Modelling and Simulation of Liquid-Vapor Phase Transition

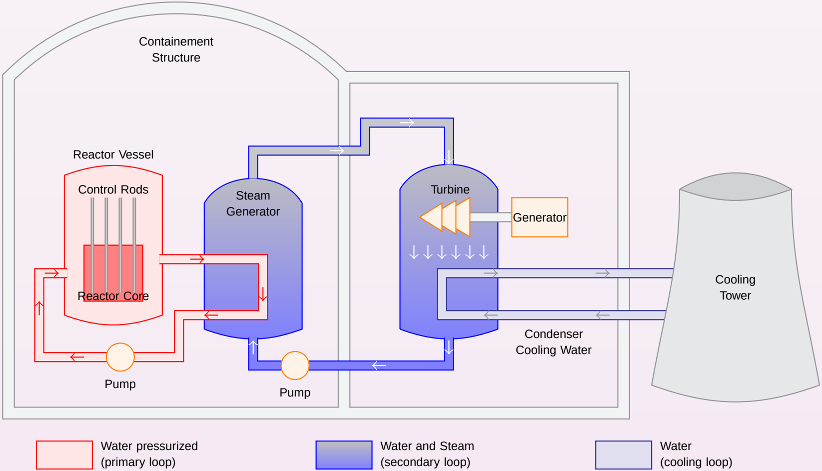
A Boiling Crisis Study Contribution

Gloria Faccanoni[1,2] **Grégoire Allaire**[1,2] **Samuel Kokh**[2]

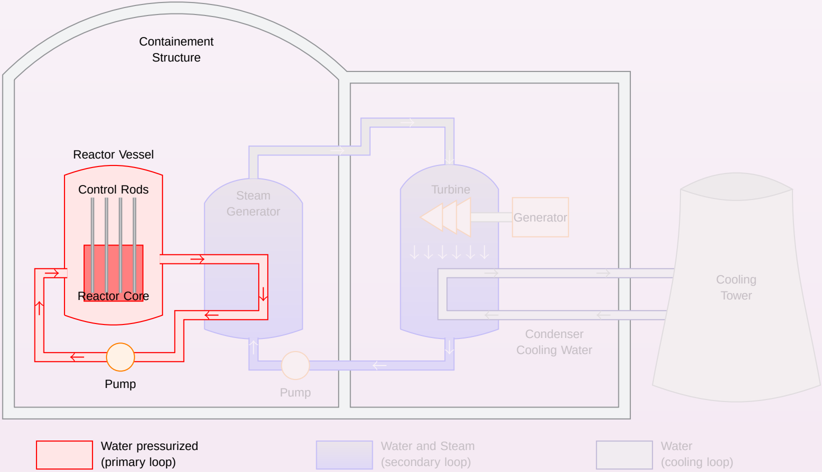
[1]**École Polytechnique - CMAP**

[2]**CEA Saclay - SFME/LETR**

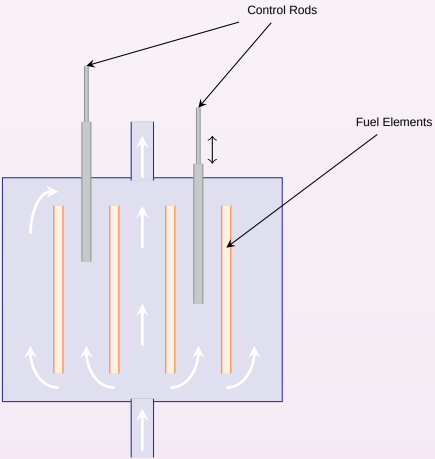
Pressurized Water Reactor



Pressurized Water Reactor



Core of a Pressurized Water Reactor



Core of a Pressurized Water Reactor

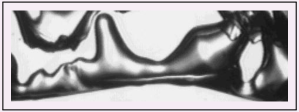
Boiling Crisis

Phenomenon

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

Nucleate Boiling

Film Boiling



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

Outline

Outline

EULER SYSTEM

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

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

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

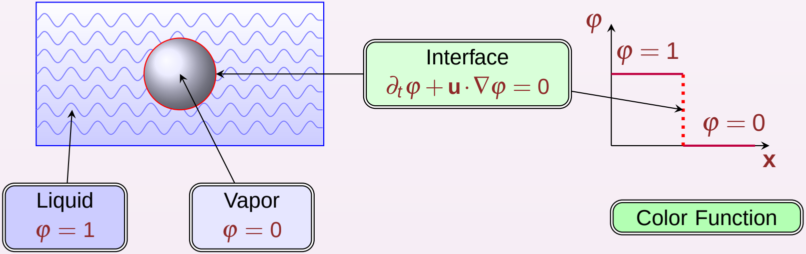
EULER SYSTEM

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

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

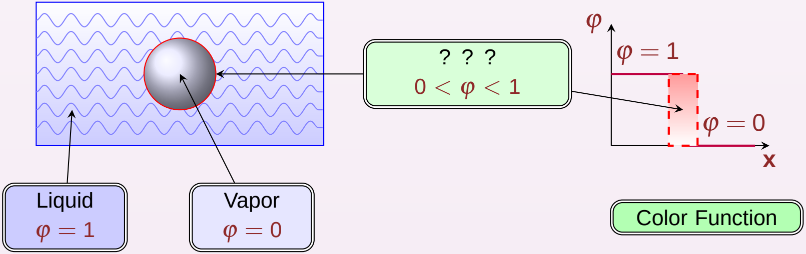
$\boxed{(\rho,\varepsilon)\mapsto P}$ pressure law.

Liquid-Vapor Interface



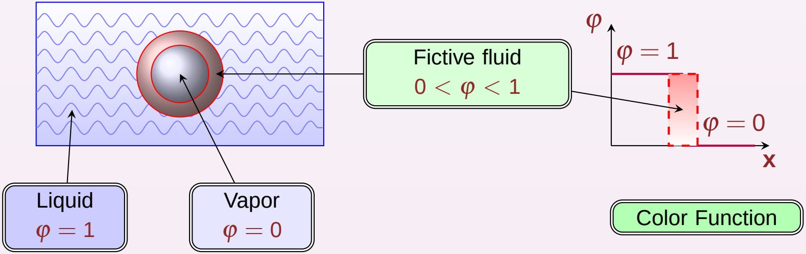
$$(\rho, \varepsilon) \mapsto P = \begin{cases} P^{\text{liq}} & \text{if } \varphi = 1; \\ P^{\text{vap}} & \text{if } \varphi = 0. \end{cases}$$

Liquid-Vapor Interface



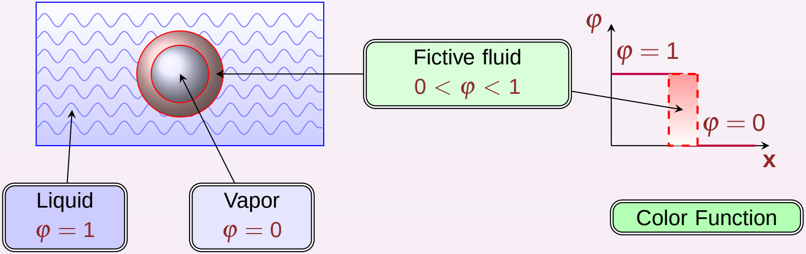
$$(\rho,\varepsilon) \mapsto P = \begin{cases} P^{\text{liq}} & \text{if } \varphi = 1; \\ ??? & \text{if } 0 < \varphi < 1; \\ P^{\text{vap}} & \text{if } \varphi = 0. \end{cases}$$

Liquid-Vapor Interface



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

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 ($\rightsquigarrow \not\varphi$)
- coherence with classical thermodynamics [H. Callen]

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

τ_α specific volume
ε_α specific internal energy

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

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

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

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

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

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

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

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

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

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

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

EOS WITHOUT PHASE CHANGE

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

EOS WITHOUT PHASE CHANGE

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

ENTROPY WITHOUT PHASE CHANGE

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

$$P = \left(\left.\frac{\partial\sigma}{\partial\varepsilon}\right|_{\tau;y,z,\psi}\right)^{-1} \left.\frac{\partial\sigma}{\partial\tau}\right|_{\varepsilon;y,z,\psi}$$

EOS without Phase Change

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

Entropy without phase change

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

$$P = \left(\left.\frac{\partial\sigma}{\partial\varepsilon}\right|_{\tau;y,z,\psi}\right)^{-1} \left.\frac{\partial\sigma}{\partial\tau}\right|_{\varepsilon;y,z,\psi}$$

EOS WITHOUT PHASE CHANGE

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

ENTROPY WITHOUT PHASE CHANGE

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

$$P = \left(\left.\frac{\partial\sigma}{\partial\varepsilon}\right|_{\tau;y,z,\psi}\right)^{-1} \left.\frac{\partial\sigma}{\partial\tau}\right|_{\varepsilon;y,z,\psi}$$

EOS with Phase Change

Entropy without Ph.Ch.

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

→

Entropy at equilibrium

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

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

Optimization Problem:

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

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^*)

EOS with Phase Change

Entropy without Ph.Ch.

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

→

Entropy at equilibrium

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

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

Optimization Problem:

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

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

Solution: (z^*, y^*, ψ^*)

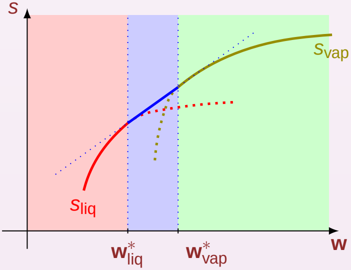
EOS with Phase Change

Entropy without Ph.Ch.

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

Entropy at equilibrium

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



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

Optimization Problem:

$$s^{\mathrm{eq}}(\mathbf{w}) \stackrel{\mathrm{def}}{=} \max_{z,y,\psi\in[0,1]^3} \sigma(\mathbf{w}, z, y, \psi) = \mathrm{co}\left\{ \max\left\{ s_1(\mathbf{w}), s_2(\mathbf{w}) \right\} \right\}$$

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^*)

EOS with Phase Change

Entropy without Ph.Ch.

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

Entropy at equilibrium

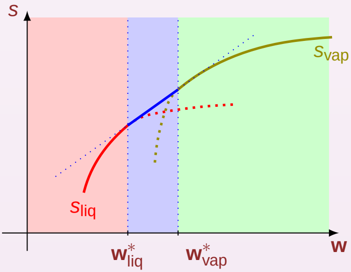
$\mathbf{w} \mapsto s^{eq}$

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

Optimization Problem:

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

$$= \operatorname{co}\{\max\{s_1(\mathbf{w}), s_2(\mathbf{w})\}\}$$



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^*)

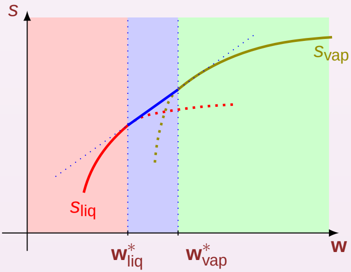
EOS with Phase Change

Entropy without Ph.Ch.

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

Entropy at equilibrium

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



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

Optimization Problem:

$$s^{eq}(\mathbf{w}) \stackrel{\text{def}}{=} \max_{z,y,\psi \in [0,1]^3} \sigma(\mathbf{w}, z, y, \psi)$$
$$= \text{co}\{\max\{s_1(\mathbf{w}), s_2(\mathbf{w})\}\}$$

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^*)

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

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

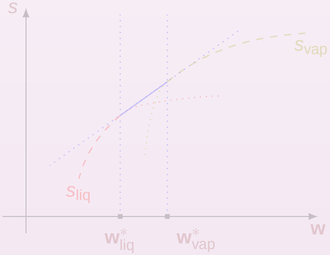
$$\begin{cases} P_{\text{liq}}(\mathbf{w}_{\text{liq}}) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ T_{\text{liq}}(\mathbf{w}_{\text{liq}}) = T_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ g_{\text{liq}}(\mathbf{w}_{\text{liq}}) = g_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{\text{liq}}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

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

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

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

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



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

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

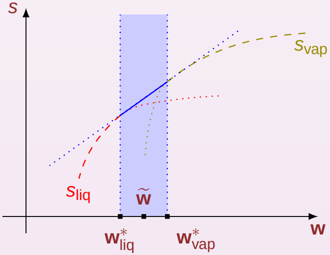
$$\begin{cases} P_{\text{liq}}(\mathbf{w}_{\text{liq}}) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ T_{\text{liq}}(\mathbf{w}_{\text{liq}}) = T_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ g_{\text{liq}}(\mathbf{w}_{\text{liq}}) = g_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{\text{liq}}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

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

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

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

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



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

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

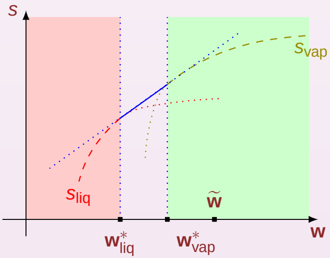
$$\begin{cases} P_{\text{liq}}(\mathbf{w}_{\text{liq}}) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ T_{\text{liq}}(\mathbf{w}_{\text{liq}}) = T_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ g_{\text{liq}}(\mathbf{w}_{\text{liq}}) = g_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{\text{liq}}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

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

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

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

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



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

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

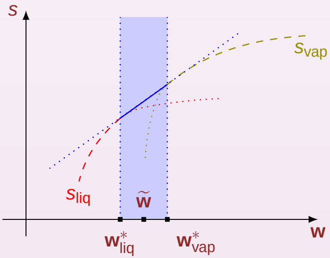
$$\begin{cases} P_{\text{liq}}(\mathbf{w}_{\text{liq}}) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ T_{\text{liq}}(\mathbf{w}_{\text{liq}}) = T_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ g_{\text{liq}}(\mathbf{w}_{\text{liq}}) = g_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{\text{liq}}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

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

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

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

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



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

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

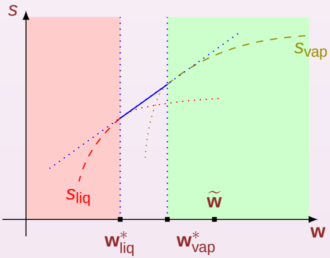
$$\begin{cases} P_{liq}(\mathbf{w}_{liq}) = P_{vap}(\mathbf{w}_{vap}) \\ T_{liq}(\mathbf{w}_{liq}) = T_{vap}(\mathbf{w}_{vap}) \\ g_{liq}(\mathbf{w}_{liq}) = g_{vap}(\mathbf{w}_{vap}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{liq} + (1-y)\mathbf{w}_{vap} \end{cases}$$

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

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

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

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



Dynamic Liquid-Vapor Phase Change

Euler System

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

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

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

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

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

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

Dynamic Liquid-Vapor Phase Change

Euler System

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

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

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

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

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

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

Dynamic Liquid-Vapor Phase Change

Euler System

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

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

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

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

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

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

Outline

How to simulate the Liu solution

- Exact Riemann Solver (cf. [A. Voß] for Van der Waals EOS)
- Viscuous Solver (the Liu solution is the only solution that has a viscuous profile) (cf. [S. Jaouen] for Perfect Gas EOS with $c_{v_{\text{liq}}} = c_{v_{\text{vap}}}$)
- Solver(s) based on Relaxation Approach [F. Coquel, B. Perthame], [Th. Barberon, Ph. Helluy], [Ph. Helluy, N. Seguin], [F. Coquel, F. Caro, D. Jamet, S. Kokh],...

Relaxation Approach

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

Relaxation Approach

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

Relaxation Approach

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

Equilibrium System

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

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

Relaxation Approach

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

Augmented System

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

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

Equilibrium System

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

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

Relaxation Approach

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

Augmented System

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

In the interface

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

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

Equilibrium System

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

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

Relaxation Approach

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

Augmented System

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

In the interface

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

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

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

Equilibrium System

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

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

Relaxation Approach

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

Augmented System

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

In the interface

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

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

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

Equilibrium System

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

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

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

Numerical Scheme

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

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

❶ $\mu_j = +\infty$

$\Downarrow$

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

Aug. System: 5-eq. iso-T
Num. Scheme: op. splitting
Conv.: [G. Allaire and all.]
Surf. Tens.: [J. U. Brackbill and all.]
Heat: 2D implicit

❷ $\mu_j = 0$

$\Downarrow$

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

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

Numerical Scheme

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

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

❶ $\mu_j = +\infty$

$\Downarrow$

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

Aug. System: 5-eq. iso-T
Num. Scheme: op. splitting
Conv.: [G. Allaire and all.]
Surf. Tens.: [J. U. Brackbill and all.]
Heat: 2D implicit

❷ $\mu_j = 0$

$\Downarrow$

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

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

Numerical Scheme

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

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

❶ $\mu_j = +\infty$

$\Downarrow$

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

❷ $\mu_j = 0$

$\Downarrow$

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

Aug. System: 5-eq. iso-T
Num. Scheme: op. splitting
Conv.: [G. Allaire and all.]
Surf. Tens.: [J. U. Brackbill and all.]
Heat: 2D implicit

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

Numerical Scheme

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

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

❶ $\mu_j = +\infty$

$\Downarrow$

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

❷ $\mu_j = 0$

$\Downarrow$

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

Aug. System: 5-eq. iso-T

Num. Scheme: op. splitting

Conv.: [G. Allaire and all.]

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

Heat: 2D implicit

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

Numerical Scheme

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

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

❶ $\mu_j = +\infty$

$\Downarrow$

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

Aug. System: 5-eq. iso-T
Num. Scheme: op. splitting
Conv.: [G. Allaire and all.]
Surf. Tens.: [J. U. Brackbill and all.]
Heat: 2D implicit

❷ $\mu_j = 0$

$\Downarrow$

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

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

Analytical EOS

Water Example

(τ, ε) fixed

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

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

(P, T) SOLUTION OF

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

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

T SOLUTION OF

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

Analytical EOS

Water Example

(τ, ε) fixed

$(\tau_1, \varepsilon_1, \tau_2, \varepsilon_2, y)$ solution of

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

(P, T) solution of

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

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

T solution of

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

Analytical EOS

Water Example

(τ,ε) fixed

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

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

(P,T) SOLUTION OF

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

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

T SOLUTION OF

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

Analytical EOS

Water Example

(τ,ε) fixed

$(\tau_1,\varepsilon_1,\tau_2,\varepsilon_2,y)$ solution of

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

(P,T) solution of

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

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

T solution of

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

Analytical EOS

Water Example

(τ,ε) fixed

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

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

(P,T) SOLUTION OF

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

least square approximation

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

T SOLUTION OF

$$\frac{\tau-\tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T)-\tau_2^{\text{sat}}(T)}=\frac{\varepsilon-\varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T)-\varepsilon_2^{\text{sat}}(T)}$$

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

Tabulated EOS

Water Examples

(τ,ε) fixed

T solution of

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

$\wr\wr$

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

TABULATED EOS

Water Examples

(τ, ε) fixed

T SOLUTION OF

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

$$\wr\wr$$

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

least square approximations

Tabulated EOS

Water Examples

(τ,ε) fixed

T solution of

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

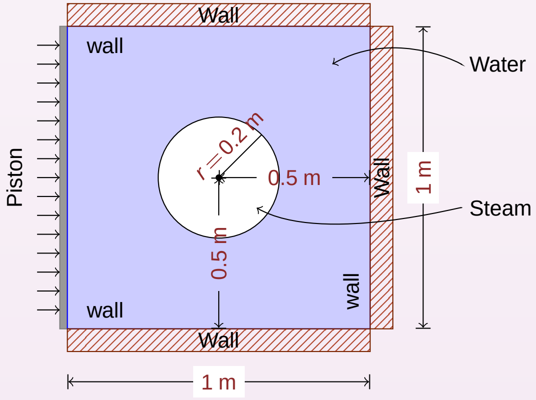
$\wr\wr$

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

least square approximations

Outline

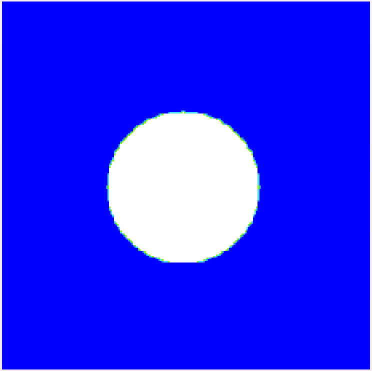
Compression of a Vapor Bubble



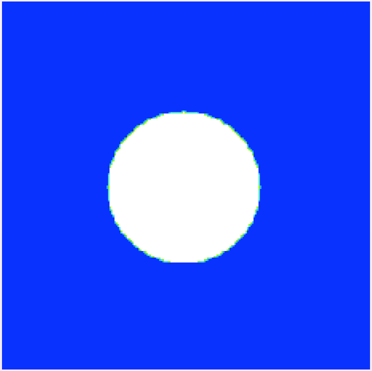
Compression of a 2D Vapor Bubble involving two Stiffened Gases for water and steam.
The piston moves towards right at constant speed $u_p = 30$ m/s.

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

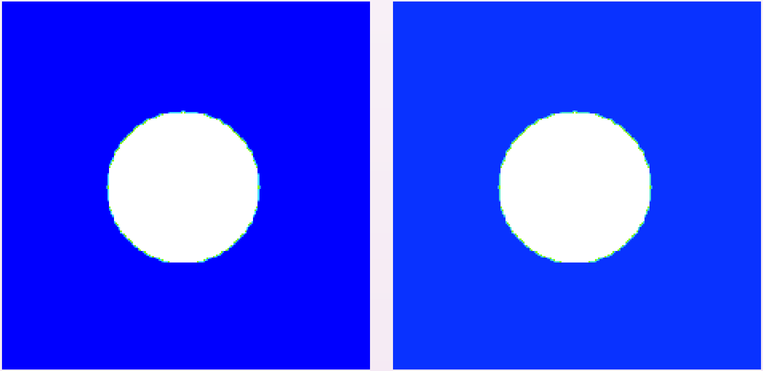


$t = 0.00$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ

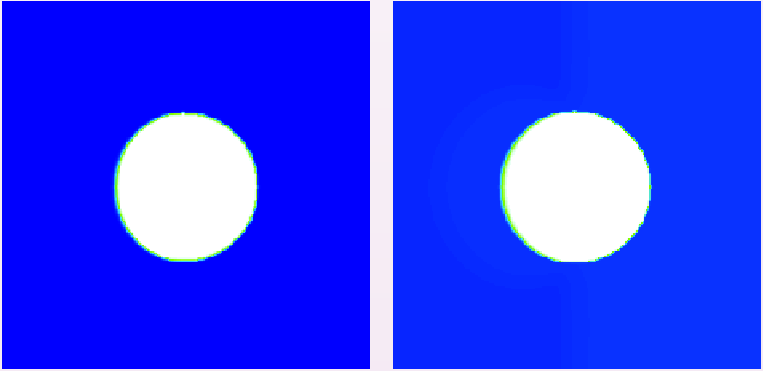


$t = 0.00$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y | Density ρ

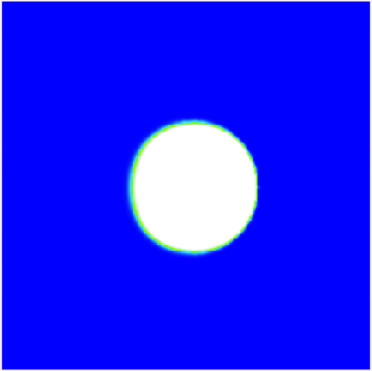


$t = 0.89$ ms

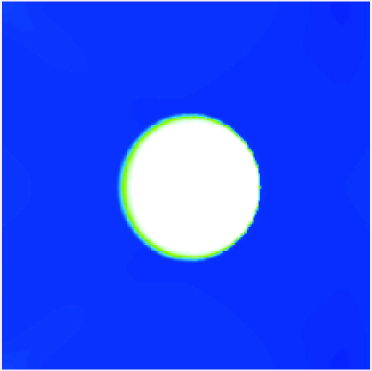
Geometry | Play | Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

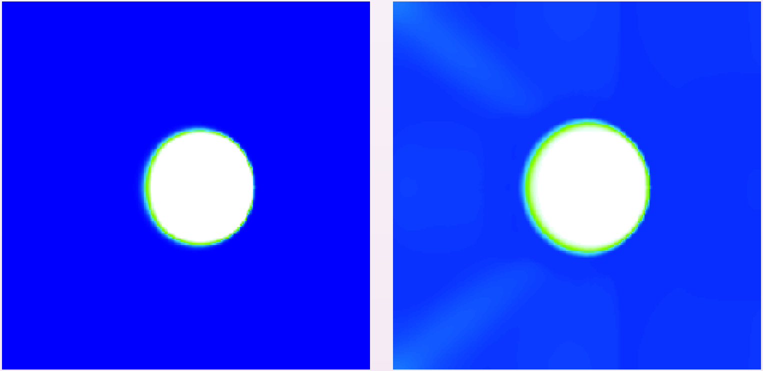


$t = 1.09$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y | Density ρ

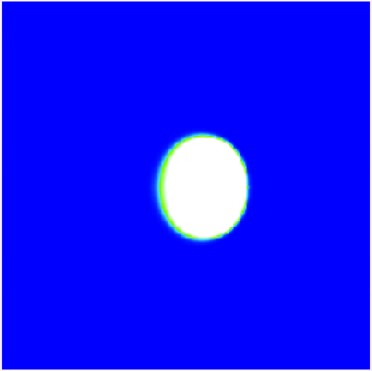


$t = 1.49$ ms

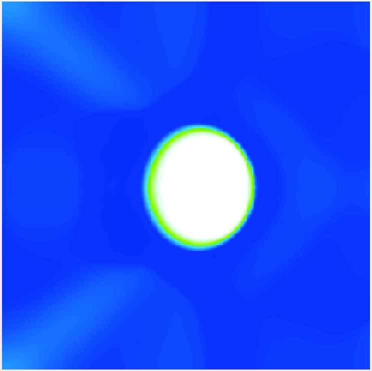
Geometry | Play | Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

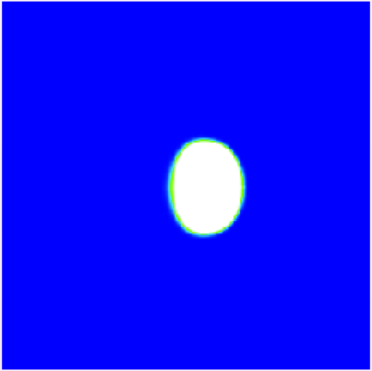


$t = 1.80$ ms

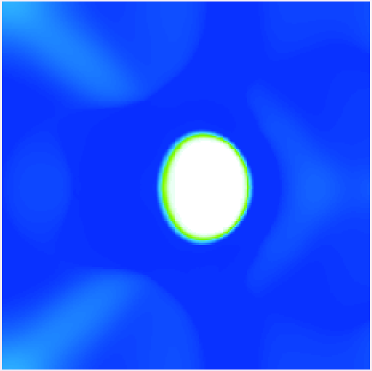
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

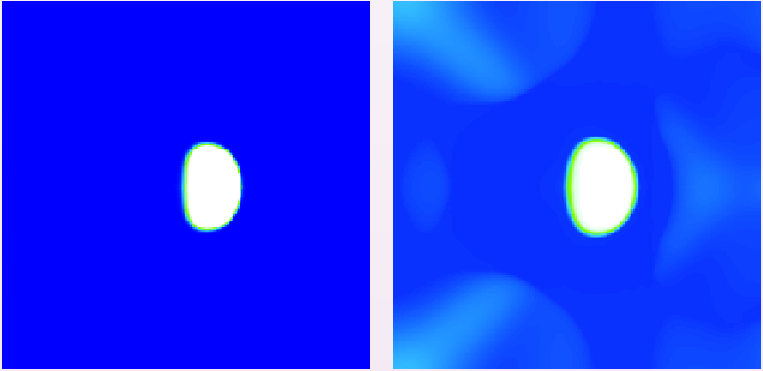


$t = 2.09$ ms

Geometry Play Skip

Compression of a Vapor Bubble

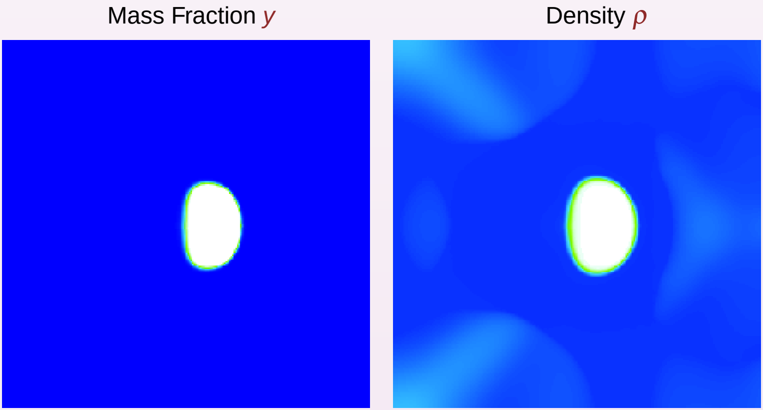
Mass Fraction y Density ρ



$t = 2.39$ ms

Geometry Play Skip

Compression of a Vapor Bubble

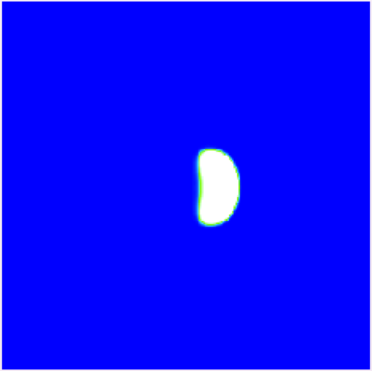


$t = 2.69$ ms

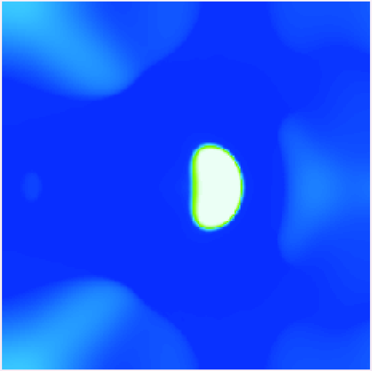
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

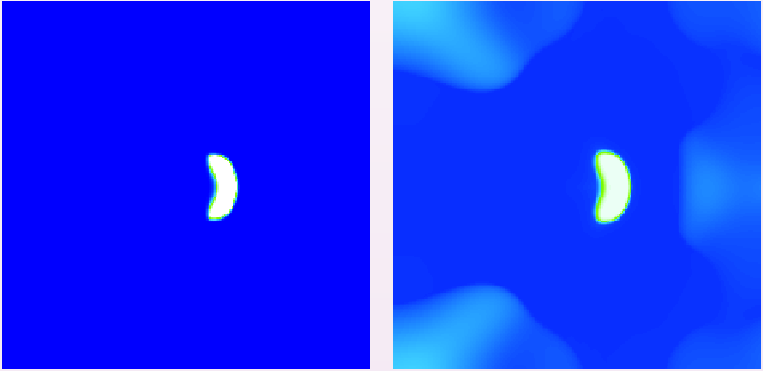


$t = 2.99$ ms

Geometry Play Skip

COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ

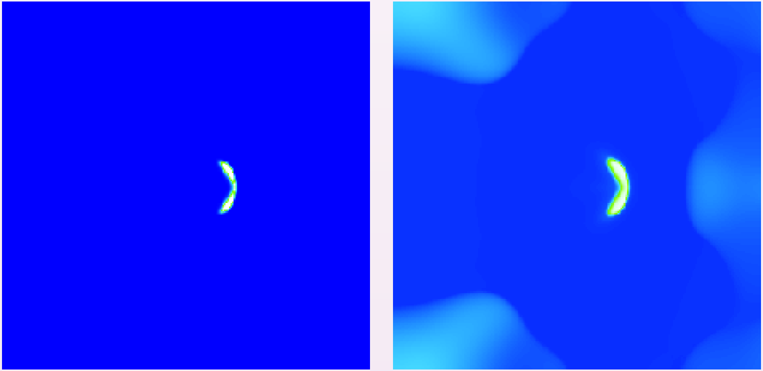


$t = 3.29$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ

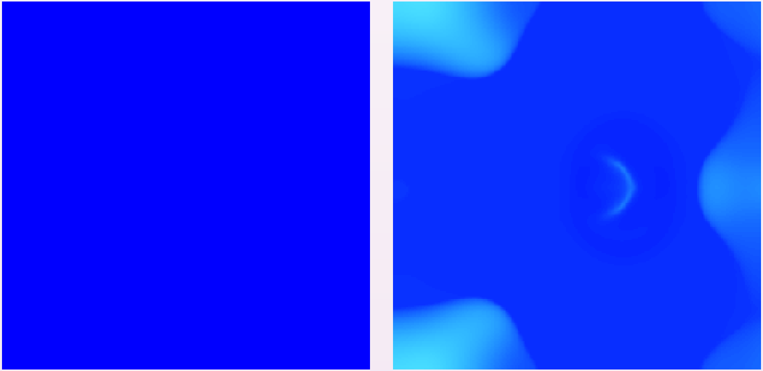


$t = 3.49$ ms

◂ Geometry ▸ Play ▸▸ Skip

COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y Density ρ

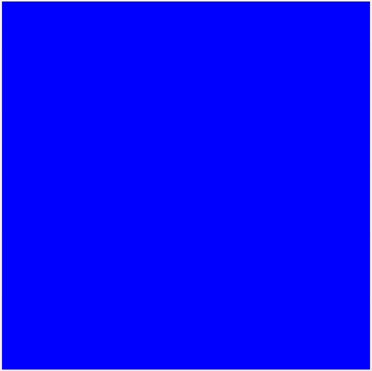


$t = 3.60$ ms

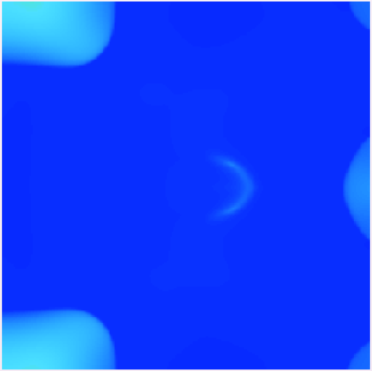
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

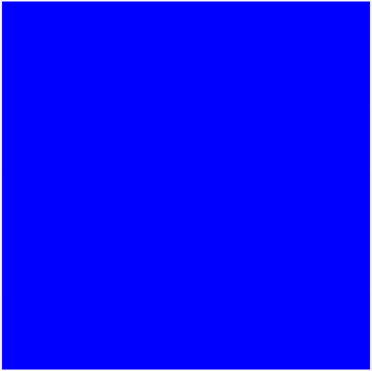


$t = 3.80$ ms

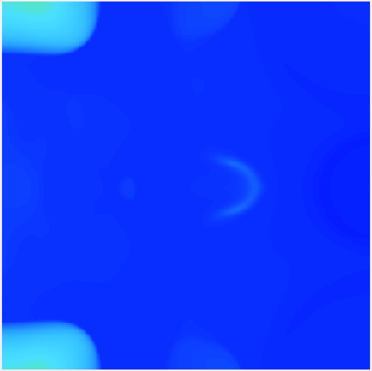
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

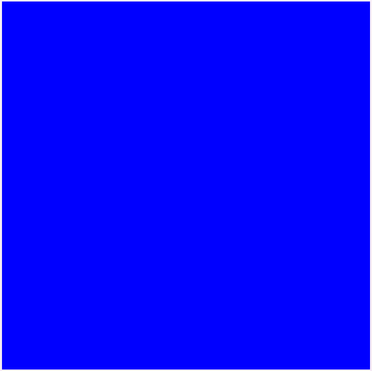


$t = 3.99$ ms

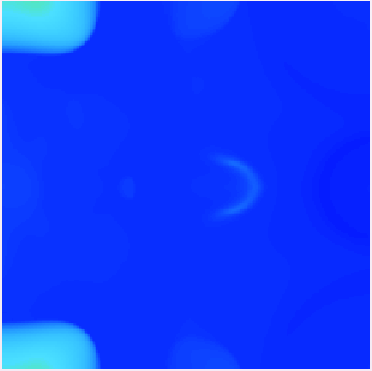
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



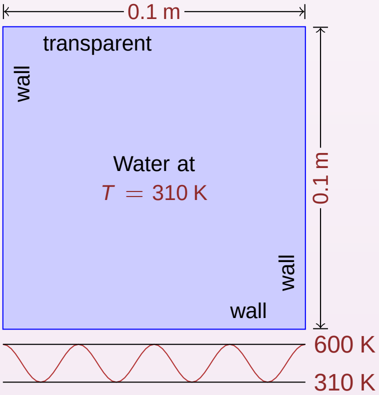
Density ρ



$t = 4.10$ ms

Geometry Play Skip

Nucleating Bubbles

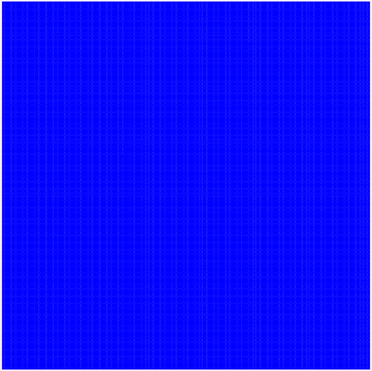


Nucleation of a 2D Vapor Bubbles involving two Stiffened Gases for water and steam. The temperature of the south wall is fixed at

$$T^{\text{wall}} = 310 + (600 - 310)(1 + \cos(6\pi x))/2.$$

Nucleating Bubbles

Mass Fraction y

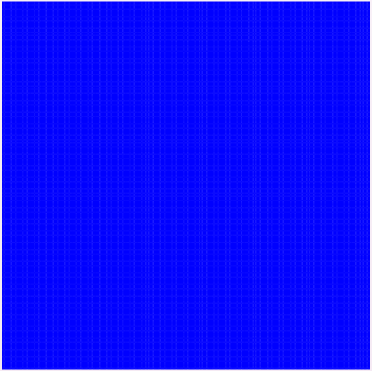


Temperature T

Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y

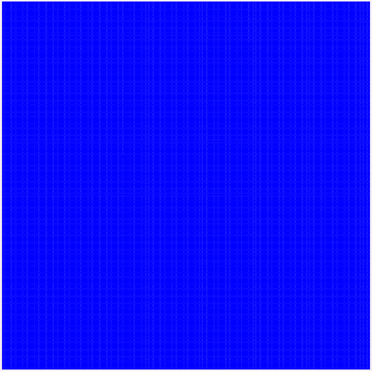


Temperature T

Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

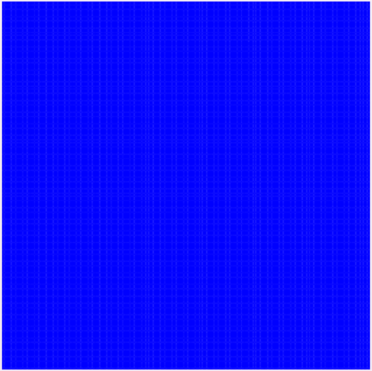


Temperature T

Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y

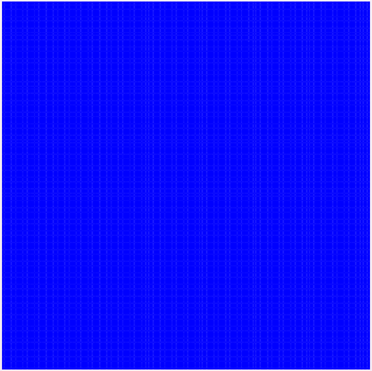


Temperature T

Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

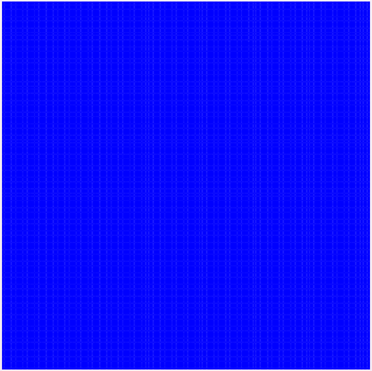


Temperature T

Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

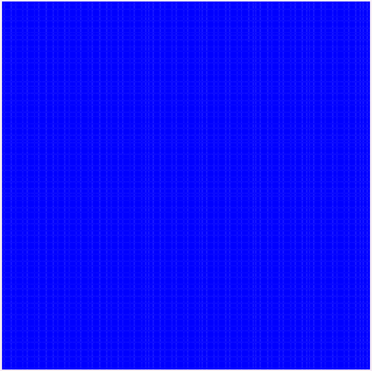


Temperature T

◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLES

Mass Fraction y

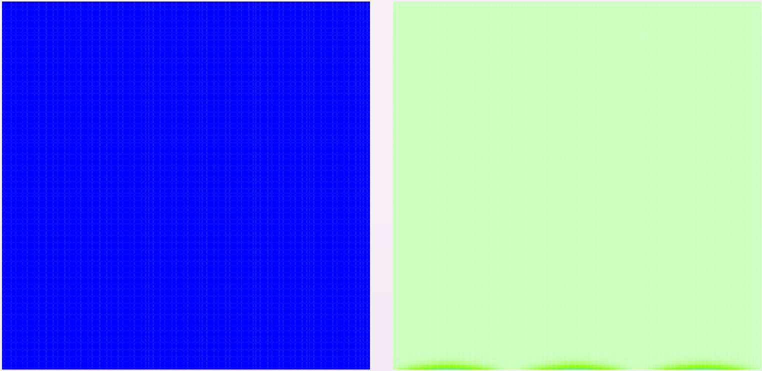


Temperature T

Geometry Play Skip

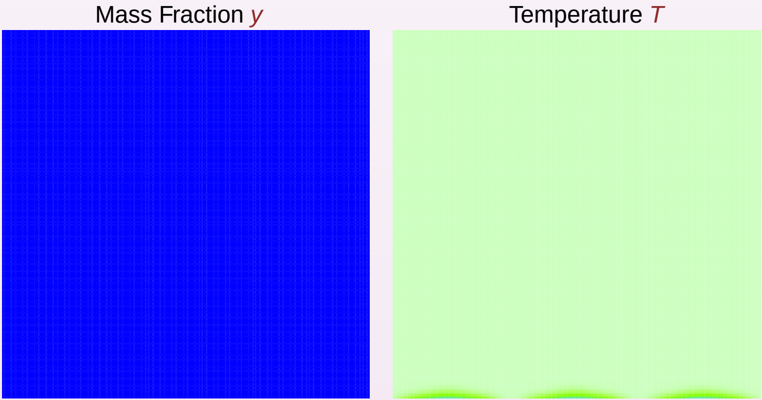
Nucleating Bubbles

Mass Fraction y Temperature T



Geometry Play Skip

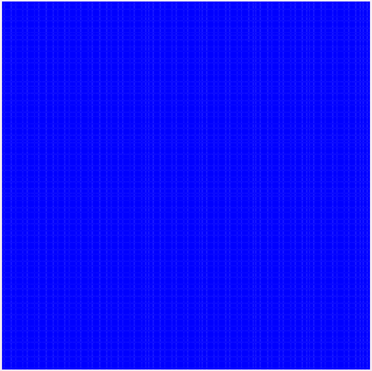
Nucleating Bubbles



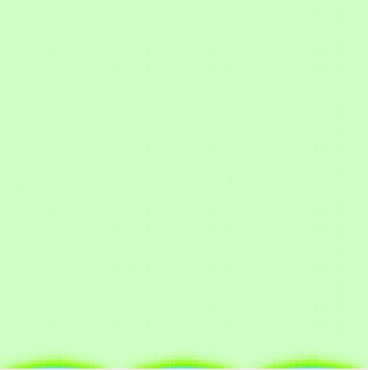
◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLES

Mass Fraction y



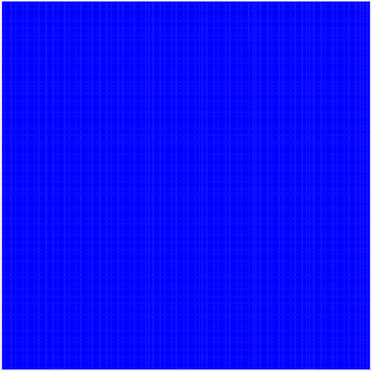
Temperature T



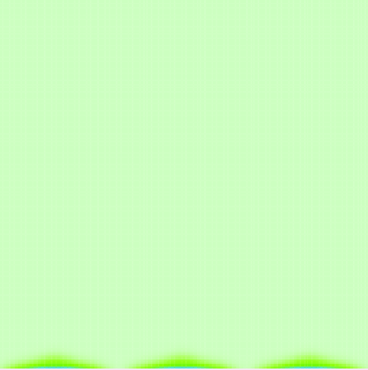
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



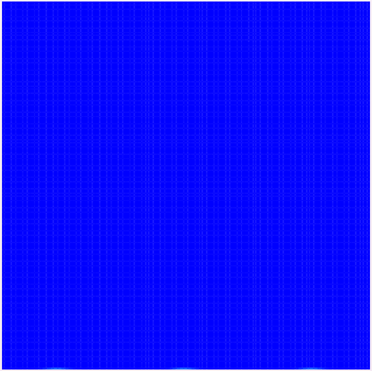
Temperature T



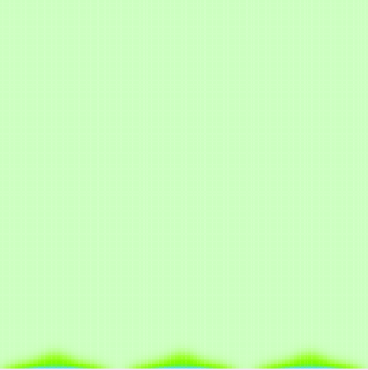
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y



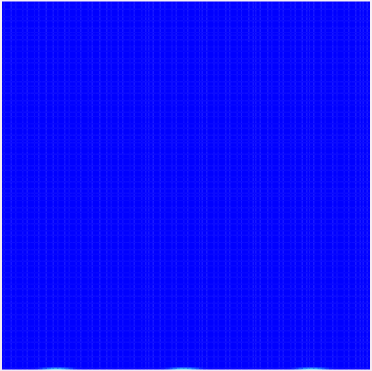
Temperature T



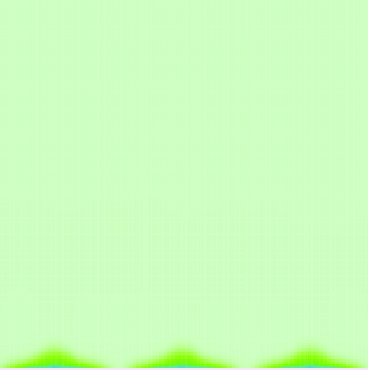
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



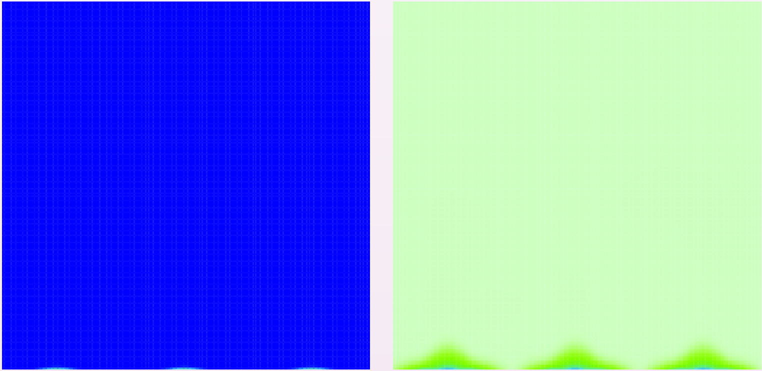
Temperature T



Geometry Play Skip

Nucleating Bubbles

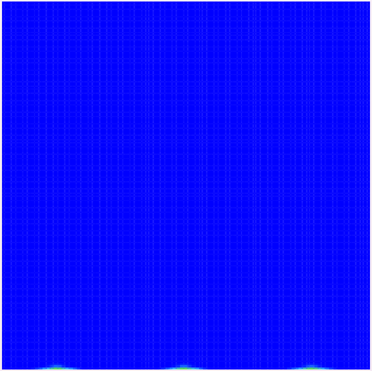
Mass Fraction y Temperature T



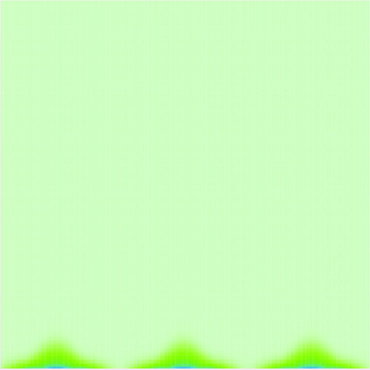
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



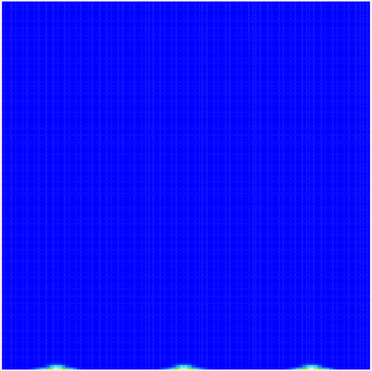
Temperature T



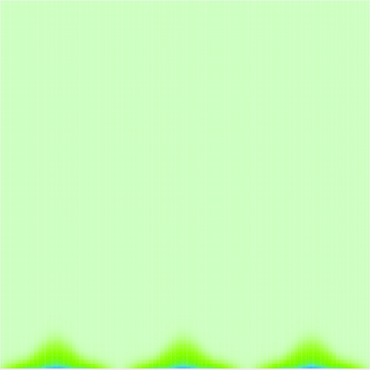
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



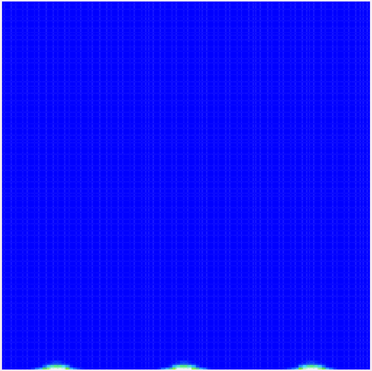
Temperature T



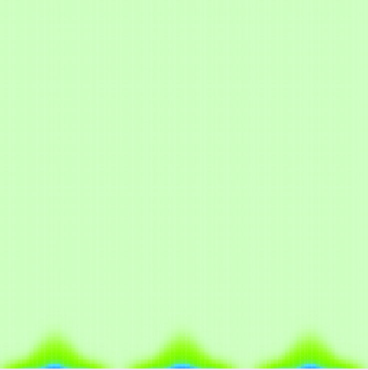
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



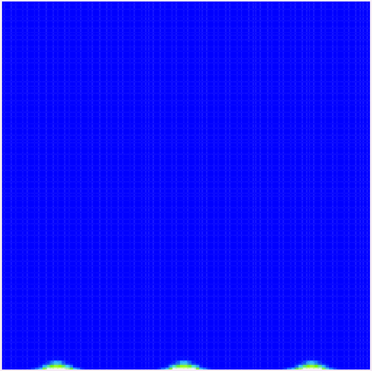
Temperature T



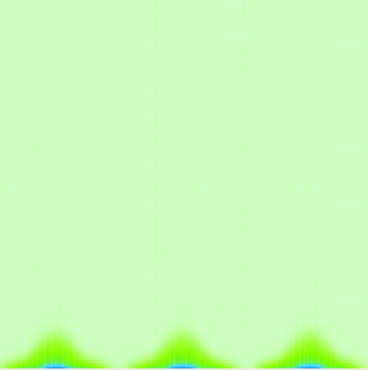
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



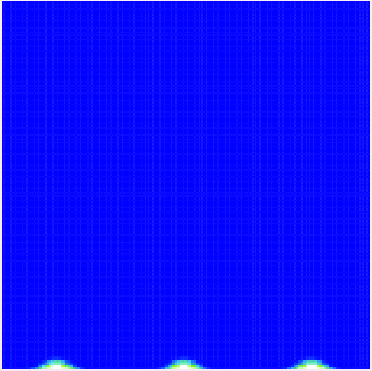
Temperature T



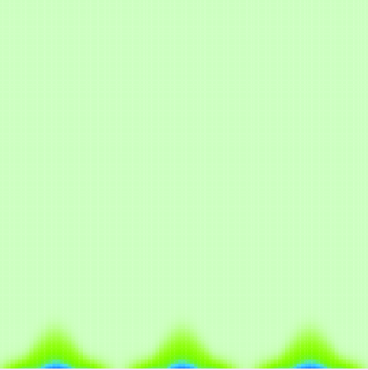
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



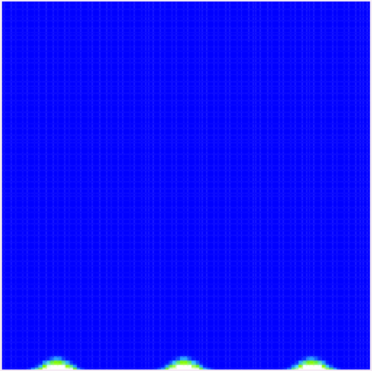
Temperature T



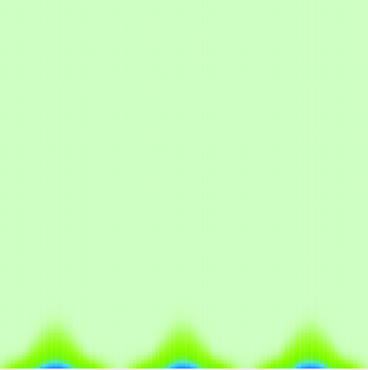
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



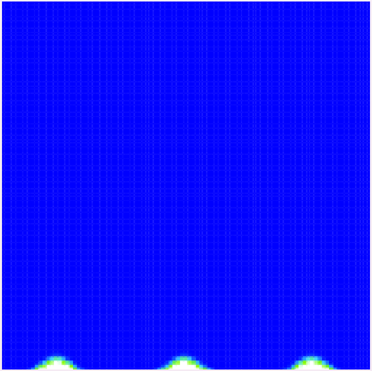
Temperature T



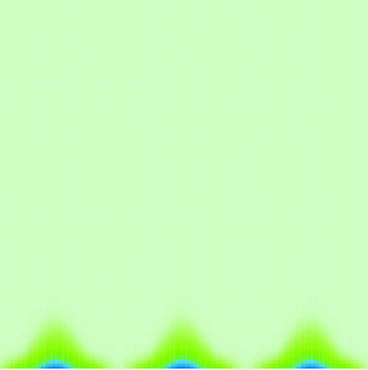
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



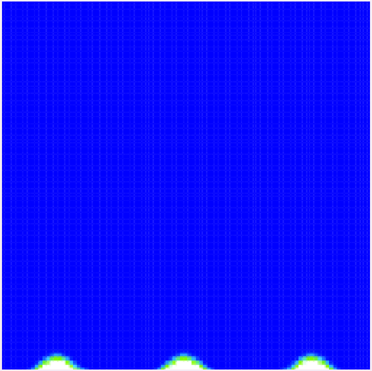
Temperature T



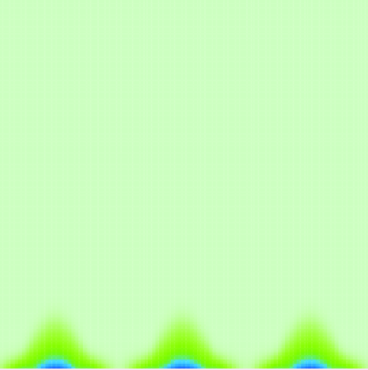
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



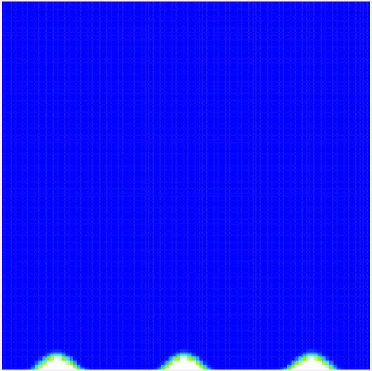
Temperature T



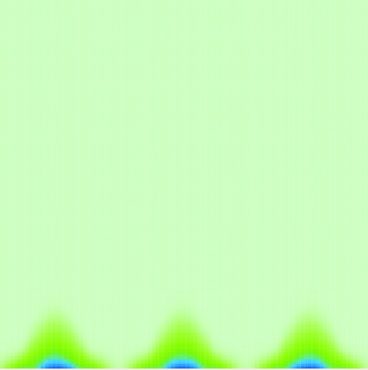
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y



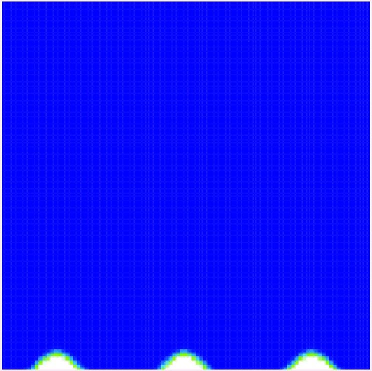
Temperature T



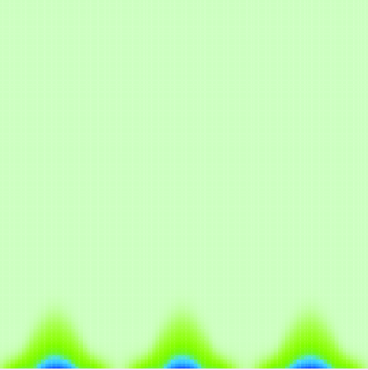
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



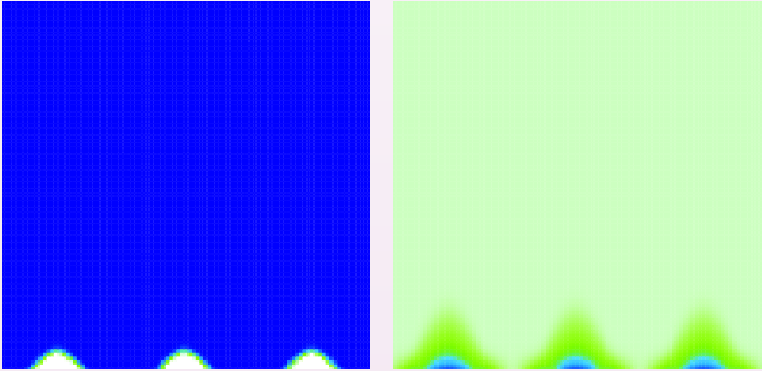
Temperature T



Geometry Play Skip

NUCLEATING BUBBLES

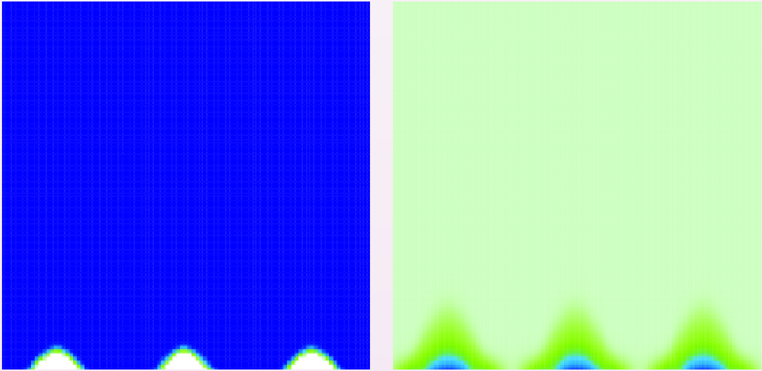
Mass Fraction y Temperature T



Geometry Play Skip

NUCLEATING BUBBLES

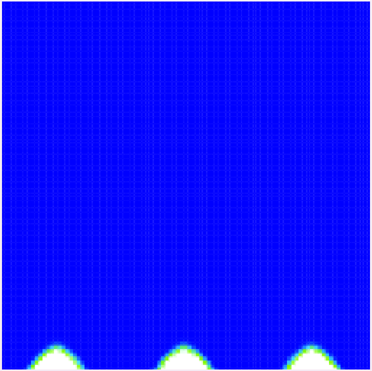
Mass Fraction y Temperature T



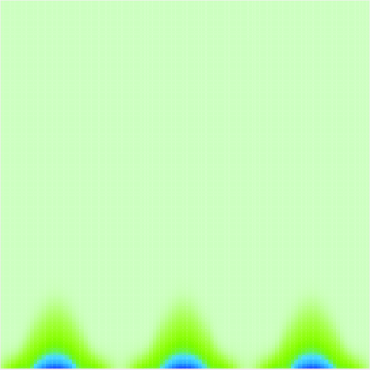
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



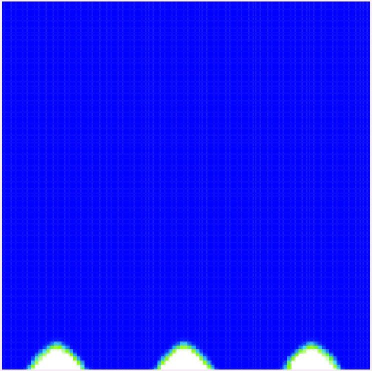
Temperature T



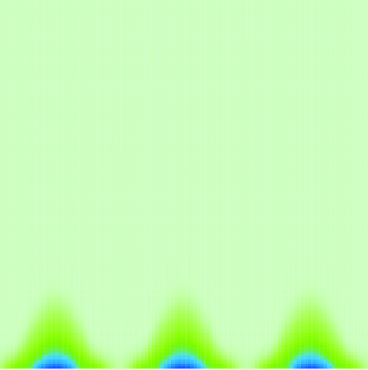
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



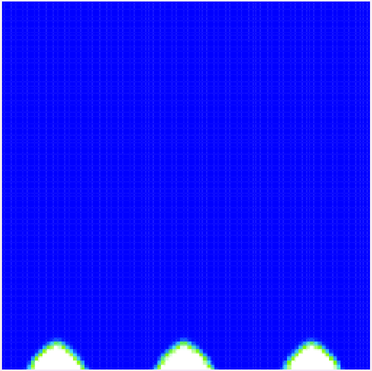
Temperature T



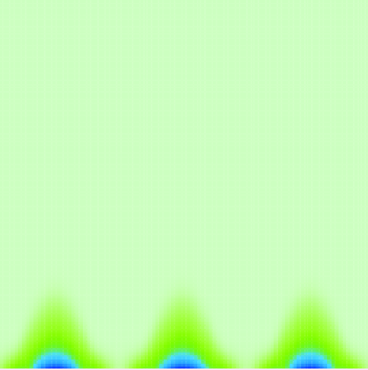
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



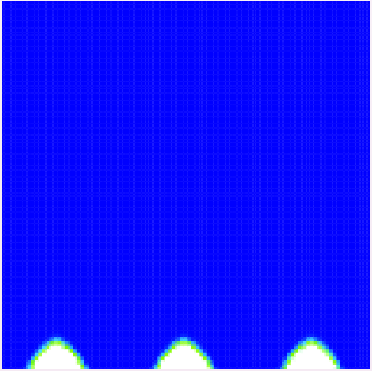
Temperature T



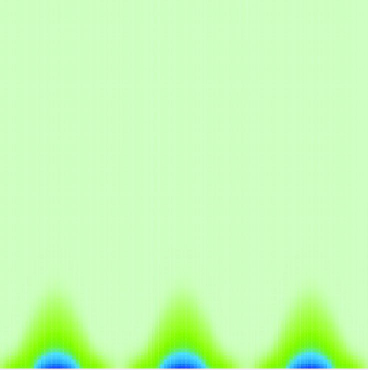
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

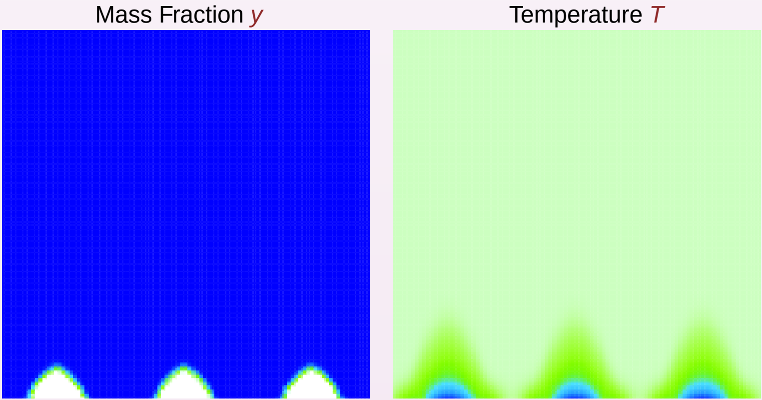


Temperature T



◂ Geometry ▸ Play ▸▸ Skip

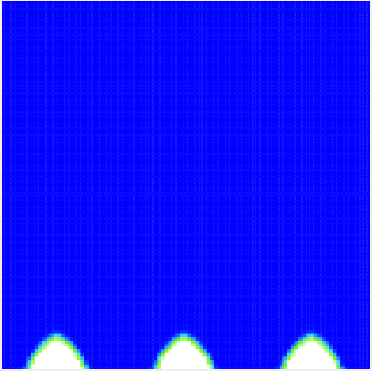
Nucleating Bubbles



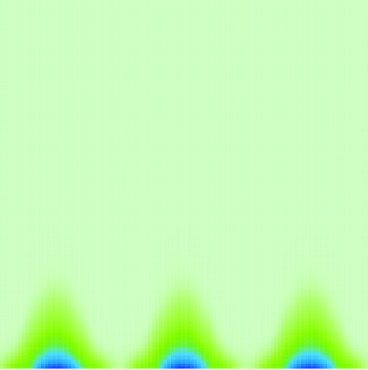
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



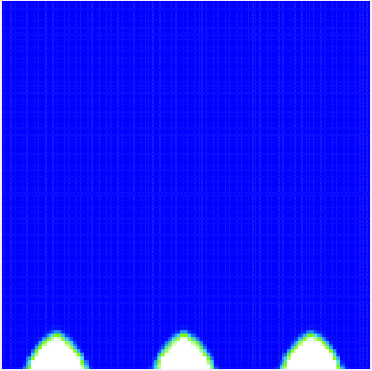
Temperature T



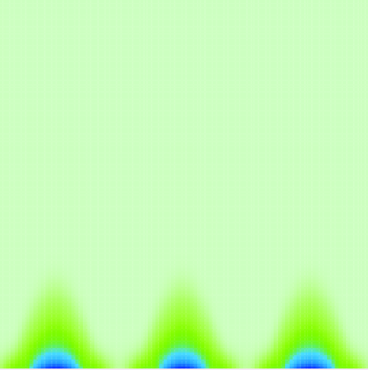
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



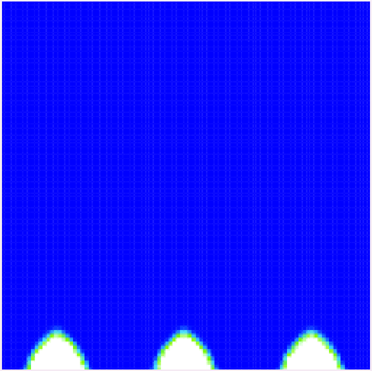
Temperature T



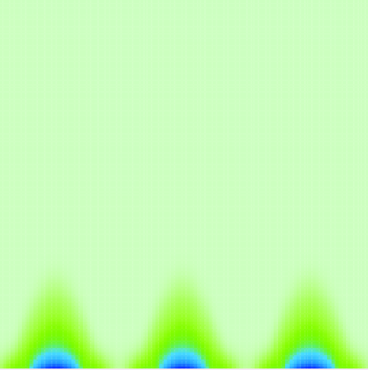
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



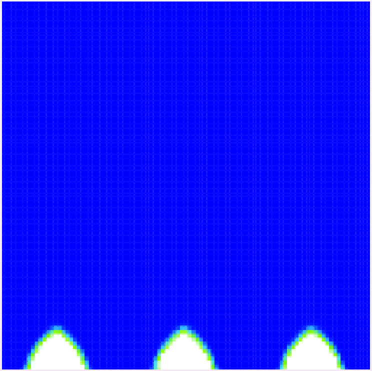
Temperature T



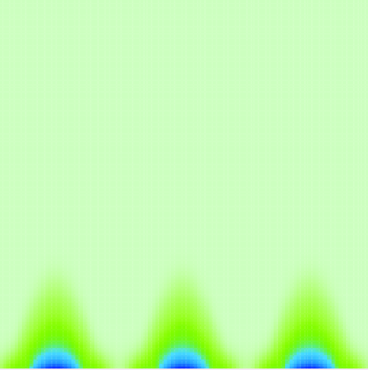
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



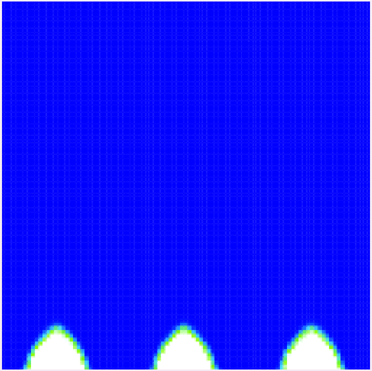
Temperature T



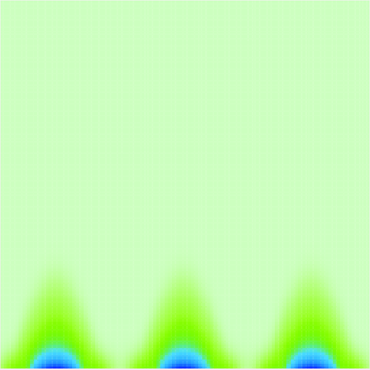
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



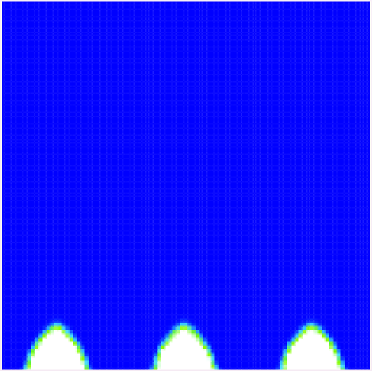
Temperature T



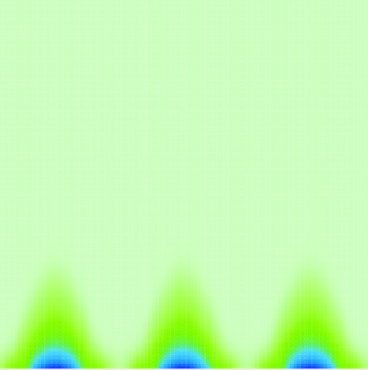
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



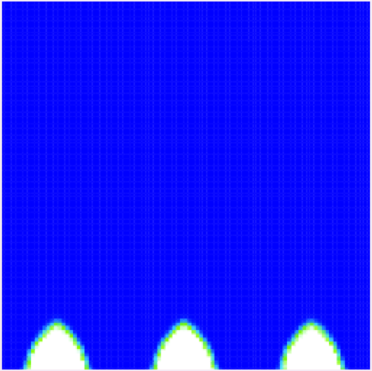
Temperature T



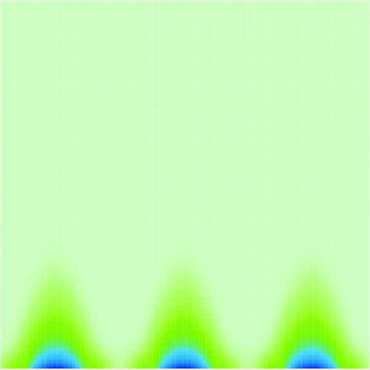
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



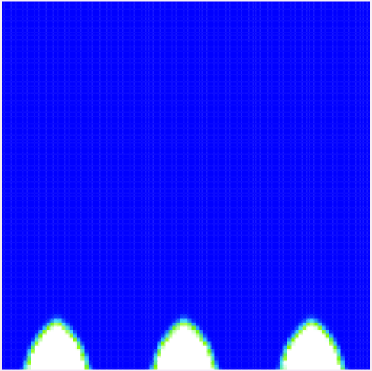
Temperature T



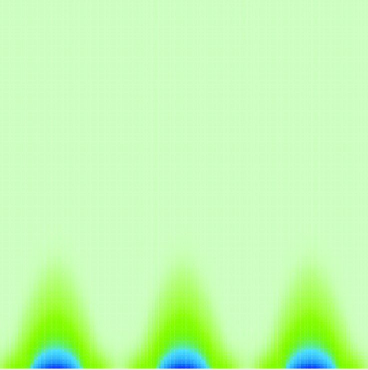
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



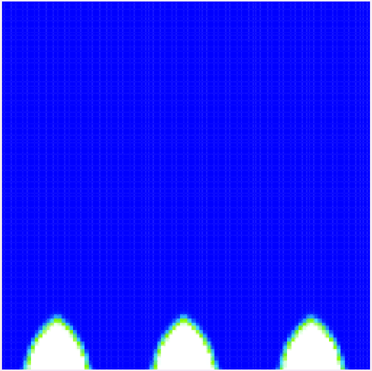
Temperature T



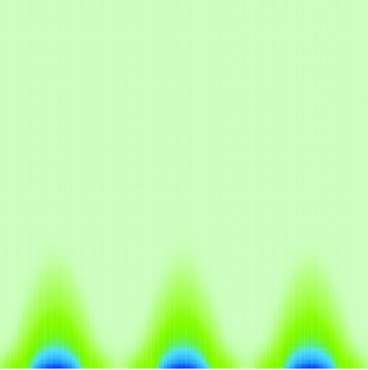
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y



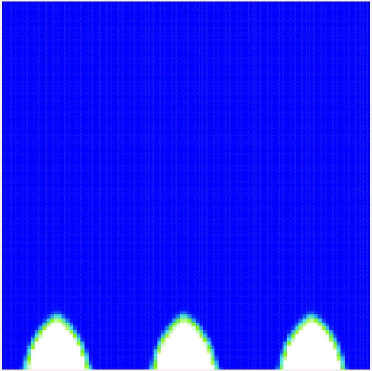
Temperature T



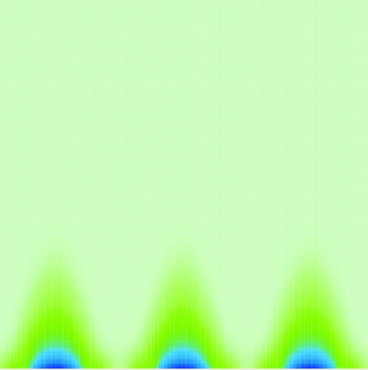
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



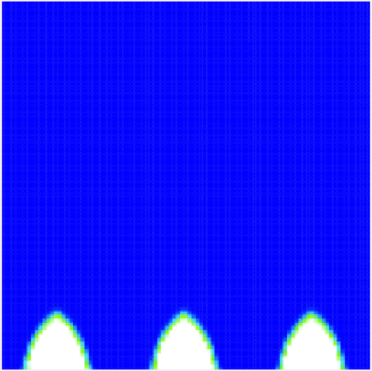
Temperature T



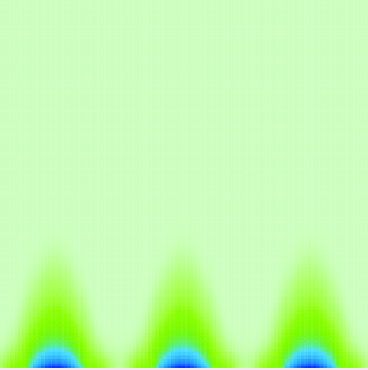
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y



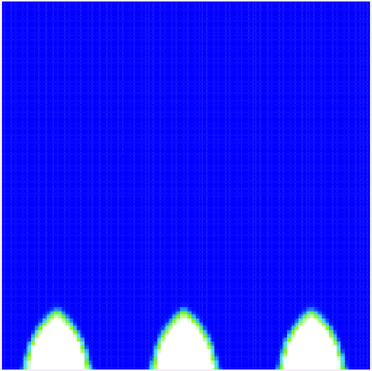
Temperature T



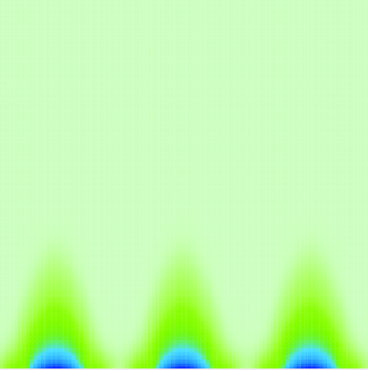
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



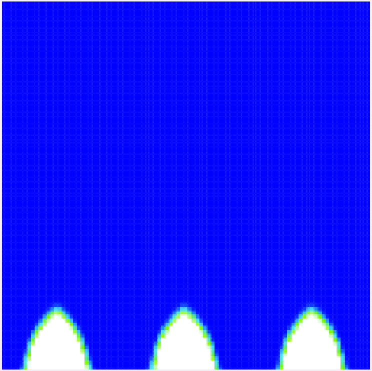
Temperature T



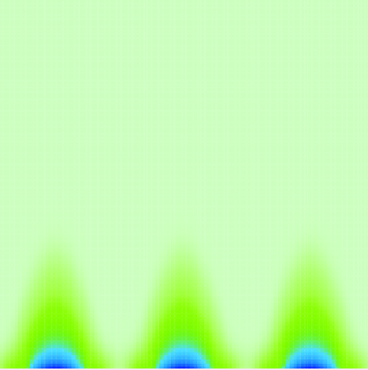
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



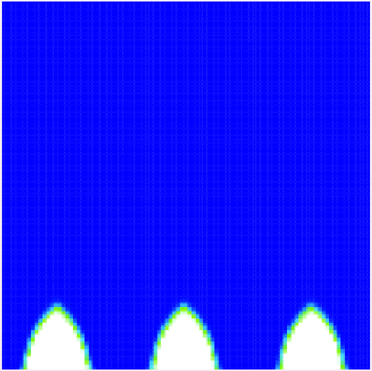
Temperature T



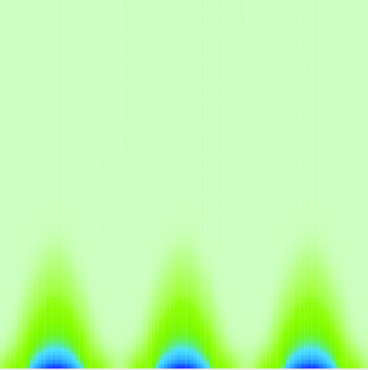
◀ Geometry ▶ Play ▶▶ Skip

Nucleating Bubbles

Mass Fraction y



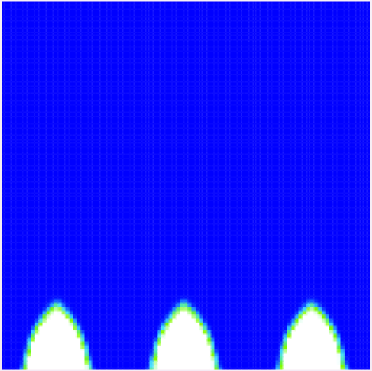
Temperature T



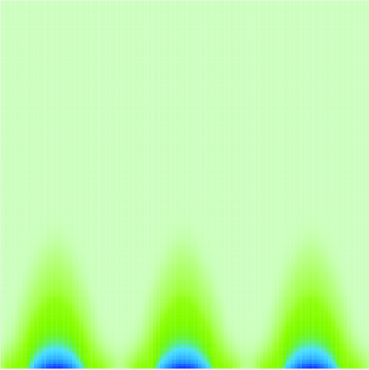
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



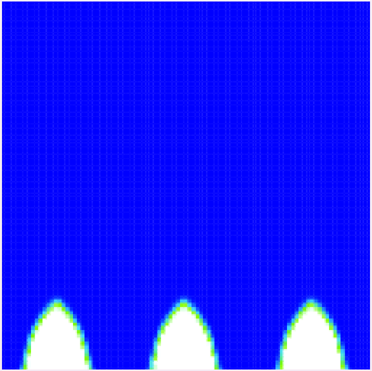
Temperature T



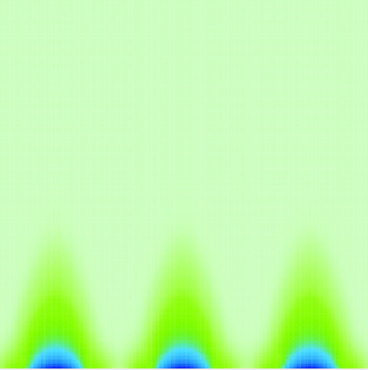
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



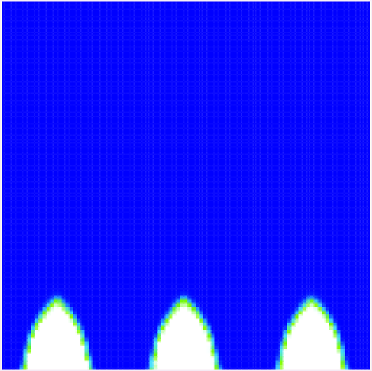
Temperature T



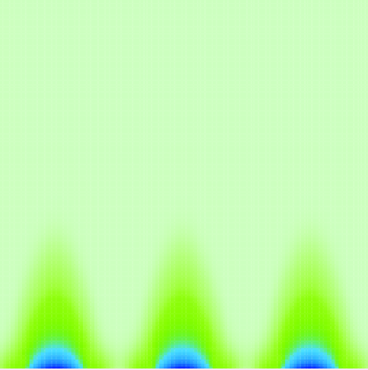
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



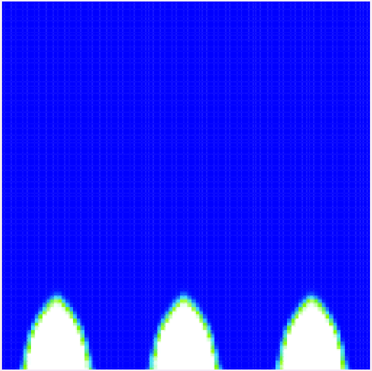
Temperature T



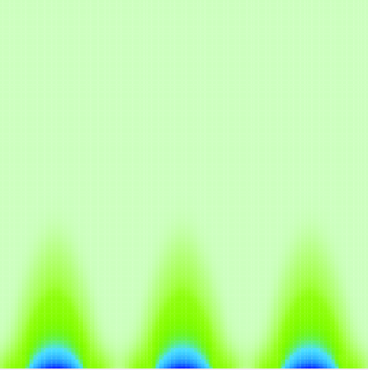
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



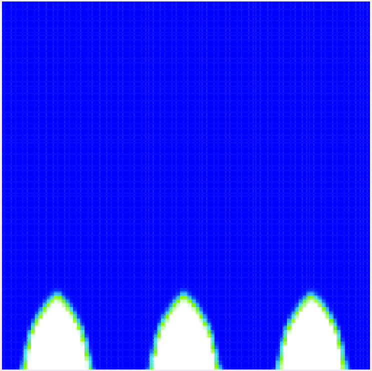
Temperature T



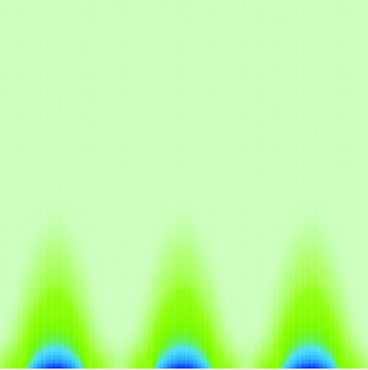
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



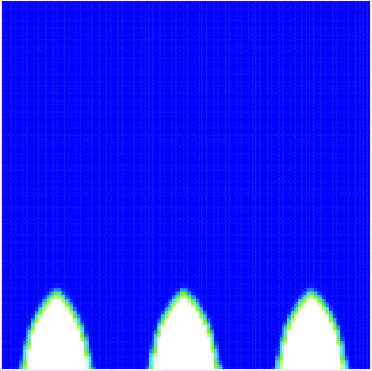
Temperature T



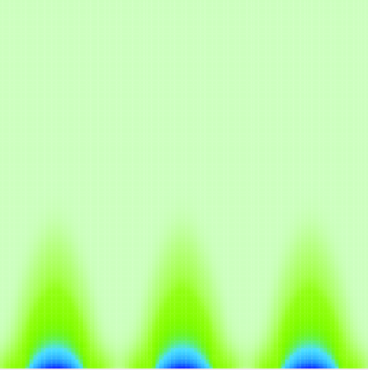
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



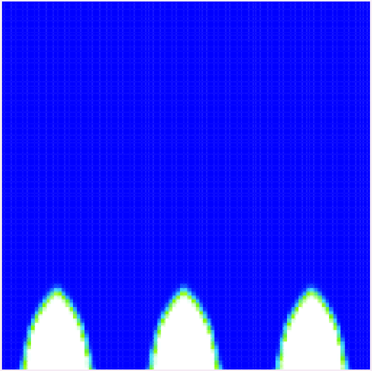
Temperature T



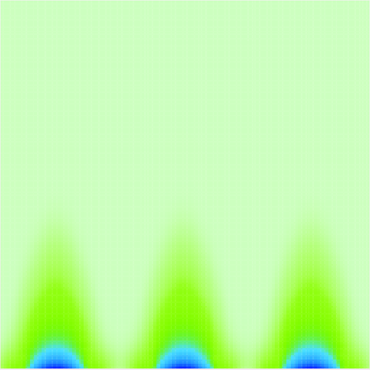
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



Temperature T



Geometry Play Skip

OUTLINE

Liquid-Vapor Phase Transition

- Diffuse Interface Model
  - global EOS always at equilibrium (entropy maximization),
  - strict hyperbolicity of the Euler system,
  - uniqueness of Liu solution for the Riemann problem;
- Relaxation Approach
  - 6 (or 5) equation system with relaxation terms;
- Numerical Method
  - operator splitting,
  - general approximate construction of global EOS (and resolution of projection step).

LIQUID-VAPOR PHASE TRANSITION

- Diffuse Interface Model
    - global EOS always at equilibrium (entropy maximization),
    - strict hyperbolicity of the Euler system,
    - uniqueness of Liu solution for the Riemann problem;
- Relaxation Approach
    - 6 (or 5) equation system with relaxation terms;
- Numerical Method
    - operator splitting,
    - general approximate construction of global EOS (and resolution of projection step).

LIQUID-VAPOR PHASE TRANSITION

- Diffuse Interface Model
  - global EOS always at equilibrium (entropy maximization),
  - strict hyperbolicity of the Euler system,
  - uniqueness of Liu solution for the Riemann problem;
- Relaxation Approach
  - 6 (or 5) equation system with relaxation terms;
- Numerical Method
  - operator splitting,
  - general approximate construction of global EOS (and resolution of projection step).

Speed of sound

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

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

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

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

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

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

Return

Speed of sound

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

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

- for all **w** pure phase state

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

- for all **w** equilibrium mixture state

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

Speed of sound

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

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

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

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

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

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

Return

Speed of sound

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

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

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

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

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

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

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

Return

SPEED OF SOUND

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

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

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

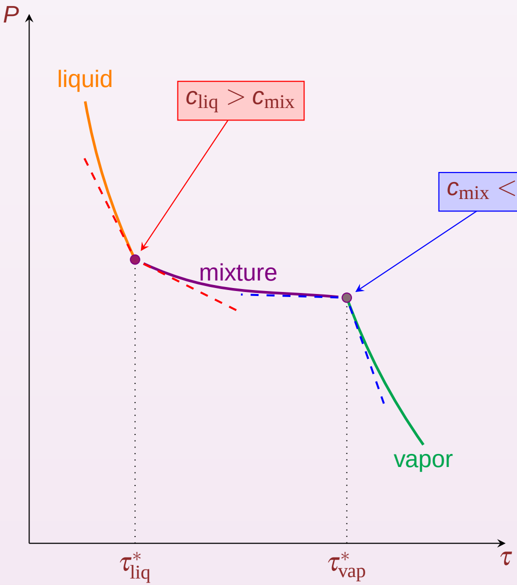
$$\mathbf{v}^T \, \mathrm{d}^2 s^{eq}(\mathbf{w}) \, \mathbf{v} < 0 \quad \forall \, \mathbf{v} \neq 0,$$

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

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

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

Isentropic curves



Stiffened Gas for Water

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

Phase	c_v [J/(kg·K)]	γ	π [Pa]	q [J/kg]	m [J/(kg·K)]
Water	1816.2	2.35	10^9	-1167.056×10^3	-32765.55596
Steam	1040.14	1.43	0	2030.255×10^3	-33265.65947

TABLE: Parameters proposed by [Le Metayer] for water.

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

$$\left.\begin{array}{l} T^i = 278\text{K}\dots610\text{K},\\ g_1(P,T^i)=g_2(P,T^i)\Rightarrow P^{\text{sat}}(T^i)\end{array}\right\}\Rightarrow\mathfrak{A}=\left\{\left(T^i,P^{\text{sat}}(T^i)\right)\right\}_{i=0}^{83}$$

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

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

Return

Stiffened Gas for Water

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

Phase	c_v [J/(kg·K)]	γ	π [Pa]	q [J/kg]	m [J/(kg·K)]
Water	1816.2	2.35	10^9	-1167.056×10^3	-32765.55596
Steam	1040.14	1.43	0	2030.255×10^3	-33265.65947

TABLE: Parameters proposed by [Le Metayer] for water.

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

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

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

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

Return

Stiffened Gas for Water

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

Phase	c_v [J/(kg · K)]	γ	π [Pa]	q [J/kg]	m [J/(kg · K)]
Water	1816.2	2.35	10^9	-1167.056×10^3	-32765.55596
Steam	1040.14	1.43	0	2030.255×10^3	-33265.65947

TABLE: Parameters proposed by [Le Metayer] for water.

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

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

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

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

Return

Stiffened Gas for Water

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

Phase	c_v [J/(kg·K)]	γ	π [Pa]	q [J/kg]	m [J/(kg·K)]
Water	1816.2	2.35	10^9	-1167.056×10^3	-32765.55596
Steam	1040.14	1.43	0	2030.255×10^3	-33265.65947

TABLE: Parameters proposed by [Le Metayer] for water.

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

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

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

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

Return

Water Tabulated EOS

		Volume (m^3/kg)		Internal Energy (kJ/kg)	
T (K)	P^{sat} (MPa)	τ_{liq}^{sat}	τ_{vap}^{sat}	ε_{liq}^{sat}	ε_{vap}^{sat}
275	0,00069845	0,0010001	181,60	7,7590	2377,5
278	0,00086349	0,0010001	148,48	20,388	2381,6
281	0,0010621	0,0010002	122,01	32,996	2385,7
284	0,0012999	0,0010004	100,74	45,586	2389,8
287	0,0015835	0,0010008	83,560	58,162	2393,9
290	0,0019200	0,0010012	69,625	70,727	2398,0
293	0,0023177	0,0010018	58,267	83,284	2402,1
296	0,0027856	0,0010025	48,966	95,835	2406,2
299	0,0033342	0,0010032	41,318	108,38	2410,3
302	0,0039745	0,0010041	35,002	120,92	2414,4
305	0,0047193	0,0010050	29,764	133,46	2418,4
308	0,0055825	0,0010060	25,403	146	2422,5
311	0,0065792	0,0010071	21,759	158,54	2426,5
314	0,0077262	0,0010082	18,702	171,08	2430,5
317	0,0090418	0,0010094	16,129	183,62	2434,5
320	0,010546	0,0010107	13,954	196,16	2438,5
...	...	...	...	...	...

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

Return

Water Tabulated EOS

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

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

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

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