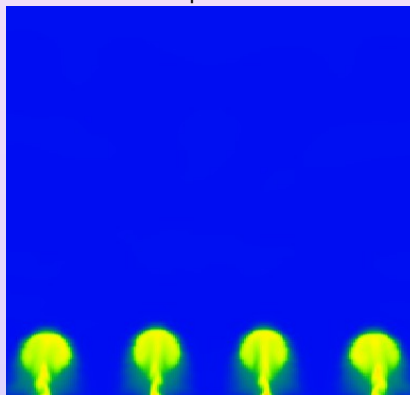
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Film

Mass Fraction y



Temperature T



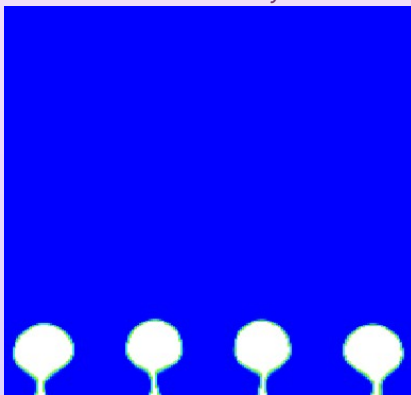
◀ Geometry

▶ Play

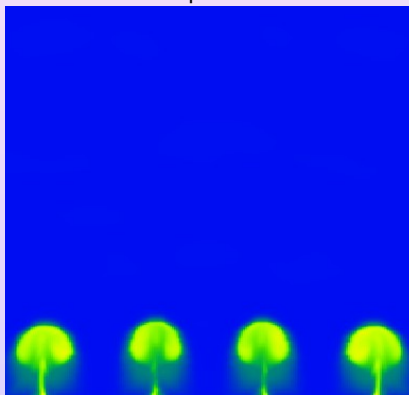
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Film

Mass Fraction y



Temperature T



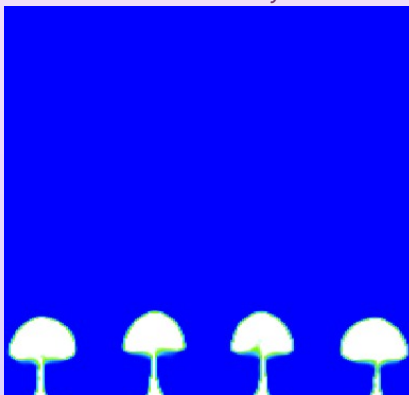
◀ Geometry

▶ Play

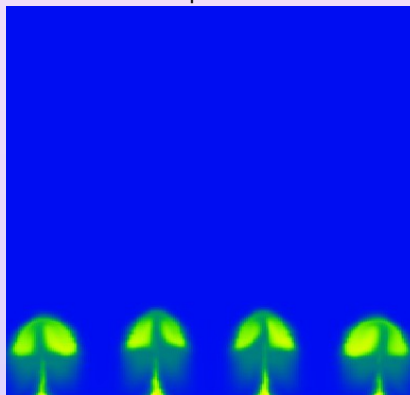
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Film

Mass Fraction y



Temperature T



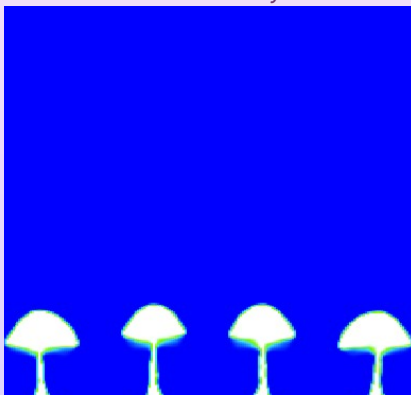
◀ Geometry

▶ Play

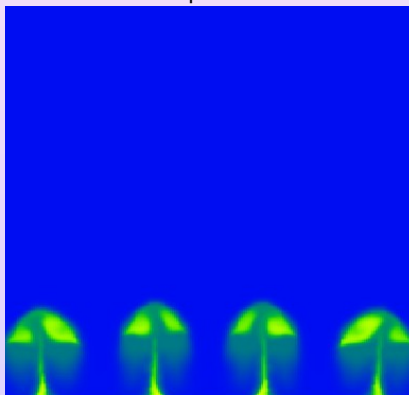
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Film

Mass Fraction y



Temperature T



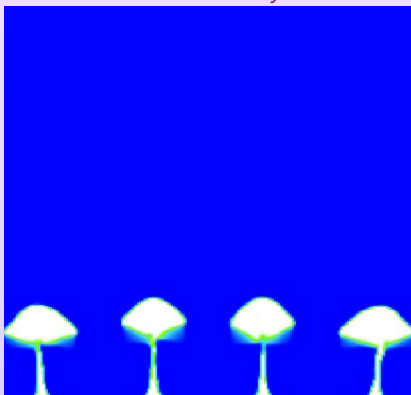
◀ Geometry

▶ Play

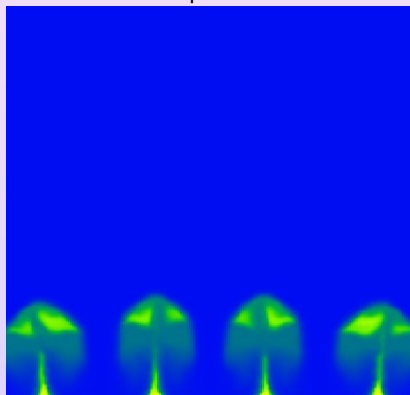
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Film

Mass Fraction y



Temperature T



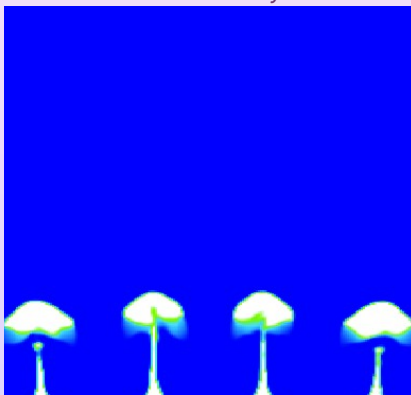
◀ Geometry

▶ Play

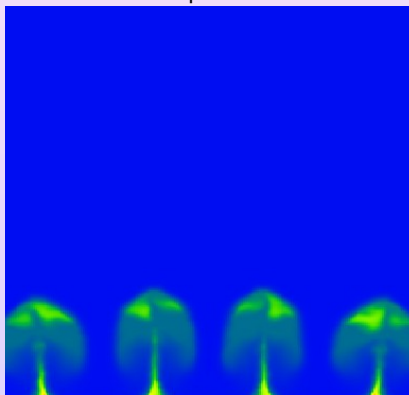
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Film

Mass Fraction y



Temperature T



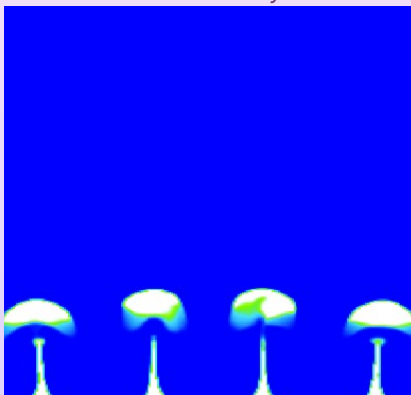
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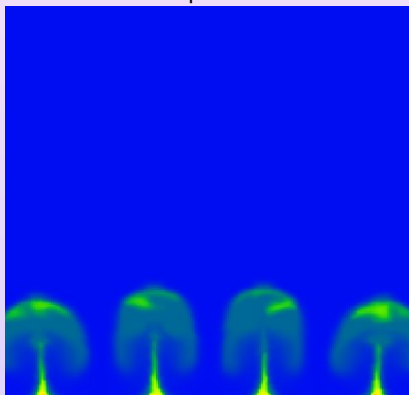
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Film

Mass Fraction y



Temperature T



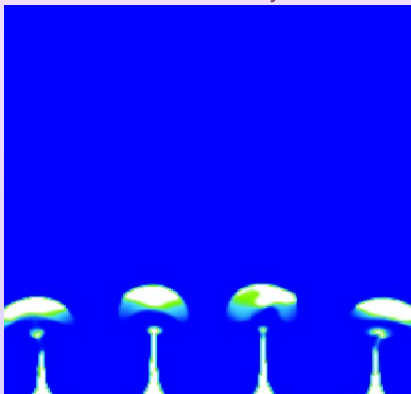
◀ Geometry

▶ Play

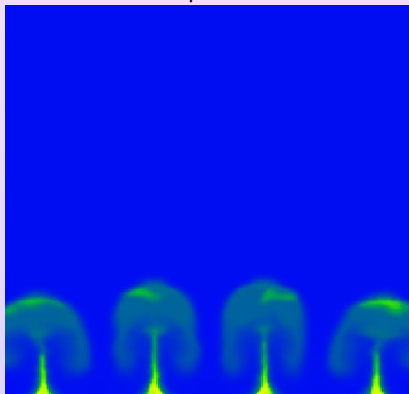
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Film

Mass Fraction y



Temperature T



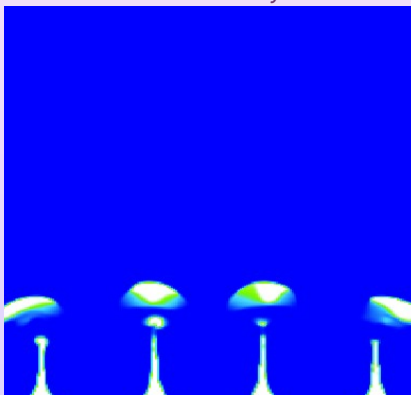
◀ Geometry

▶ Play

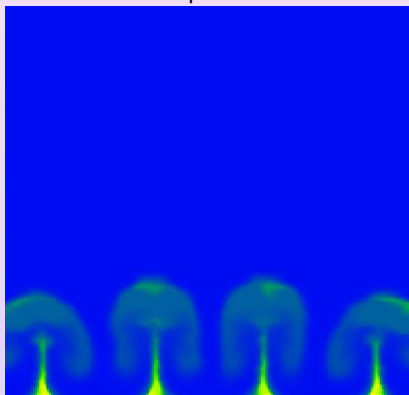
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Film

Mass Fraction y



Temperature T



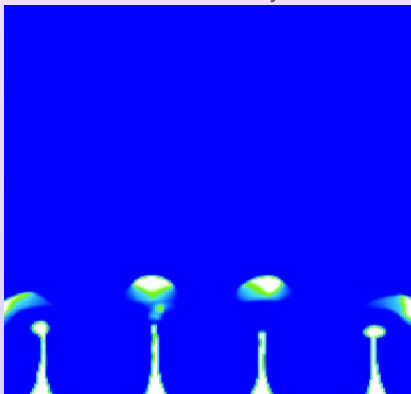
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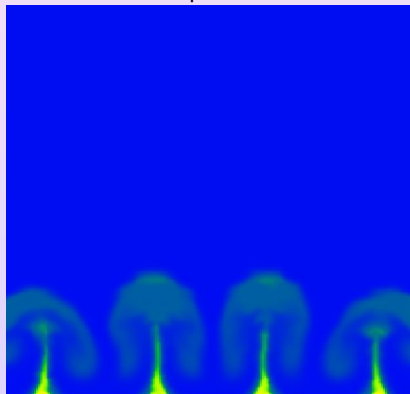
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Film

Mass Fraction y



Temperature T



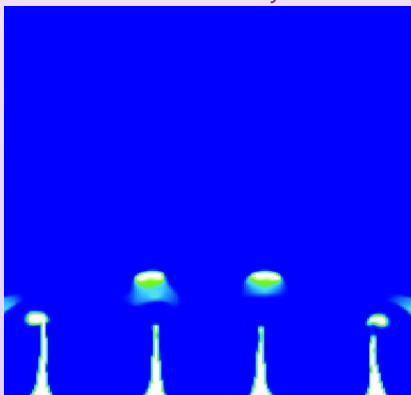
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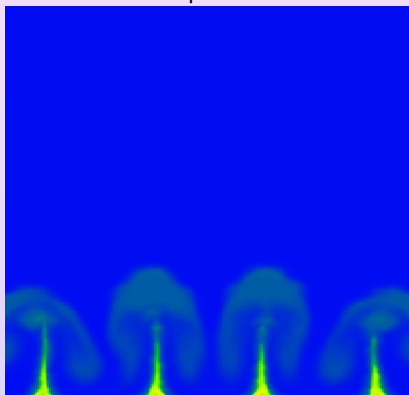
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Film

Mass Fraction y



Temperature T



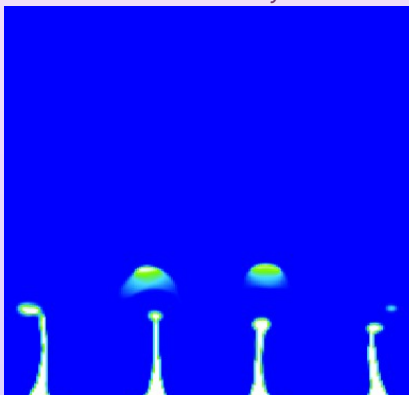
◀ Geometry

▶ Play

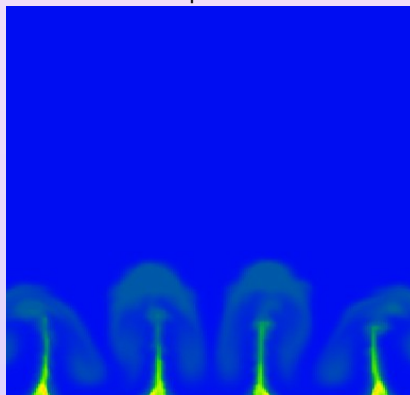
▶▶ Skip

Film

Mass Fraction y



Temperature T



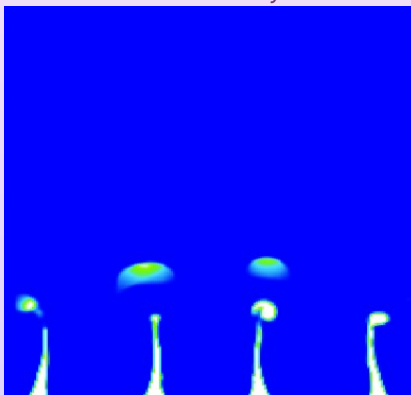
◀ Geometry

▶ Play

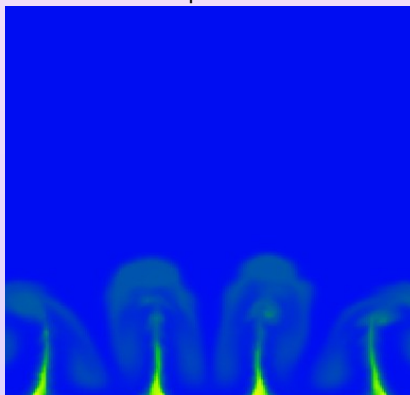
▶▶ Skip

Film

Mass Fraction y



Temperature T



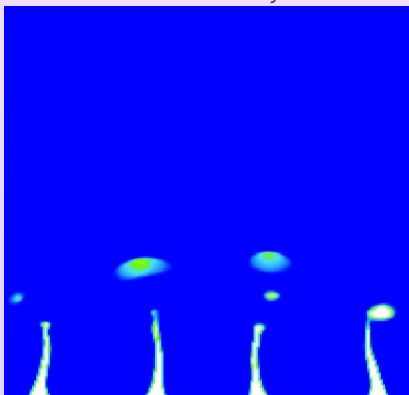
◀ Geometry

▶ Play

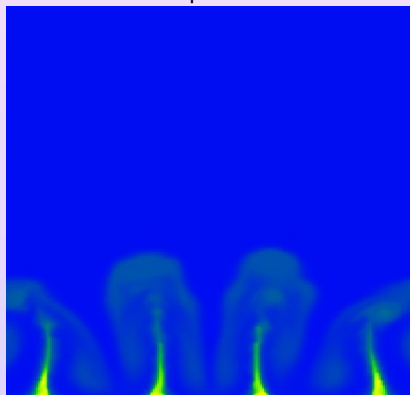
▶▶ Skip

Film

Mass Fraction y



Temperature T



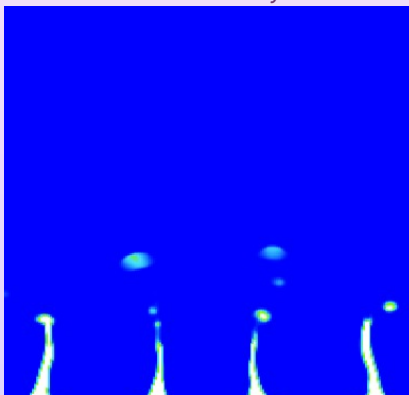
◀ Geometry

▶ Play

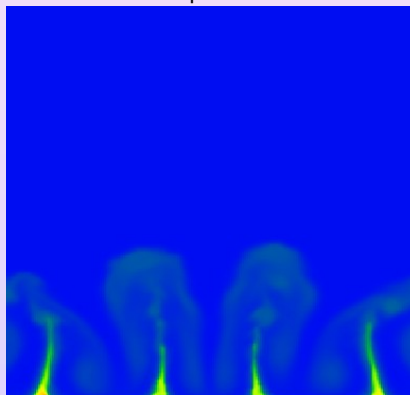
▶▶ Skip

Film

Mass Fraction y



Temperature T



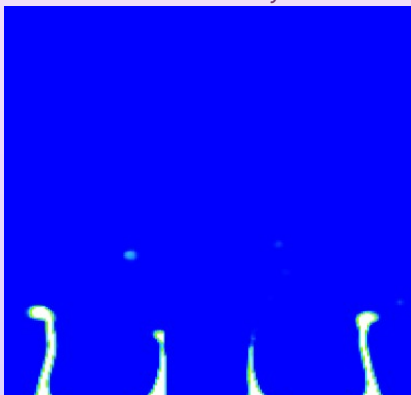
◀ Geometry

▶ Play

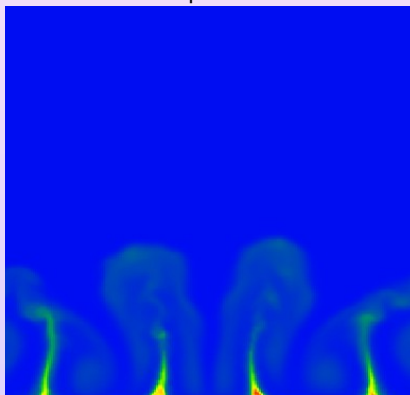
▶▶ Skip

Film

Mass Fraction y



Temperature T



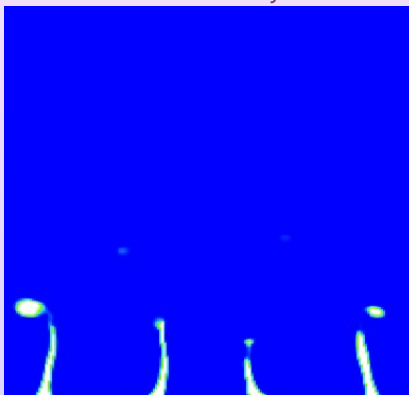
◀ Geometry

▶ Play

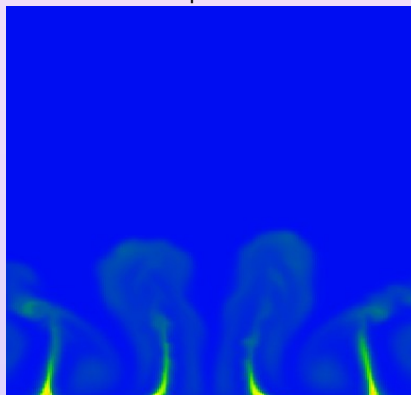
▶▶ Skip

Film

Mass Fraction y



Temperature T



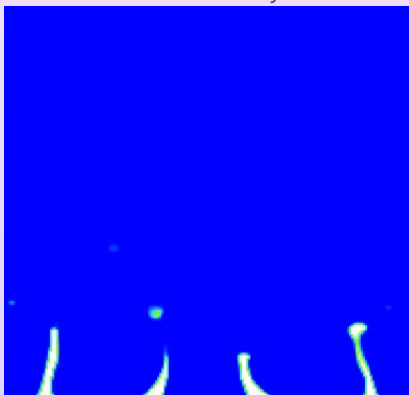
◀ Geometry

▶ Play

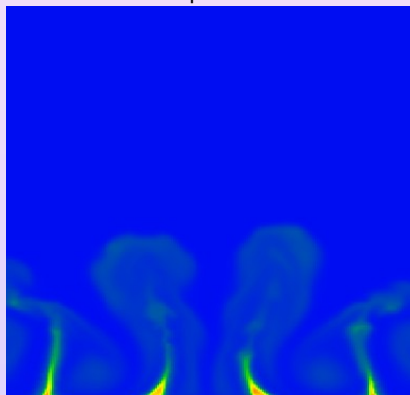
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Film

Mass Fraction y



Temperature T



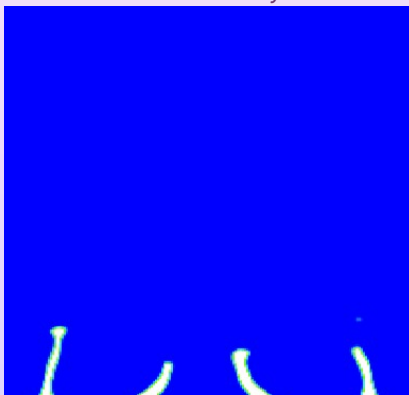
◀ Geometry

▶ Play

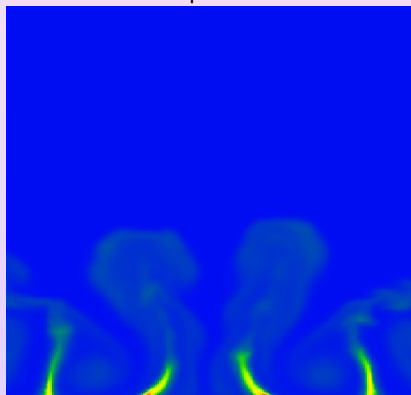
▶▶ Skip

Film

Mass Fraction y



Temperature T



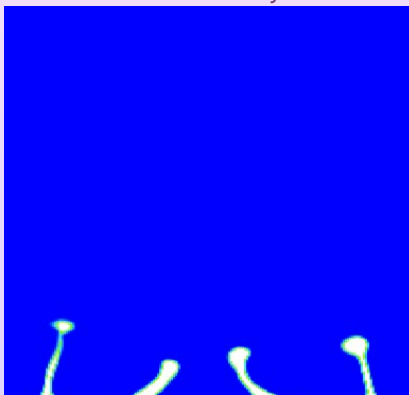
◀ Geometry

▶ Play

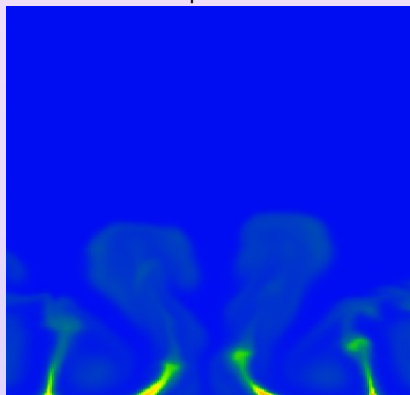
▶▶ Skip

Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

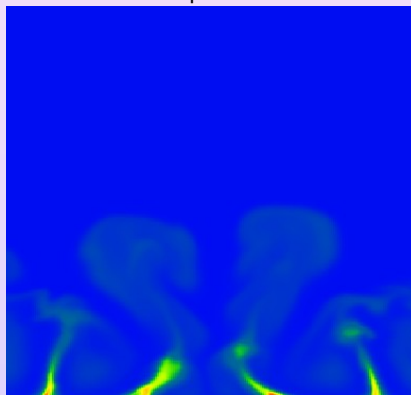
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Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

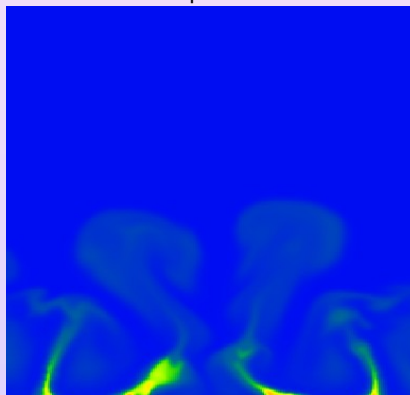
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Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

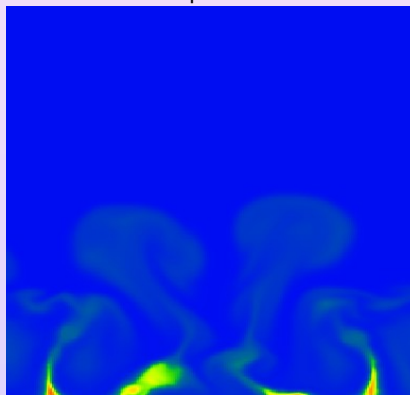
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Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

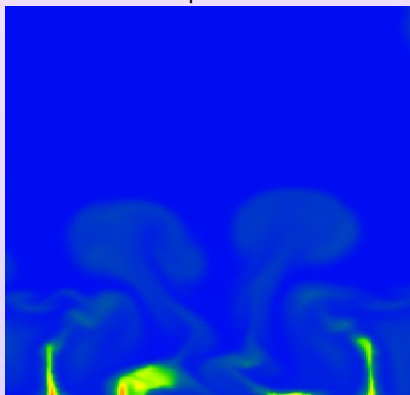
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Film

Mass Fraction y



Temperature T



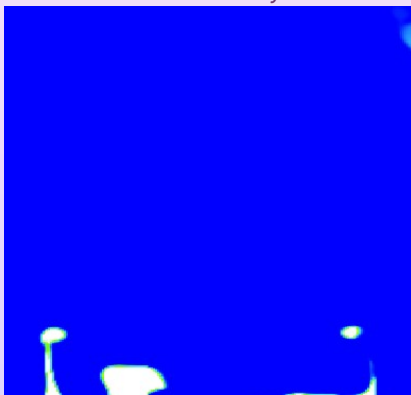
◀ Geometry

▶ Play

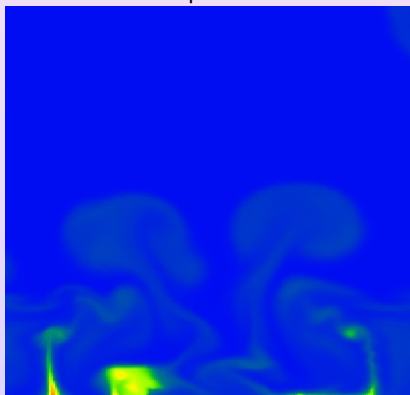
▶▶ Skip

Film

Mass Fraction y



Temperature T



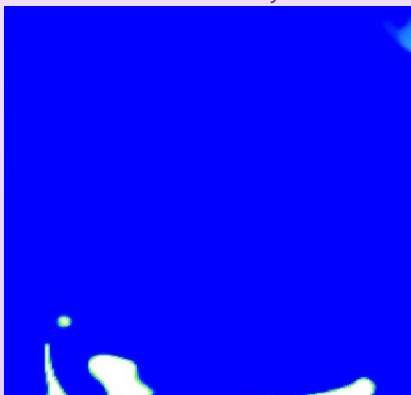
◀ Geometry

▶ Play

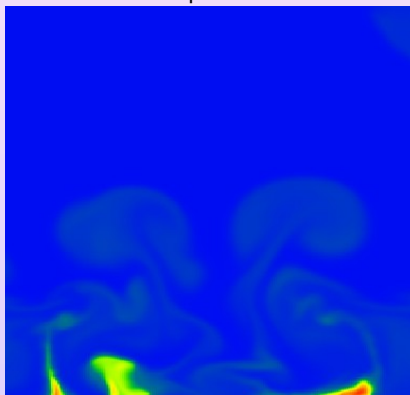
▶▶ Skip

Film

Mass Fraction y



Temperature T



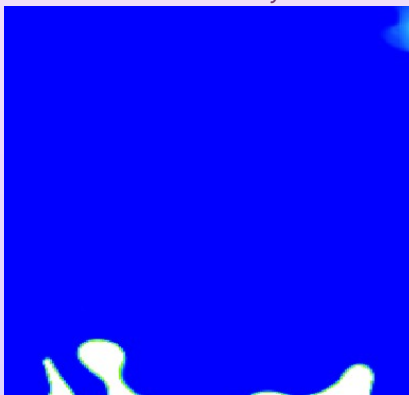
◀ Geometry

▶ Play

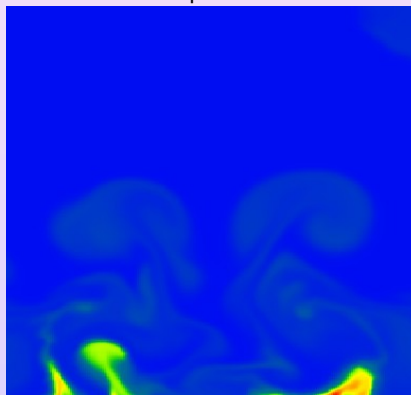
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Film

Mass Fraction y



Temperature T



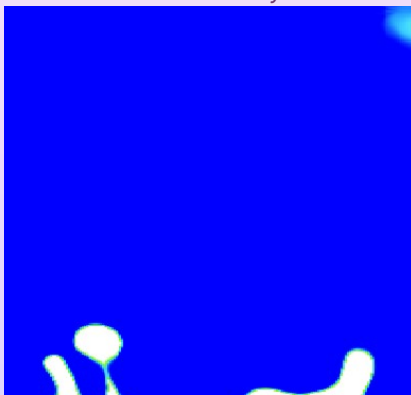
◀ Geometry

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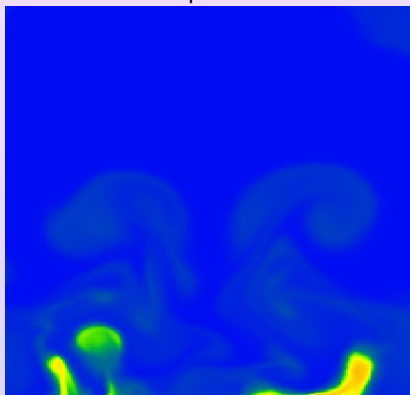
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Film

Mass Fraction y



Temperature T



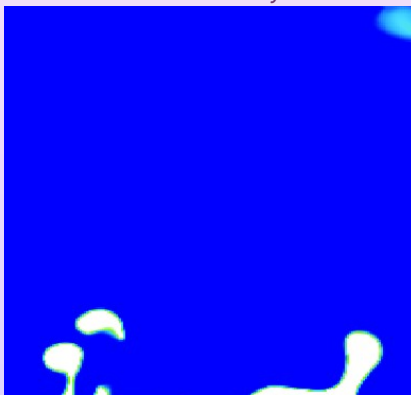
◀ Geometry

▶ Play

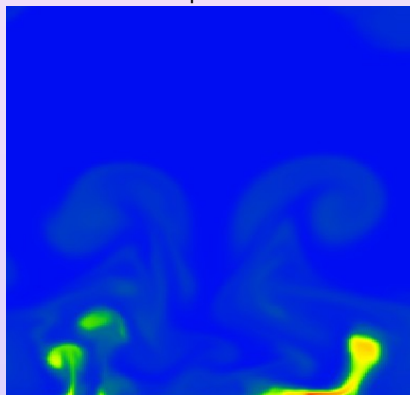
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Film

Mass Fraction y



Temperature T



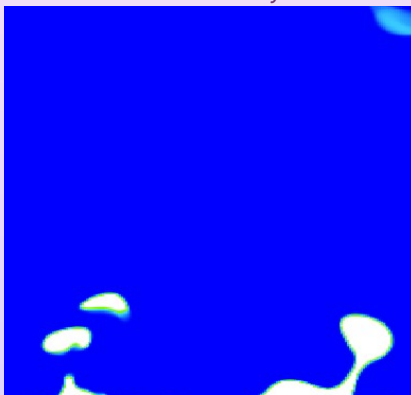
◀ Geometry

▶ Play

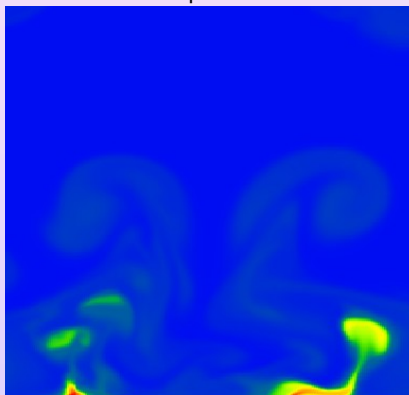
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Film

Mass Fraction y



Temperature T



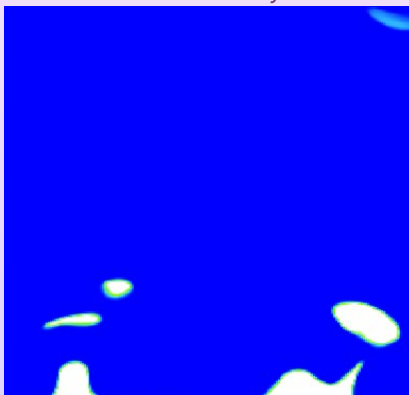
◀ Geometry

▶ Play

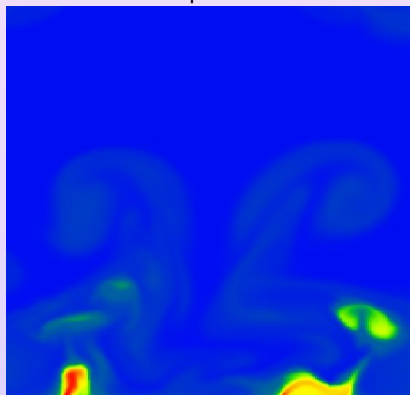
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Film

Mass Fraction y



Temperature T



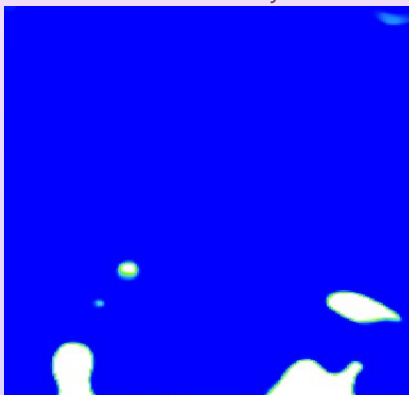
◀ Geometry

▶ Play

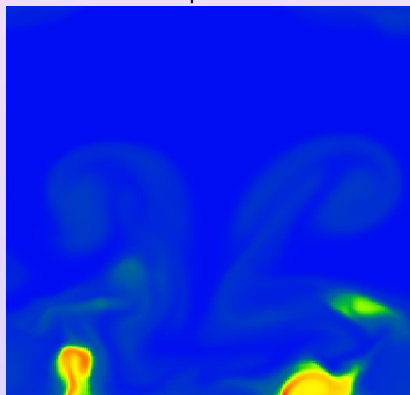
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Film

Mass Fraction y



Temperature T



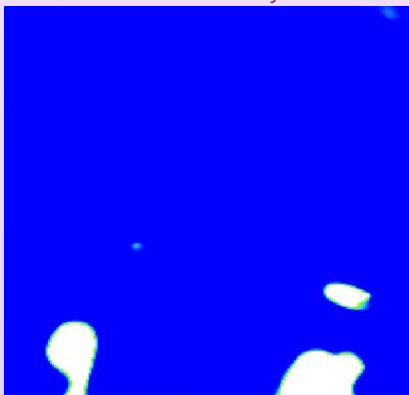
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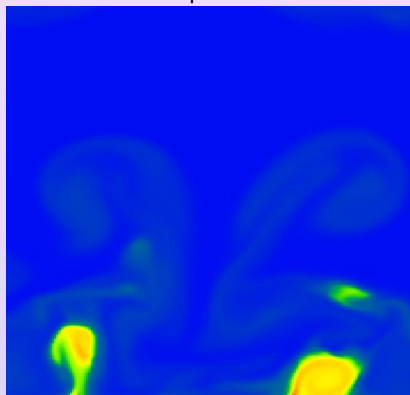
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Film

Mass Fraction y



Temperature T



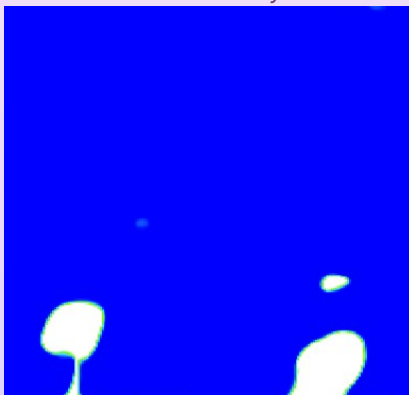
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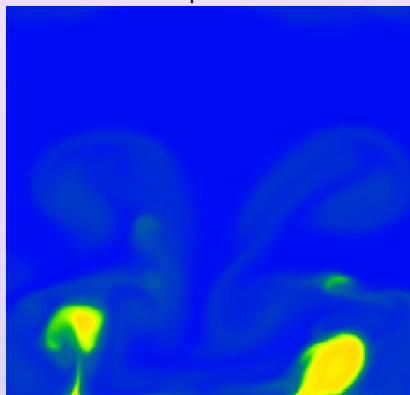
▶▶ Skip

Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

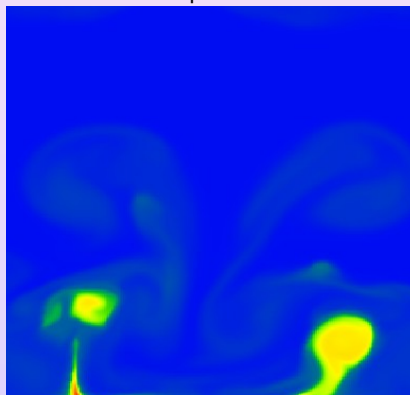
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Film

Mass Fraction y



Temperature T



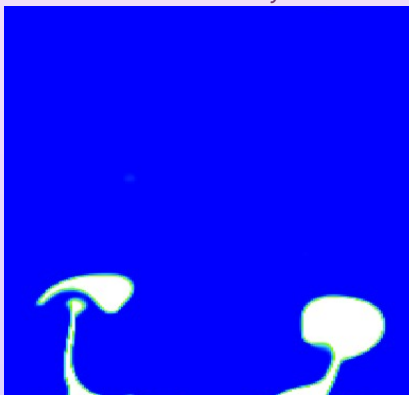
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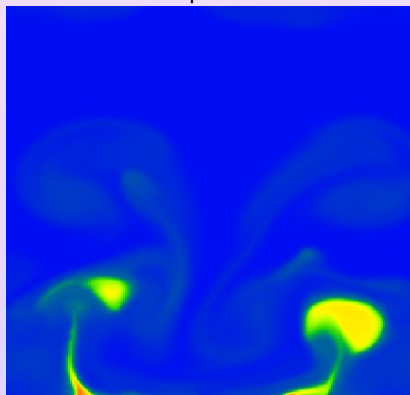
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Film

Mass Fraction y



Temperature T



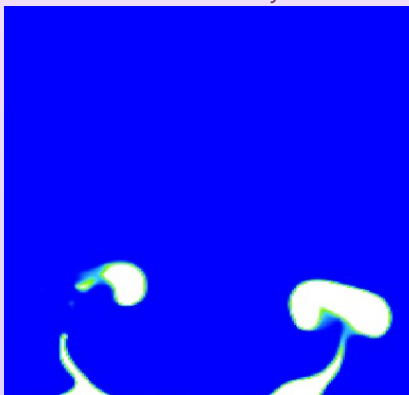
◀ Geometry

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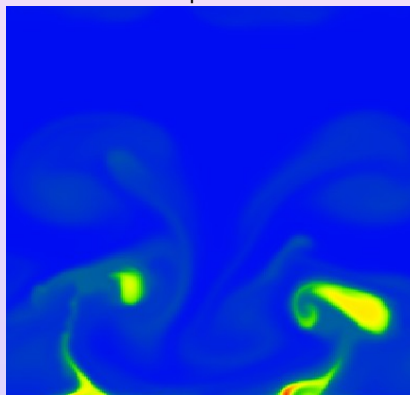
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Film

Mass Fraction y



Temperature T



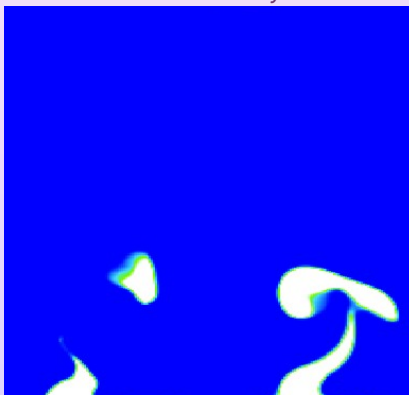
◀ Geometry

▶ Play

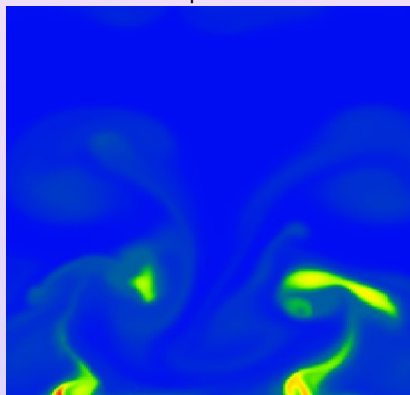
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Film

Mass Fraction y



Temperature T



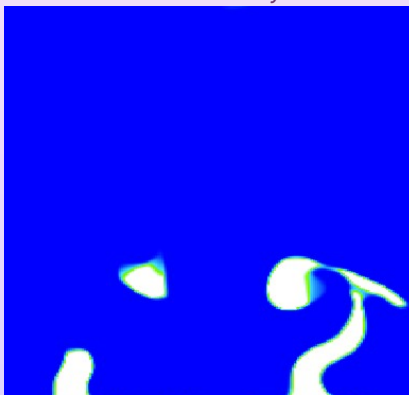
◀ Geometry

▶ Play

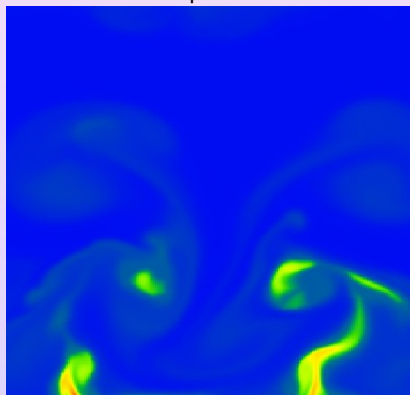
▶▶ Skip

Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

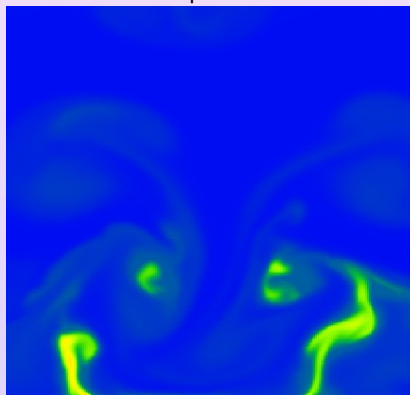
▶▶ Skip

Film

Mass Fraction y



Temperature T



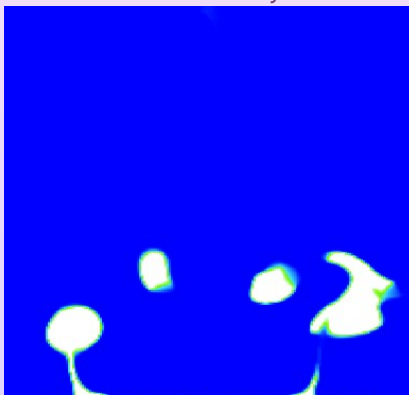
◀ Geometry

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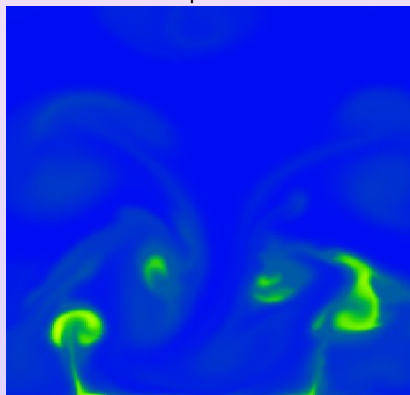
▶▶ Skip

Film

Mass Fraction y



Temperature T



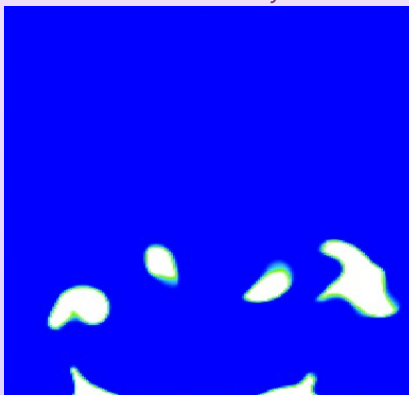
◀ Geometry

▶ Play

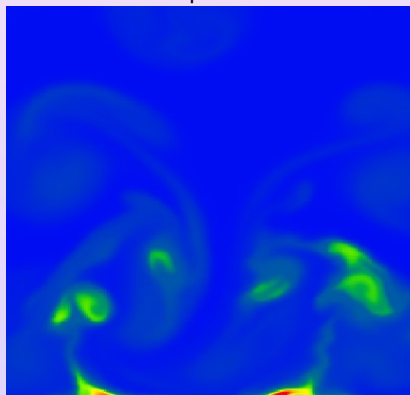
▶▶ Skip

Film

Mass Fraction y



Temperature T



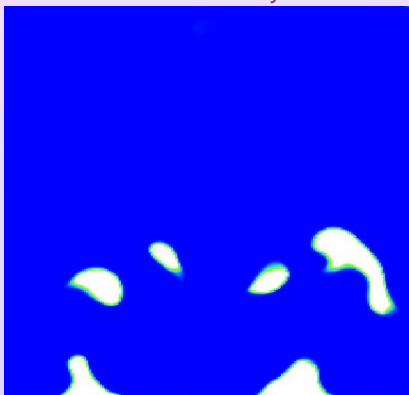
◀ Geometry

▶ Play

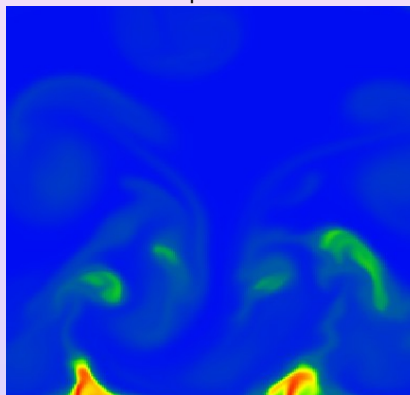
▶▶ Skip

Film

Mass Fraction y



Temperature T



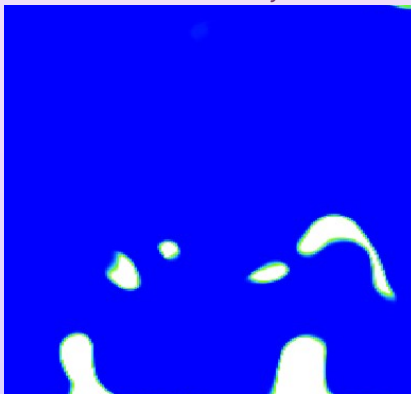
◀ Geometry

▶ Play

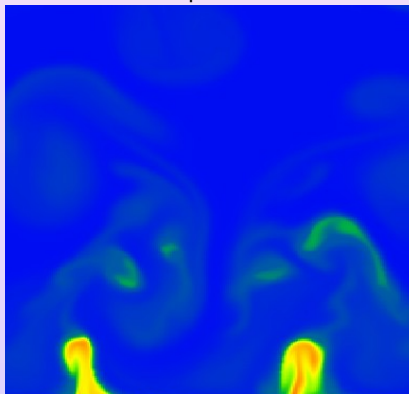
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Film

Mass Fraction y



Temperature T



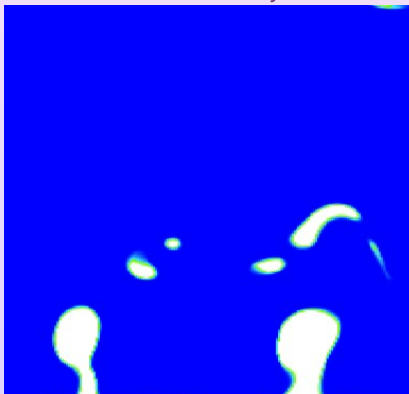
◀ Geometry

▶ Play

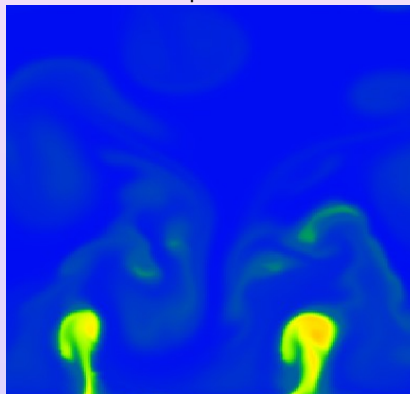
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Film

Mass Fraction y



Temperature T



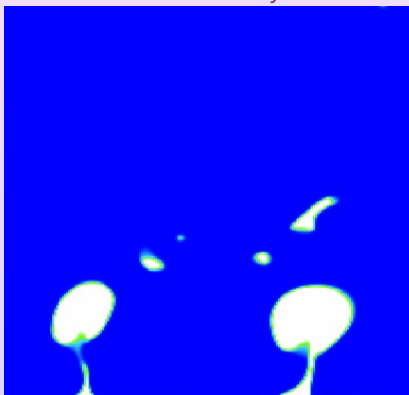
◀ Geometry

▶ Play

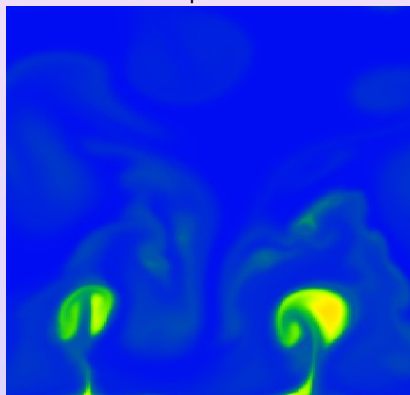
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Film

Mass Fraction y



Temperature T



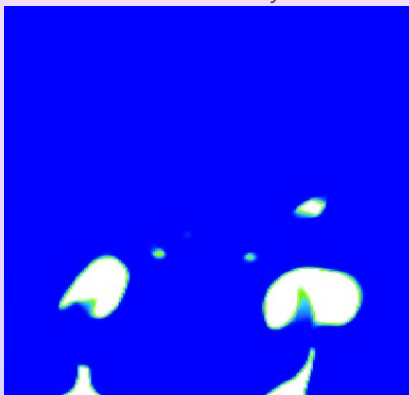
◀ Geometry

▶ Play

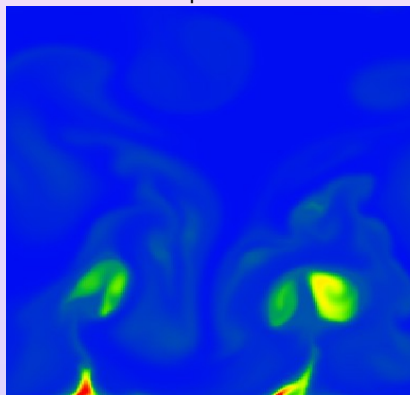
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Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

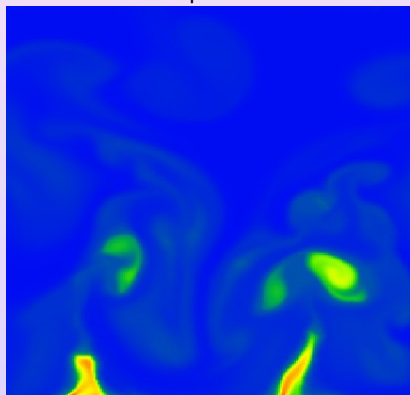
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Film

Mass Fraction y



Temperature T



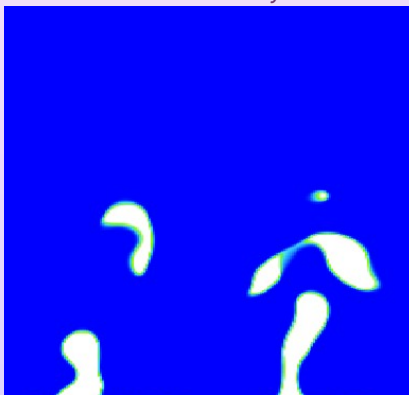
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▶ Play

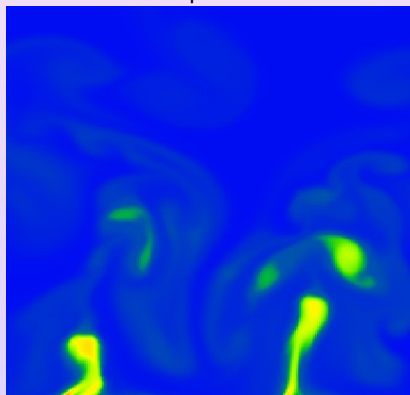
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Film

Mass Fraction y



Temperature T



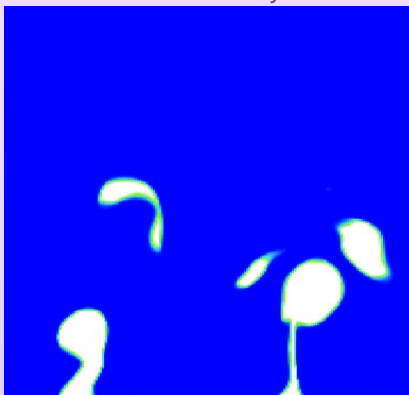
◀ Geometry

▶ Play

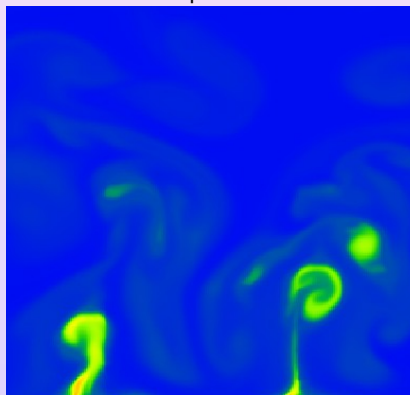
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Film

Mass Fraction y



Temperature T



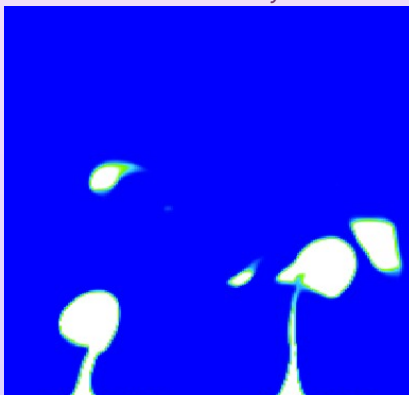
◀ Geometry

▶ Play

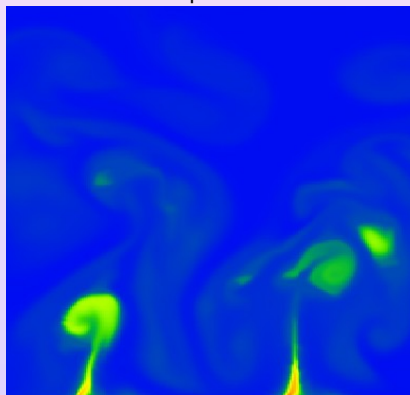
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Film

Mass Fraction y



Temperature T



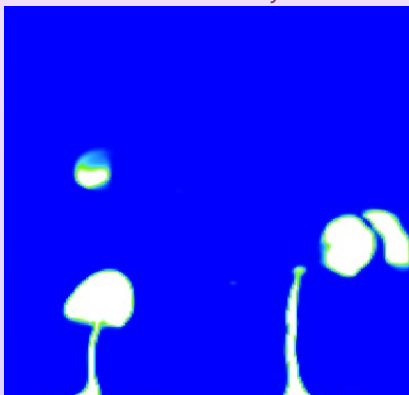
◀ Geometry

▶ Play

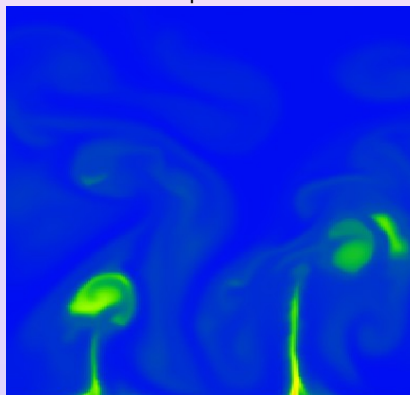
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Film

Mass Fraction y



Temperature T



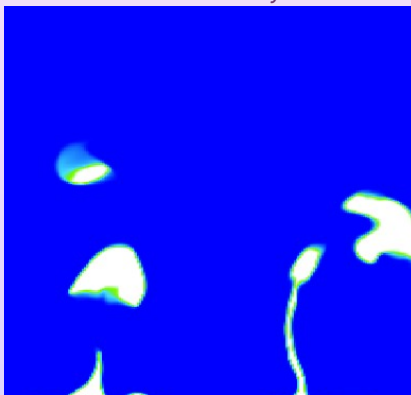
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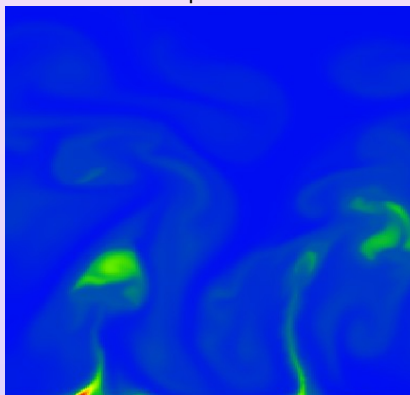
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Film

Mass Fraction y



Temperature T



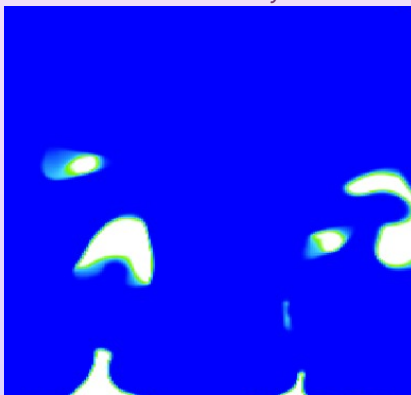
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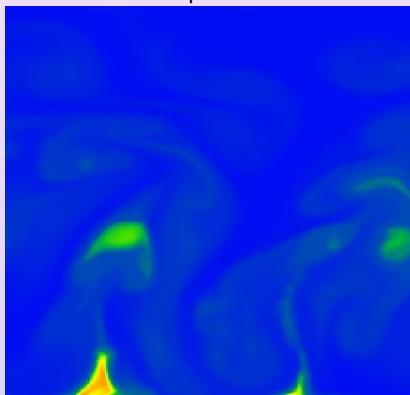
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Film

Mass Fraction y



Temperature T



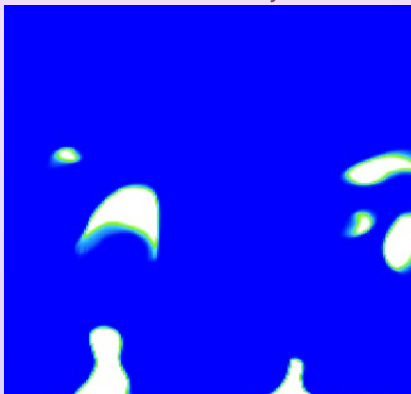
◀ Geometry

▶ Play

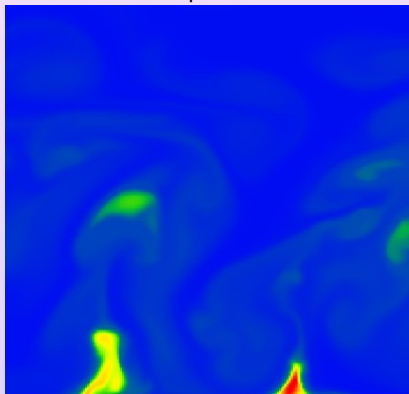
▶▶ Skip

Film

Mass Fraction y



Temperature T



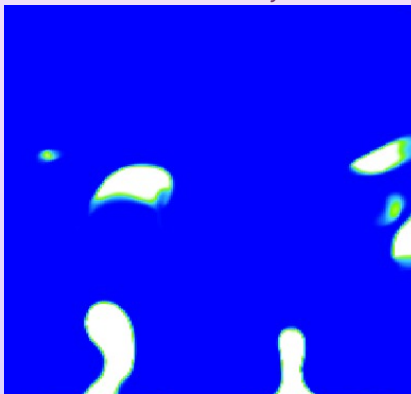
◀ Geometry

▶ Play

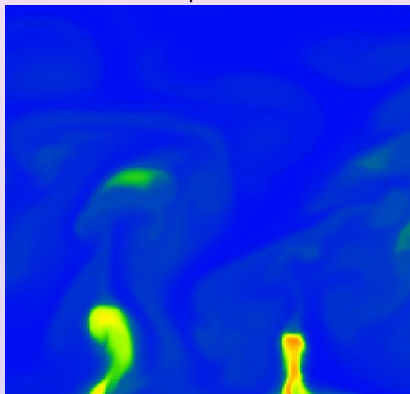
▶▶ Skip

Film

Mass Fraction y



Temperature T



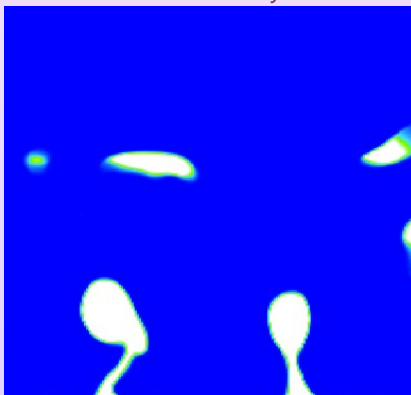
◀ Geometry

▶ Play

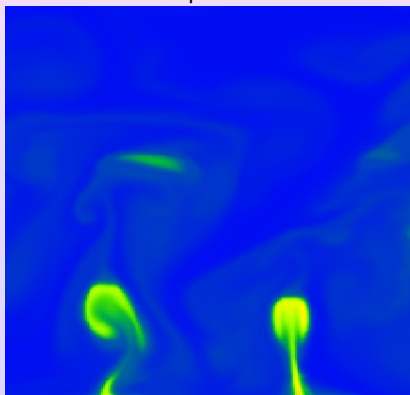
▶▶ Skip

Film

Mass Fraction y



Temperature T



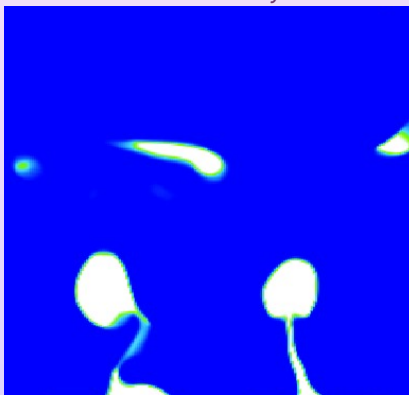
◀ Geometry

▶ Play

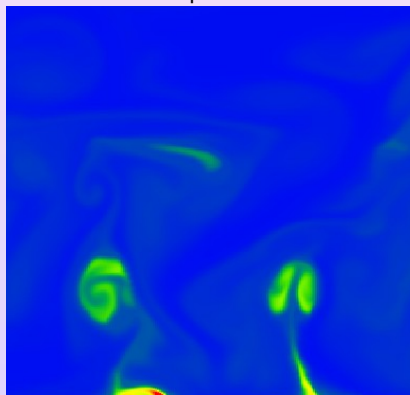
▶▶ Skip

Film

Mass Fraction y



Temperature T



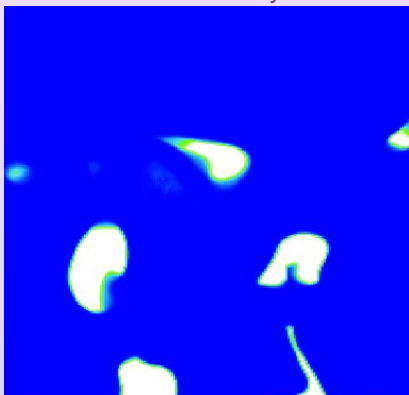
◀ Geometry

▶ Play

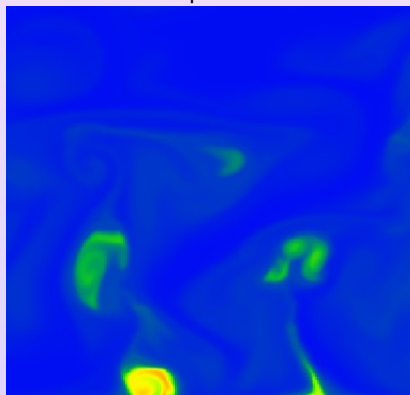
▶▶ Skip

Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

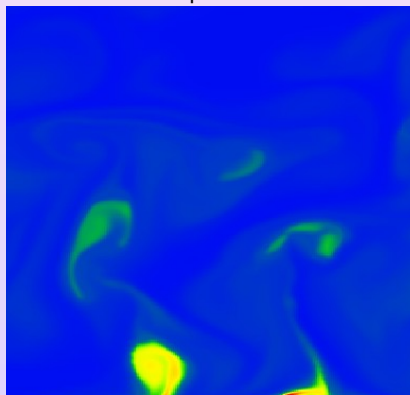
▶▶ Skip

Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

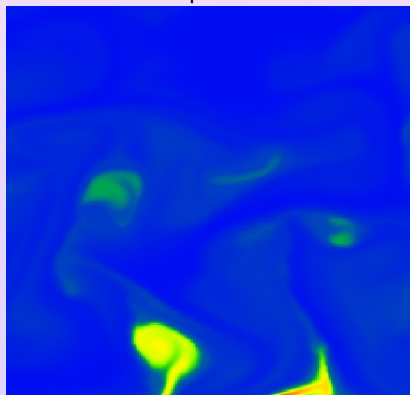
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Film

Mass Fraction y



Temperature T



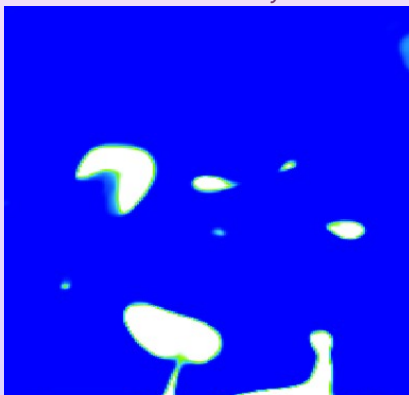
◀ Geometry

▶ Play

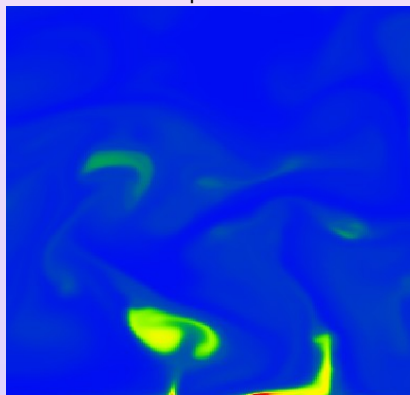
▶▶ Skip

Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

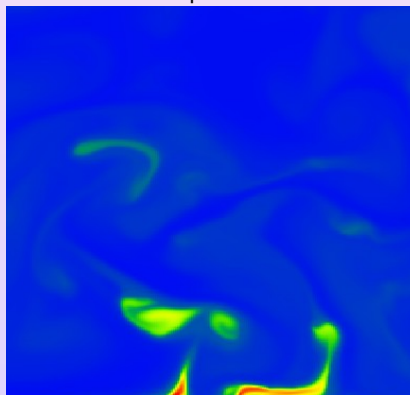
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Film

Mass Fraction y



Temperature T



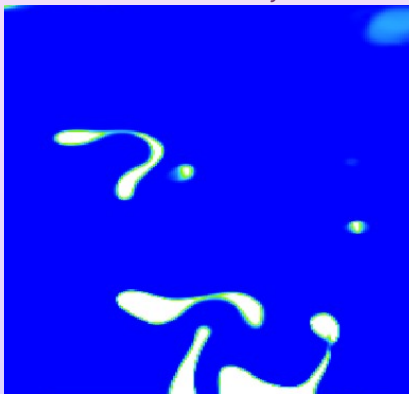
◀ Geometry

▶ Play

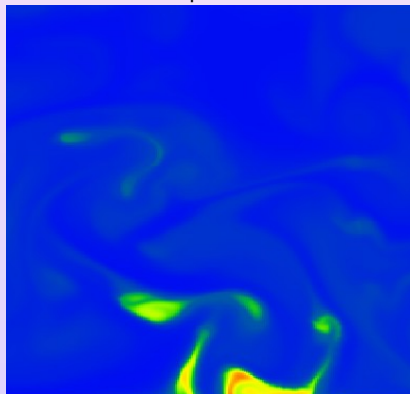
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Film

Mass Fraction y



Temperature T



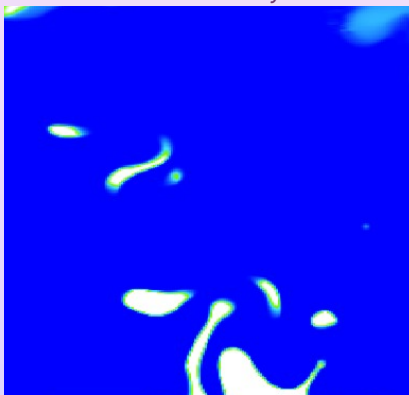
◀ Geometry

▶ Play

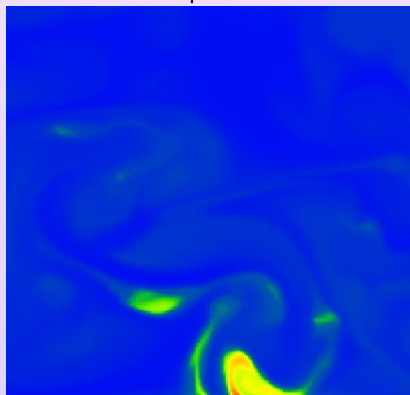
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Film

Mass Fraction y



Temperature T



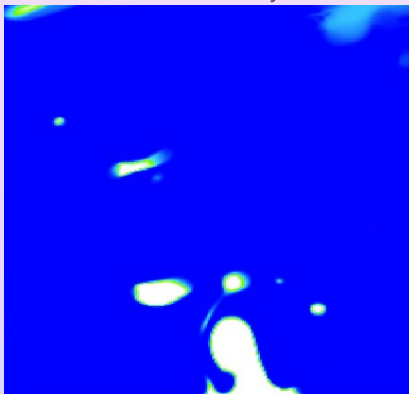
◀ Geometry

▶ Play

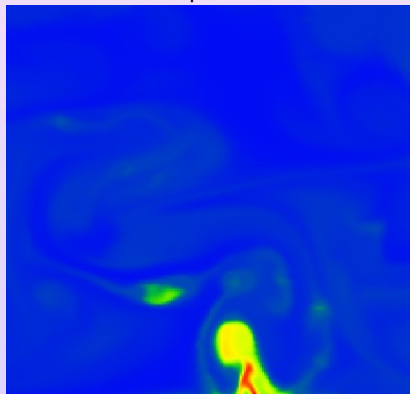
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Film

Mass Fraction y



Temperature T



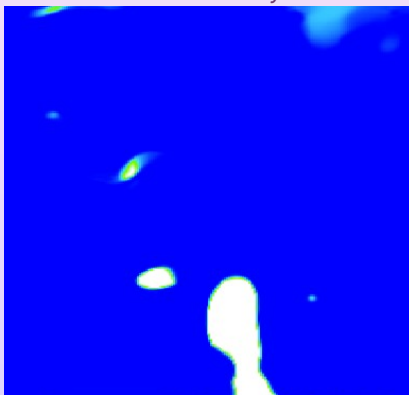
◀ Geometry

▶ Play

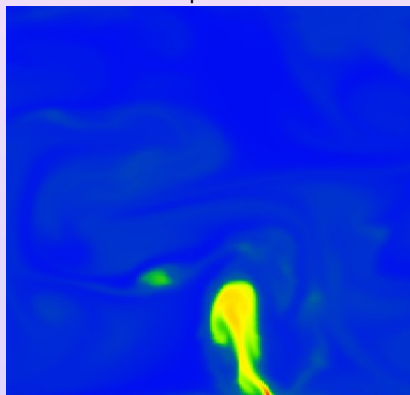
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Film

Mass Fraction y



Temperature T



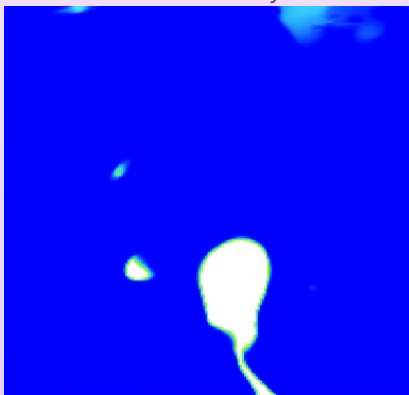
◀ Geometry

▶ Play

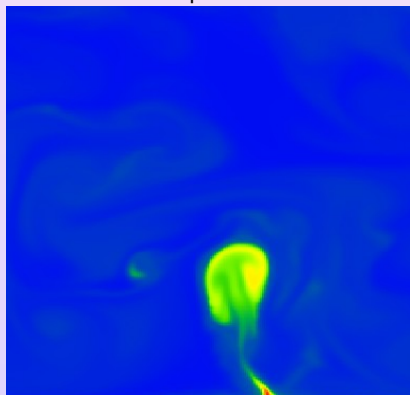
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Film

Mass Fraction y



Temperature T



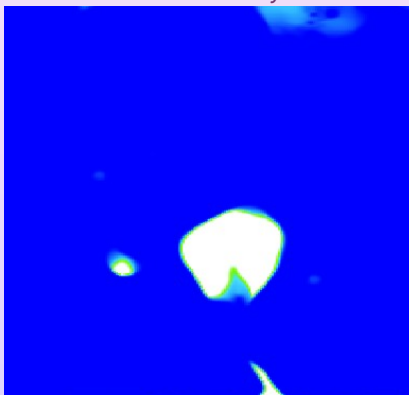
◀ Geometry

▶ Play

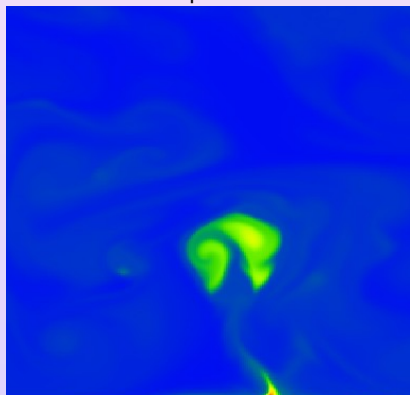
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Film

Mass Fraction y



Temperature T



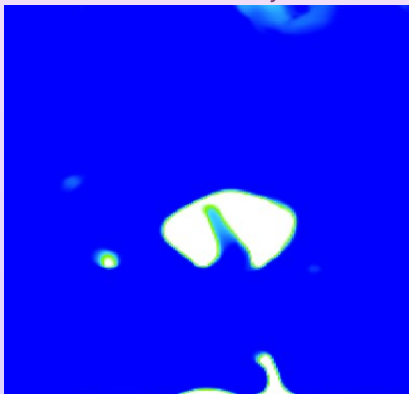
◀ Geometry

▶ Play

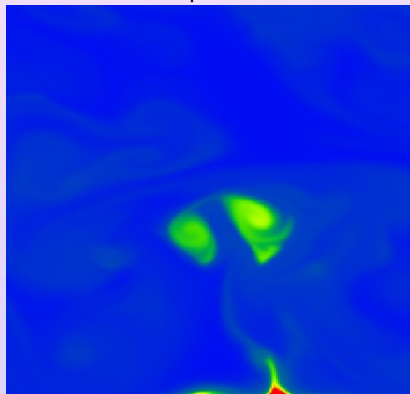
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Film

Mass Fraction y



Temperature T



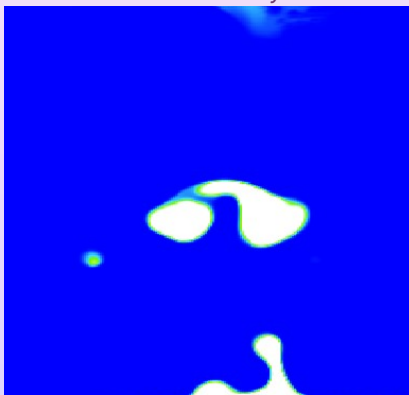
◀ Geometry

▶ Play

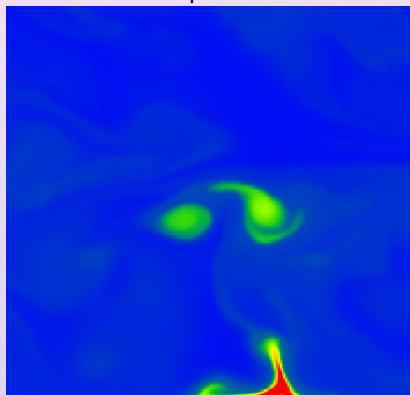
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Film

Mass Fraction y



Temperature T



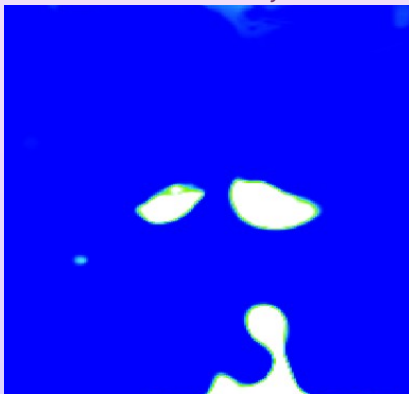
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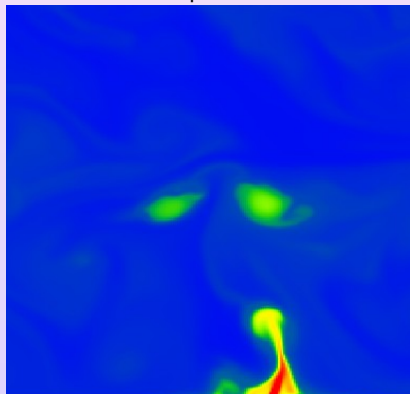
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Film

Mass Fraction y



Temperature T



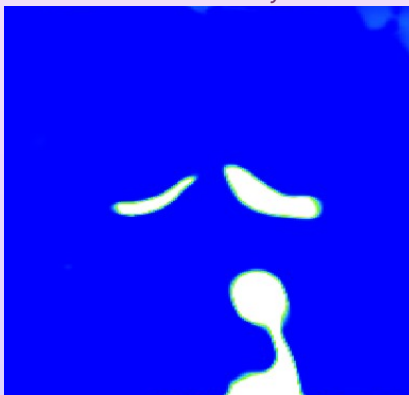
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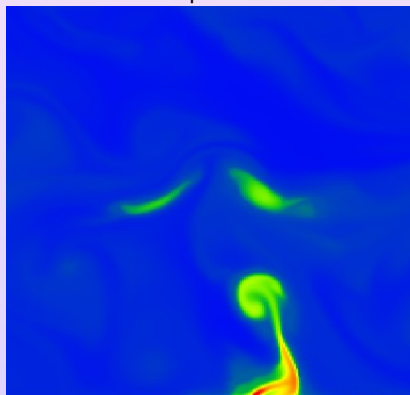
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Film

Mass Fraction y



Temperature T



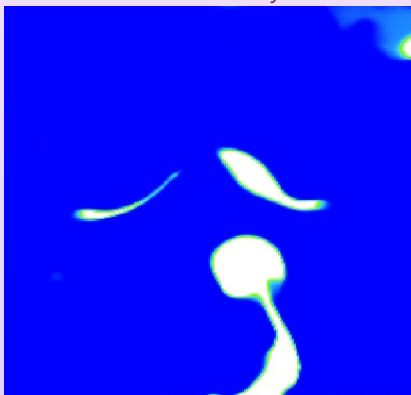
◀ Geometry

▶ Play

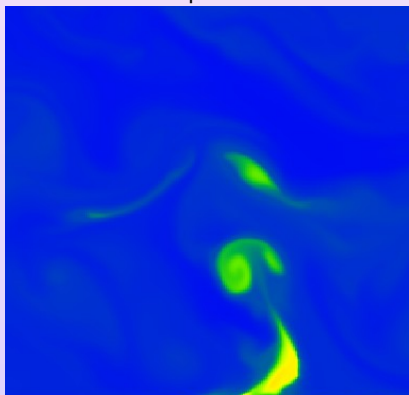
▶▶ Skip

Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

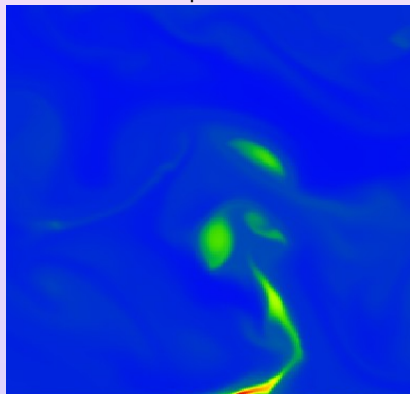
▶▶ Skip

Film

Mass Fraction y



Temperature T



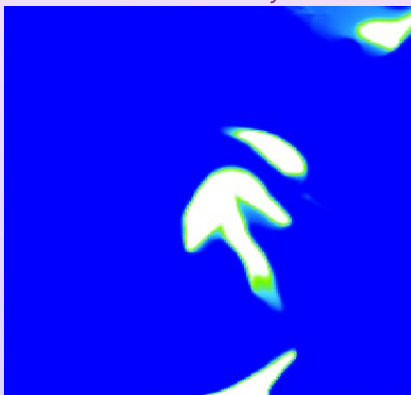
◀ Geometry

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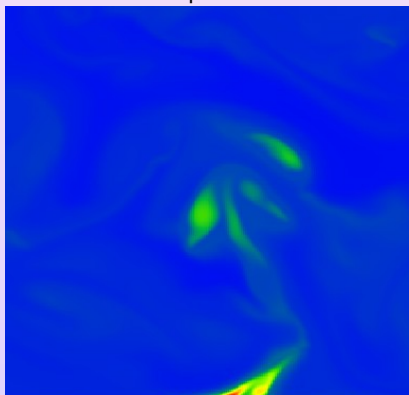
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Film

Mass Fraction y



Temperature T



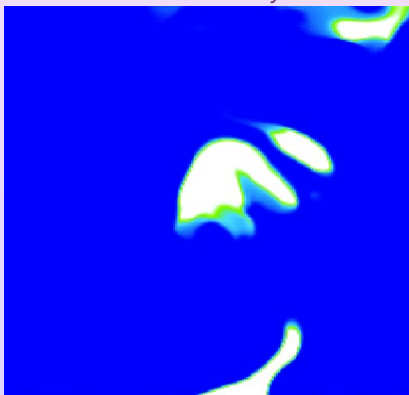
◀ Geometry

▶ Play

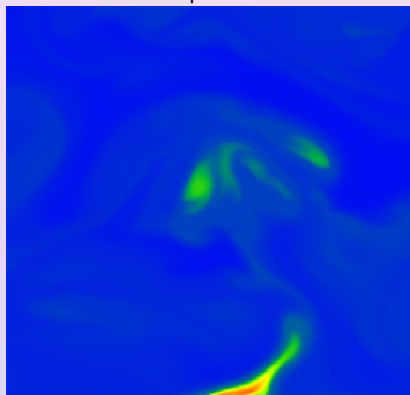
▶▶ Skip

Film

Mass Fraction y



Temperature T



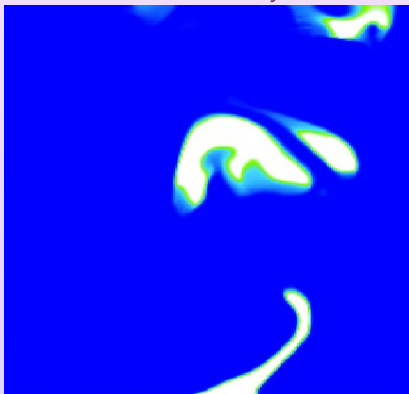
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▶ Play

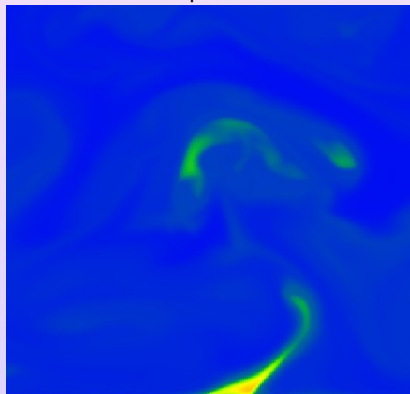
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Film

Mass Fraction y



Temperature T



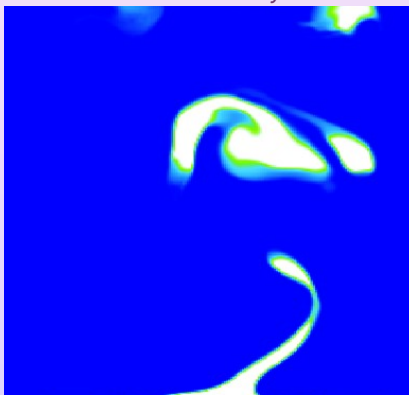
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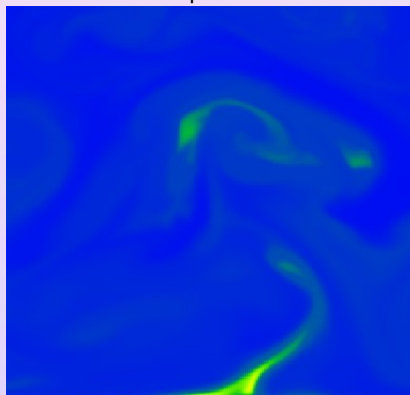
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Film

Mass Fraction y



Temperature T



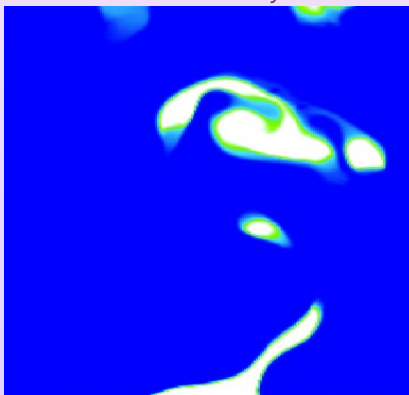
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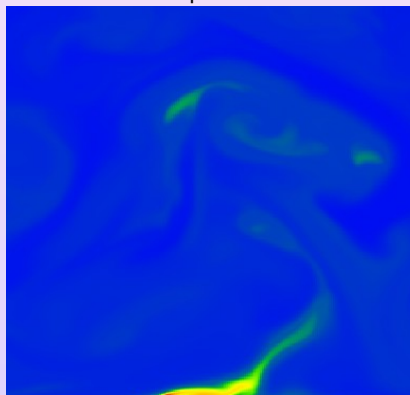
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Film

Mass Fraction y



Temperature T



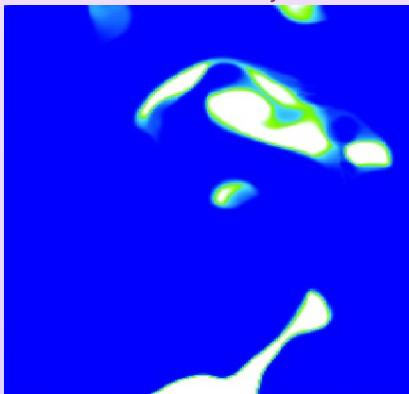
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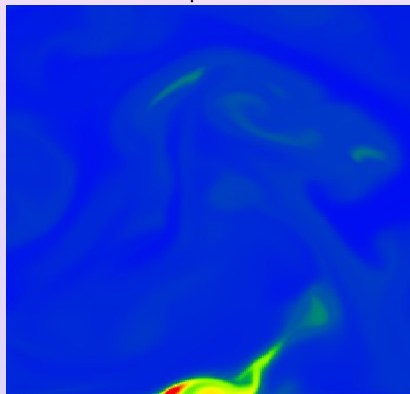
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Film

Mass Fraction y



Temperature T



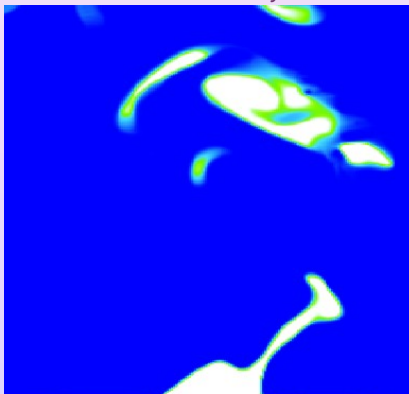
◀ Geometry

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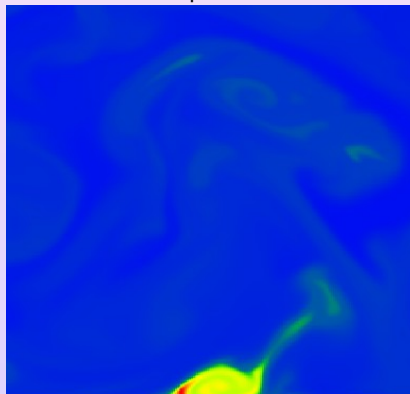
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Film

Mass Fraction y



Temperature T



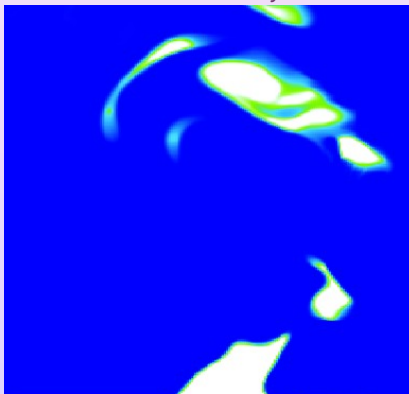
◀ Geometry

▶ Play

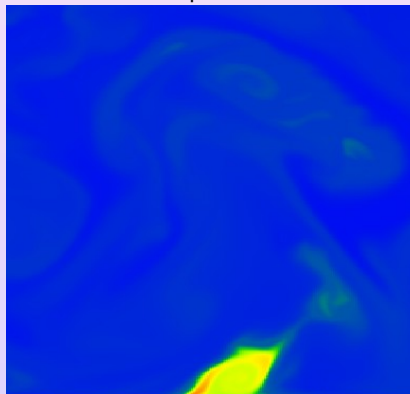
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Film

Mass Fraction y



Temperature T



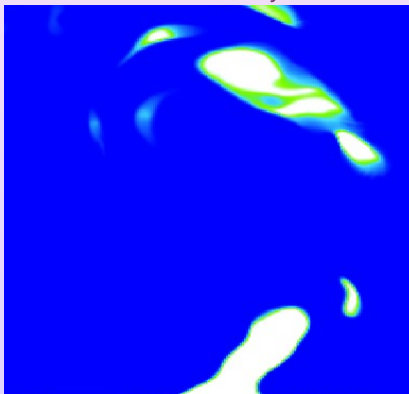
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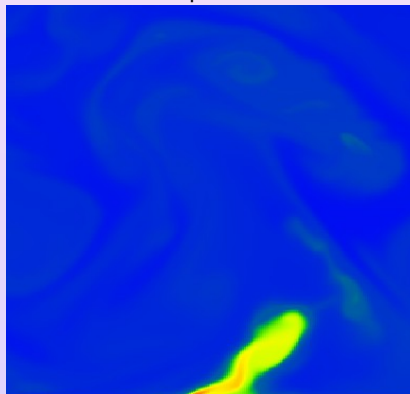
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Film

Mass Fraction y



Temperature T



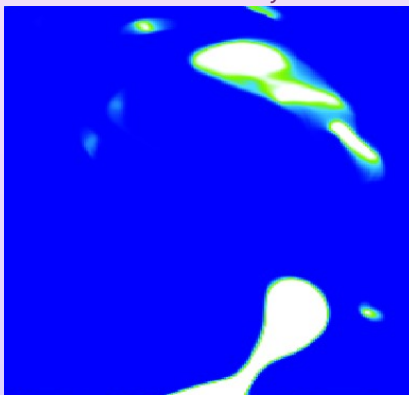
◀ Geometry

▶ Play

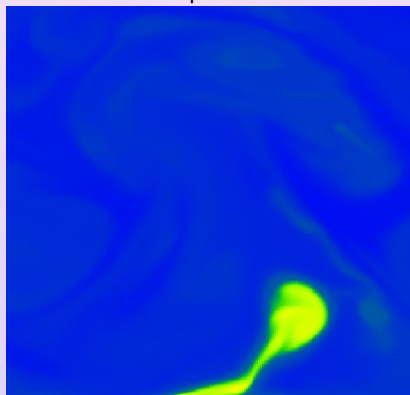
▶▶ Skip

Film

Mass Fraction y



Temperature T



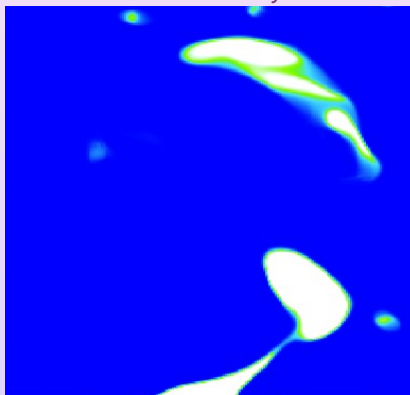
◀ Geometry

▶ Play

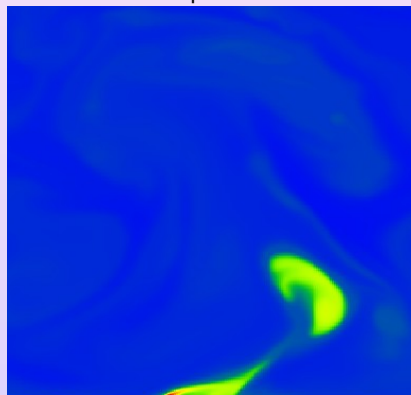
▶▶ Skip

Film

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Temperature T



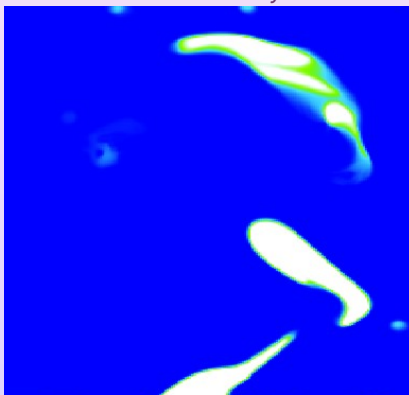
◀ Geometry

▶ Play

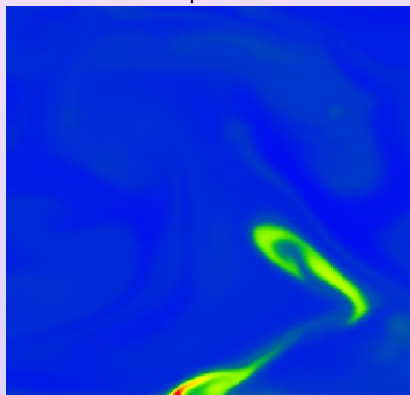
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Film

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Temperature T



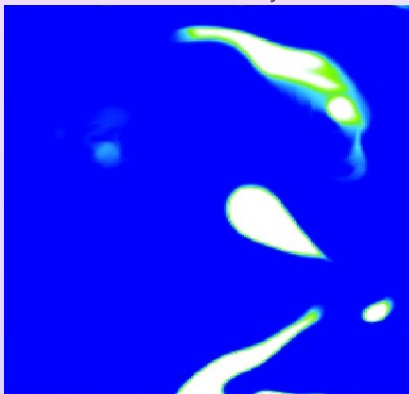
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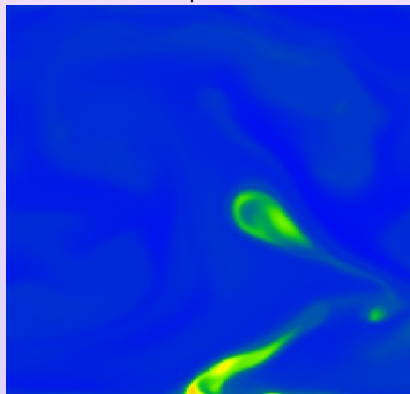
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Mass Fraction y



Temperature T



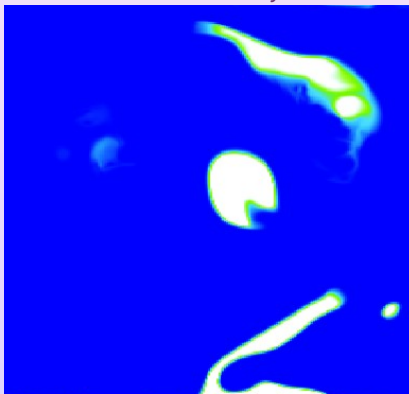
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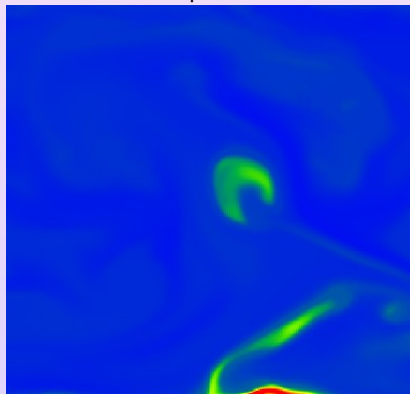
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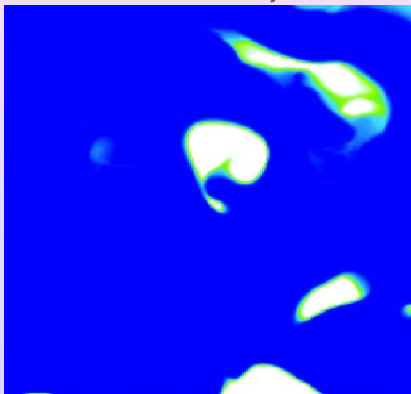
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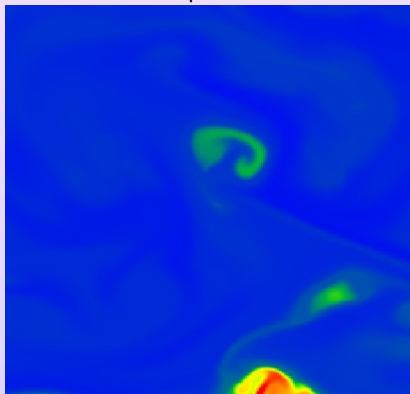
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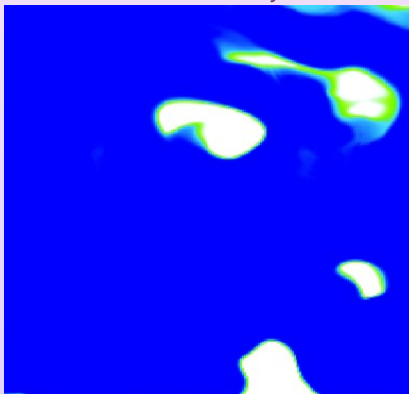
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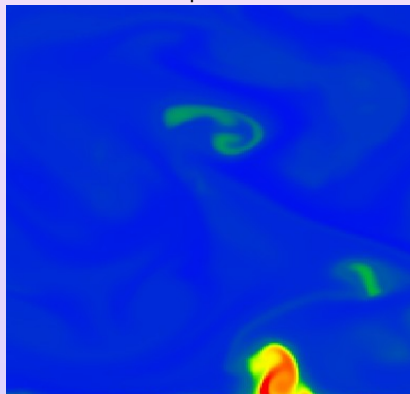
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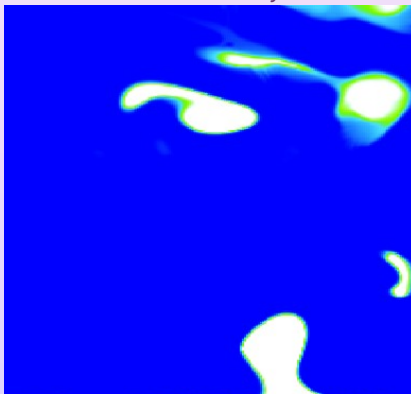
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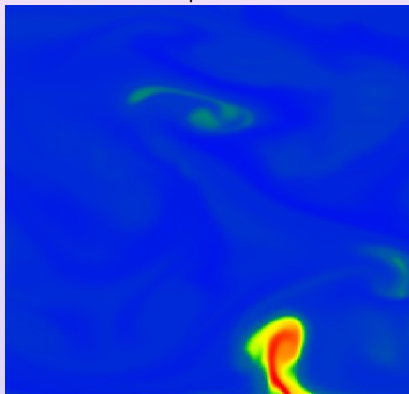
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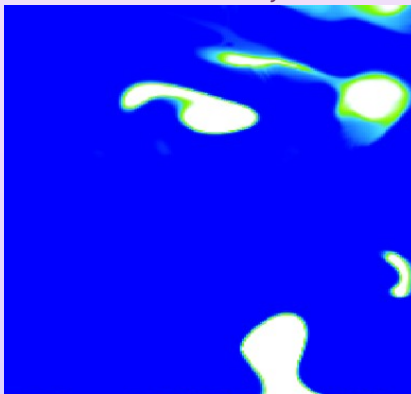
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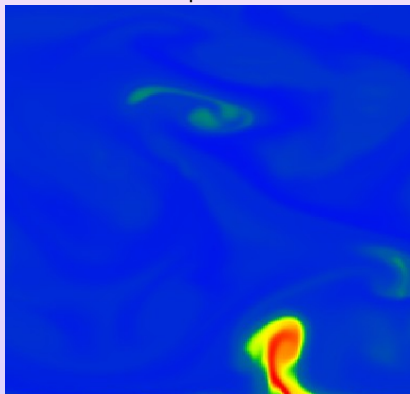
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Summary

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

Outline

1 Context

2 Model

- Equation of State WITHOUT Phase Change
- Equation of State WITH Phase Change
- The Phase Change Equation
- Conservation Laws

3 Numerical Approximation

4 Numerical Examples

5 Conclusion

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- Diffuse Interface Model

- ✓ general construction of the Equilibrium EOS (also for tabulated data),
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Appendix

- ▶ Stiffened Gas for Water
- ▶ Tabulated EOS for Water
- ▶ Speed of sound
- ▶ Isentropic curves
- ▶ Surface Tension
- ▶ Metastability
- ▶ Critical Point

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.

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

$$(P, T) \mapsto \varepsilon_\alpha = c_{v\alpha} T \frac{P + \pi_\alpha \gamma_\alpha}{P + \pi_\alpha} + q_\alpha, \quad (P, T) \mapsto \tau_\alpha = c_{v\alpha} (\gamma_\alpha - 1) \frac{T}{P + \pi_\alpha}.$$

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

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

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

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Water Tabulated EOS

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

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

$$T \mapsto \epsilon_{\text{vap}}^{\text{sat}} \approx \widehat{\epsilon}_{\text{vap}}^{\text{sat}} \stackrel{\text{def}}{=} \frac{1}{\sum_{k=0}^6 a_k T^k}$$

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Speed of sound

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

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

- for all \mathbf{w} pure phase state

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

- for all \mathbf{w} equilibrium mixture state

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

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

Speed of sound

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

HESSIAN MATRIX OF $\mathbf{w} \mapsto S^{\text{eq}}$

- for all \mathbf{w} pure phase state

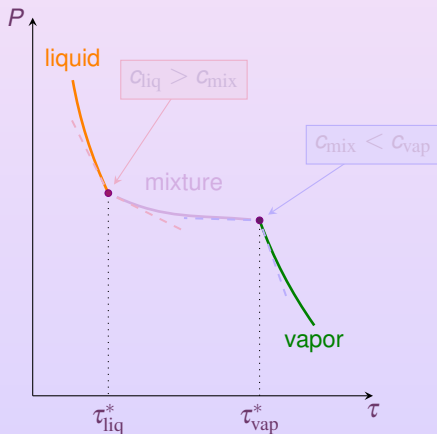
$$\mathbf{v}^T d^2 S^{\text{eq}}(\mathbf{w}) \mathbf{v} < 0 \quad \forall \mathbf{v} \neq 0,$$

- for all \mathbf{w} equilibrium mixture state

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

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

Isentropic curves



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

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

$$\mathcal{G} \stackrel{\text{def}}{=} \frac{\tau^2}{2\gamma P} \frac{\partial^2 P}{\partial \tau^2} \Big|_s$$

● Pure Phases

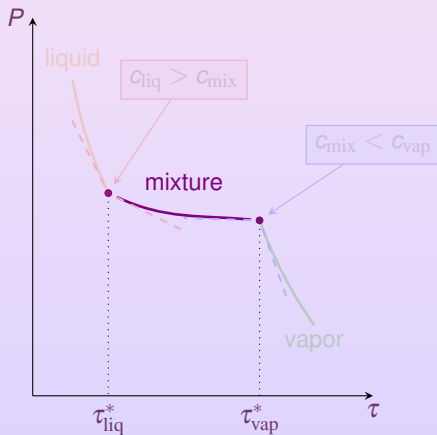
- (H) $\gamma > 0$
- (H) $\Gamma > 0$
- (H) $\mathcal{G} > 0$

● Mixture

- (P) $\gamma > 0$
- (P) $\Gamma > 0$
- (H) $\mathcal{G} > 0$

- Regularity: [J. CORREIA, P.G. LEFLOCH, M.D. THANH]
- Loss of convexity: [A. VOSS]

Isentropic curves



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

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● Pure Phases

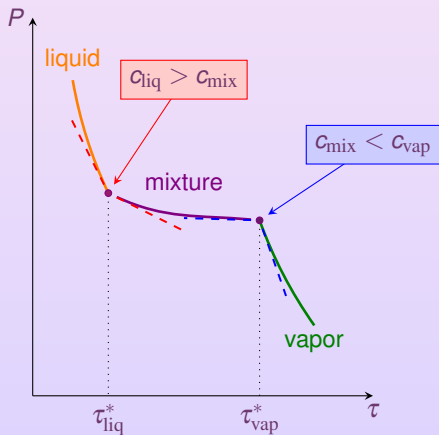
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Isentropic curves



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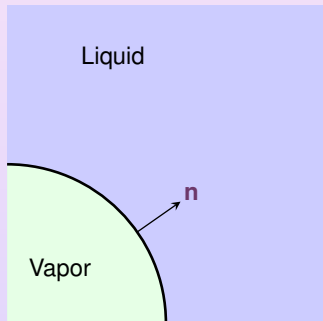
- Mixture

- (P) $\gamma > 0$
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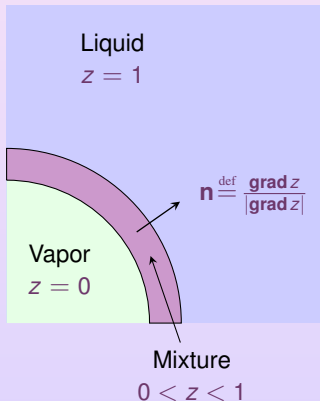
- Regularity: [J. CORREIA, P.G. LEFLOCH, M.D. THANH]
- Loss of convexity: [A. VOSS]

Continuum Surface Force (CSF) Approach

Physical Interface

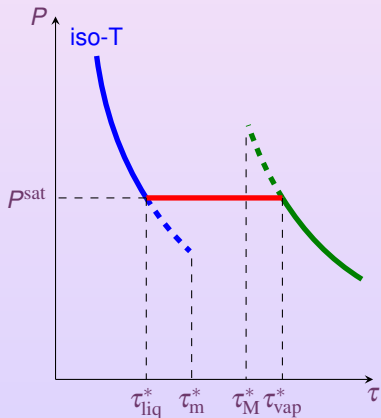


Diffuse Interface



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

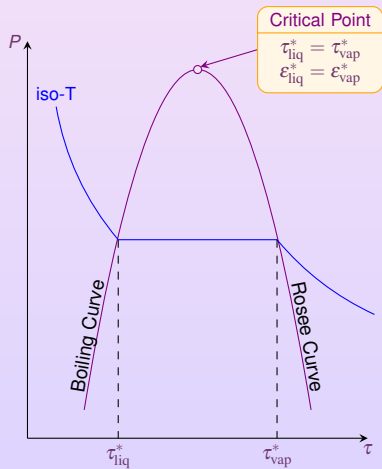
Metastability



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

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

Critical Point



PHYSIC

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

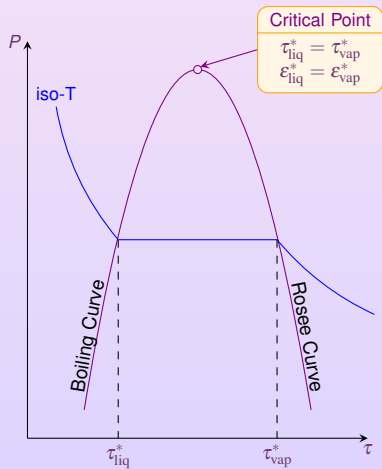
EOS

PG $\epsilon_{\text{liq}}^* = \epsilon_{\text{vap}}^* \Leftrightarrow c_{V\text{liq}} = c_{V\text{vap}}$ (indip. of T)

SG $\{\tau_i, P_i^{\text{sat},e}\}_i \rightsquigarrow (\tau, \epsilon) \mapsto P_\alpha \rightsquigarrow \tau \mapsto P^{\text{sat}}$
 $\tau_{\text{liq}}^* = \tau_{\text{vap}}^*$ but $\epsilon_{\text{liq}}^* \neq \epsilon_{\text{vap}}^*$

TAB $\{\tau_i, P_i^{\text{sat},e}\}_i \rightsquigarrow \tau \mapsto P^{\text{sat}}$
 $\{(\tau, \epsilon_i), (P_\alpha^c)_i\}_i \rightsquigarrow (\tau, \epsilon) \mapsto P_\alpha$

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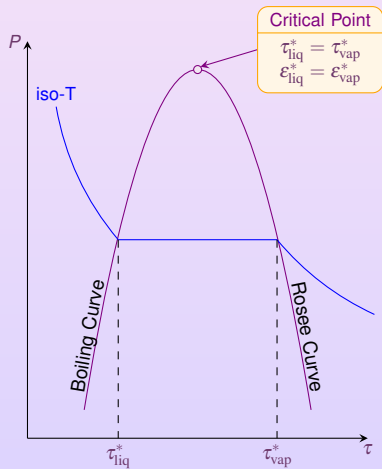
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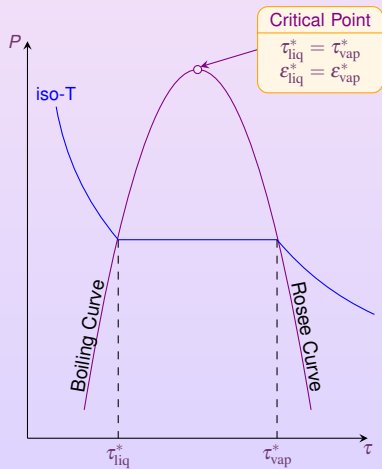
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