Modelling and Simulation of Liquid-Vapor Phase Transition

A Boiling Crisis Study Contribution

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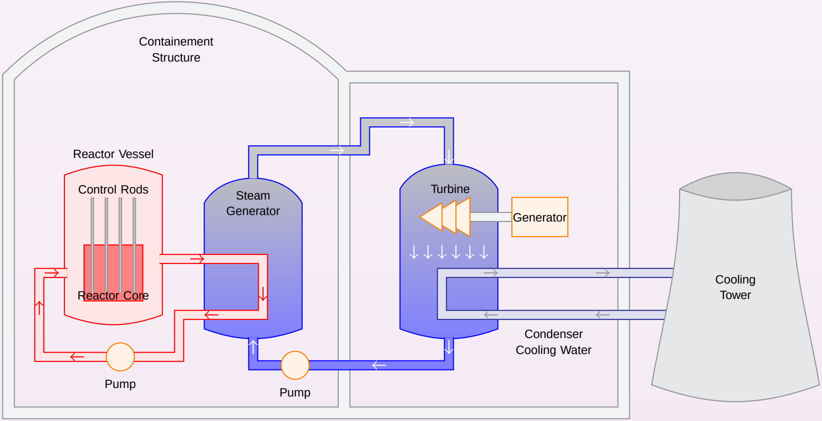
Pressurized Water Reactor

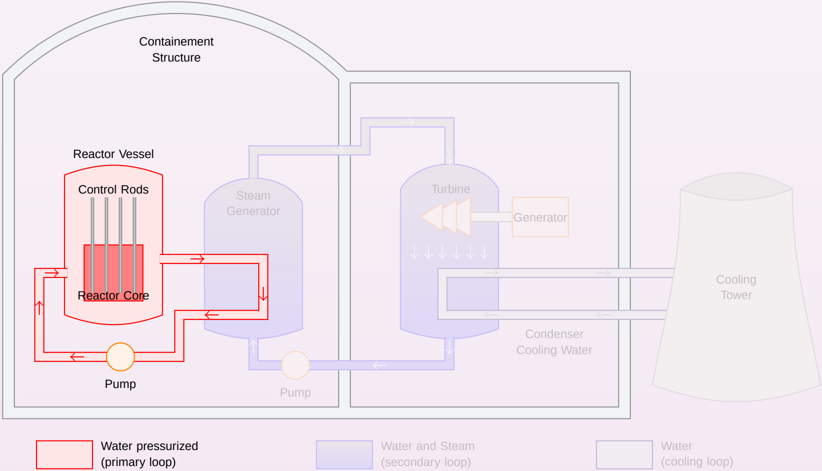


Water pressurized (primary loop)

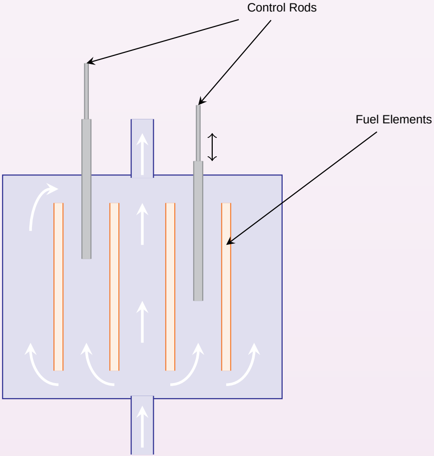
Water and Steam (secondary loop)

Water (cooling loop)

Pressurized Water Reactor



Core of a Pressurized Water Reactor



Boiling Crisis

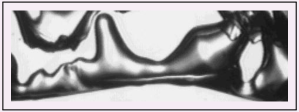
Phenomenon

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,
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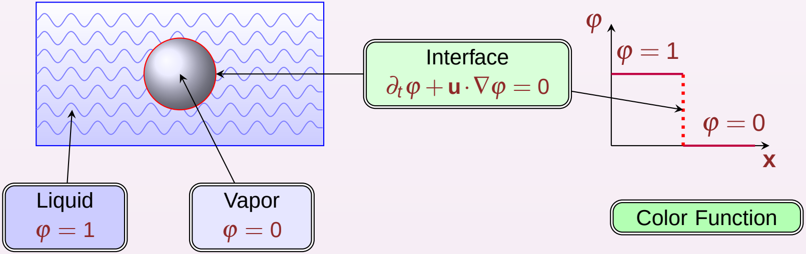
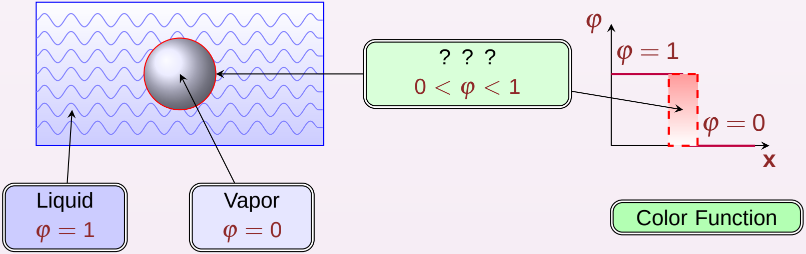
Liquid-Vapor Interface



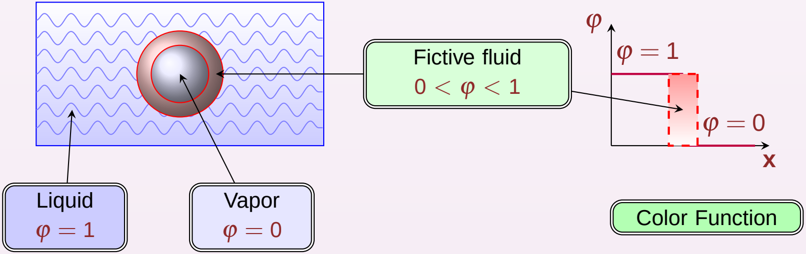
$$(\rho, \varepsilon) \mapsto P = \begin{cases} P^{\text{liq}} & \text{if } \varphi = 1; \\ P^{\text{vap}} & \text{if } \varphi = 0. \end{cases}$$

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



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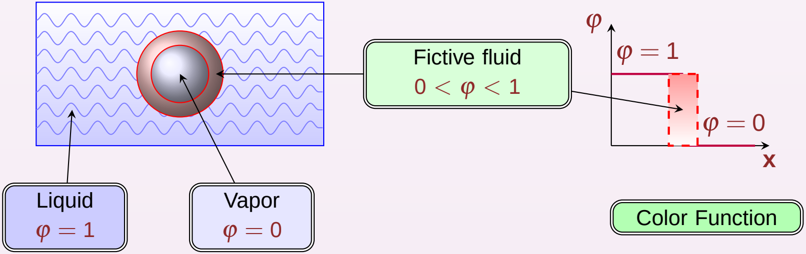

➔ Goal: define a global pressure law such that

- $(\rho, \varepsilon, \mathbf{u}, P)$ are continuous (3 zones)
- the interface position and the phase change are implicit ($\rightsquigarrow \not\varphi$)
- coherence with classical thermodynamics [H. Callen]

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

τ_α specific volume
ε_α specific internal energy

$$\Rightarrow \quad \mathbf{w}_\alpha \stackrel{\text{def}}{=} (\tau_\alpha, \varepsilon_\alpha);$$

$\mathbf{w}_\alpha \mapsto s_\alpha$ 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 $\alpha = 1, 2$

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EOS without Phase Change

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

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Entropy without phase change

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

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

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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:

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

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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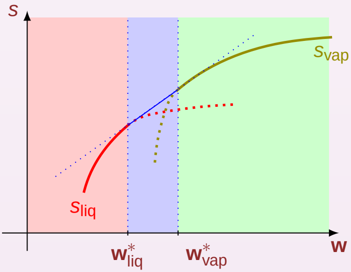

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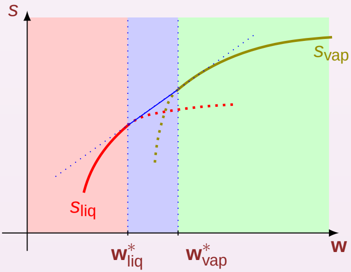

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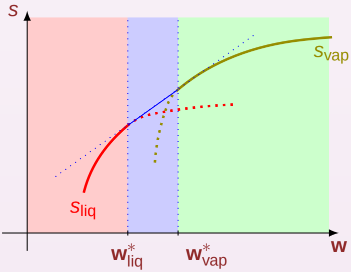

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From $\mathbf{w} \mapsto s^{\mathrm{eq}}$ to $\mathbf{w} \mapsto P^{\mathrm{eq}}$

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

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

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

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

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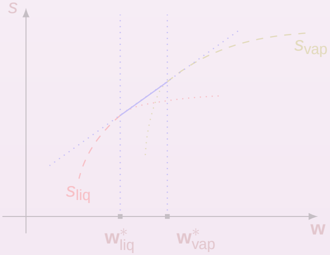

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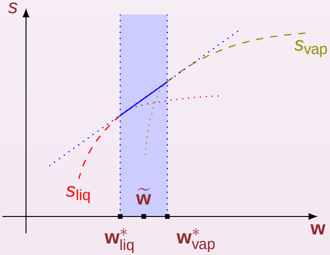

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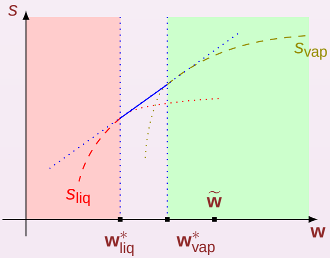

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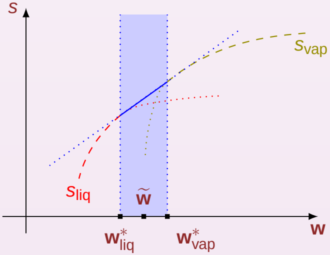

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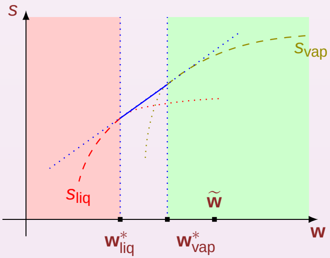

Dynamic Liquid-Vapor Phase Change

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.

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Outline

HOW TO SIMULATE THE LIU SOLUTION

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

Relaxation Approach

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

Relaxation Approach

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

Relaxation Approach

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

Equilibrium System

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

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

RELAXATION APPROACH

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

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

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

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

Augmented System

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

In the interface

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

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

Equilibrium System

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

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

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

Equilibrium System

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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

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Analytical EOS

Water Example

(τ, ε) fixed

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

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

(P, T) solution of

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

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

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ANALYTICAL EOS

Water Example

(τ, ε) fixed

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ANALYTICAL EOS

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ANALYTICAL EOS

Water Example

(τ,ε) fixed

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ANALYTICAL EOS

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least square approximation

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

T SOLUTION OF

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

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

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

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least square approximations

Tabulated EOS

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with $\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T)$ tabulated

$\wr\wr$

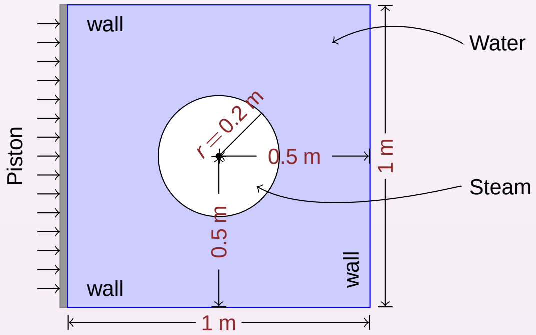
$$\frac{\tau - \widehat{\tau}_2^{\text{sat}}(T)}{\widehat{\tau}_1^{\text{sat}}(T) - \widehat{\tau}_2^{\text{sat}}(T)} = \frac{\varepsilon - \widehat{\varepsilon}_2^{\text{sat}}(T)}{\widehat{\varepsilon}_1^{\text{sat}}(T) - \widehat{\varepsilon}_2^{\text{sat}}(T)}$$

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

least square approximations

Outline

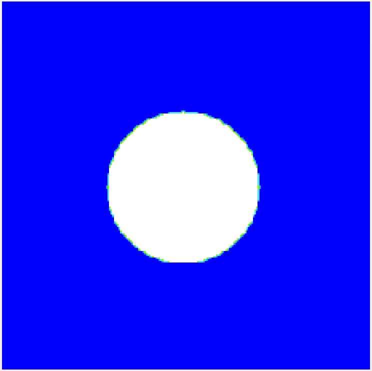
Compression of a Vapor Bubble



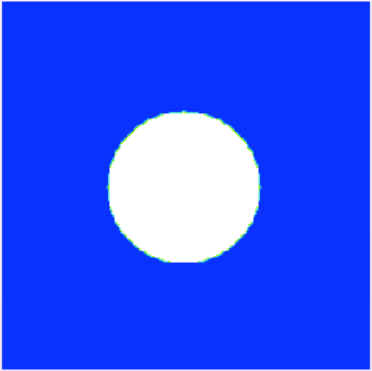
Compression of a 2D Vapor Bubble involving two Stiffened Gases for water and steam.
The piston moves towards right at constant speed $u_p = 30$ m/s.

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

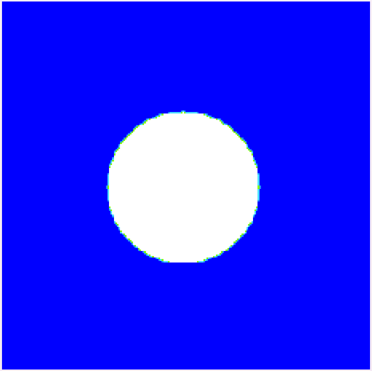


$t = 0.00$ ms

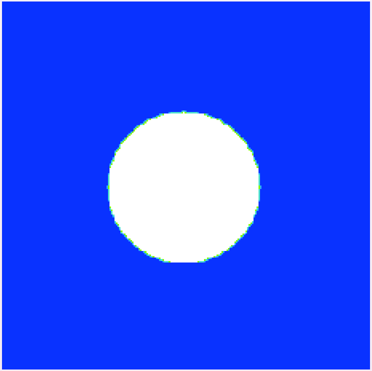
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

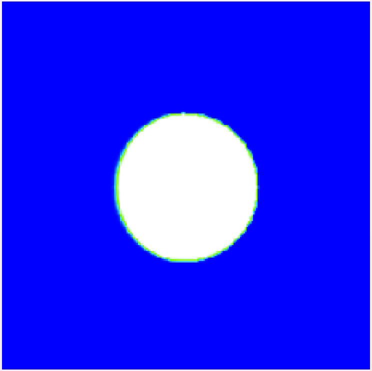


$t = 0.00$ ms

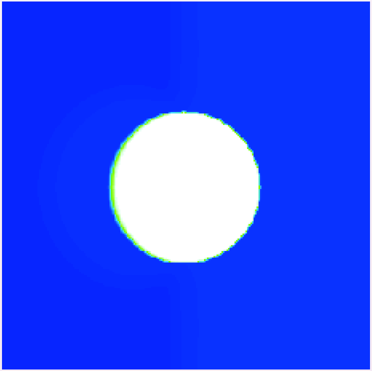
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

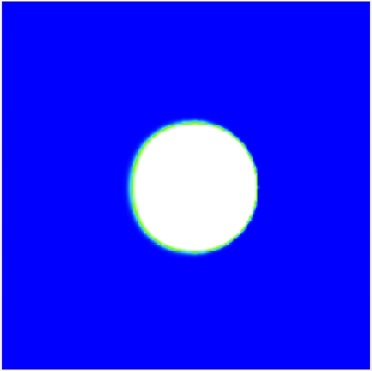


$t = 0.89$ ms

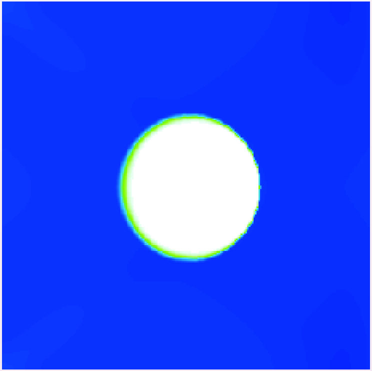
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



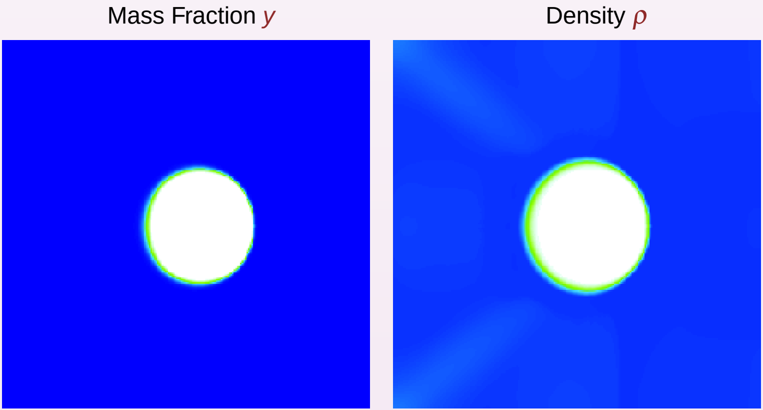
Density ρ



$t = 1.09$ ms

Geometry Play Skip

Compression of a Vapor Bubble

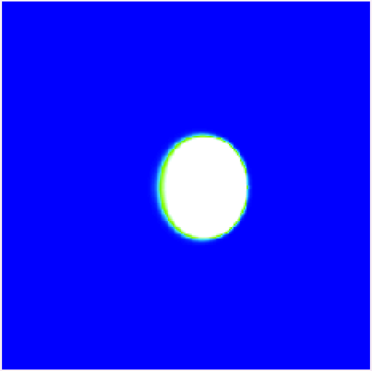


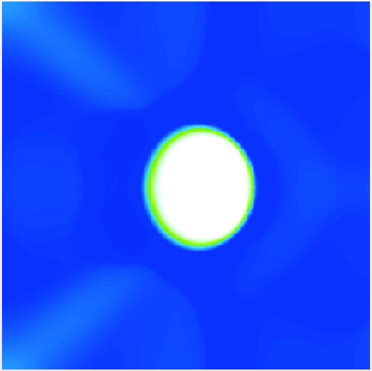
$t = 1.49$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y | Density ρ



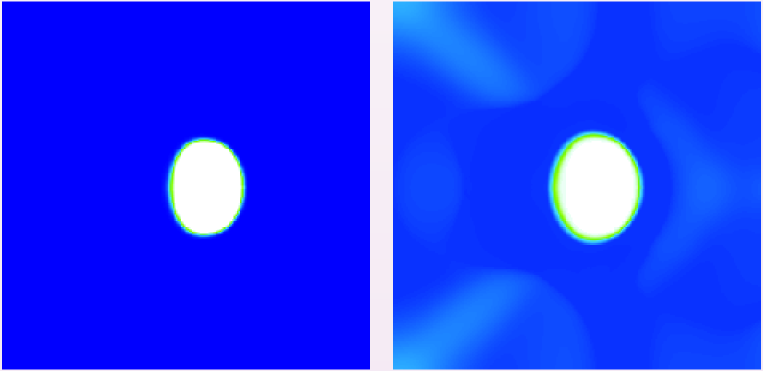


$t = 1.80$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ

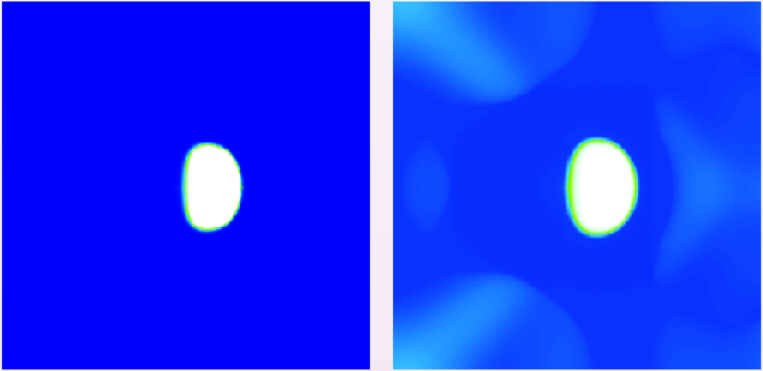


$t = 2.09$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ

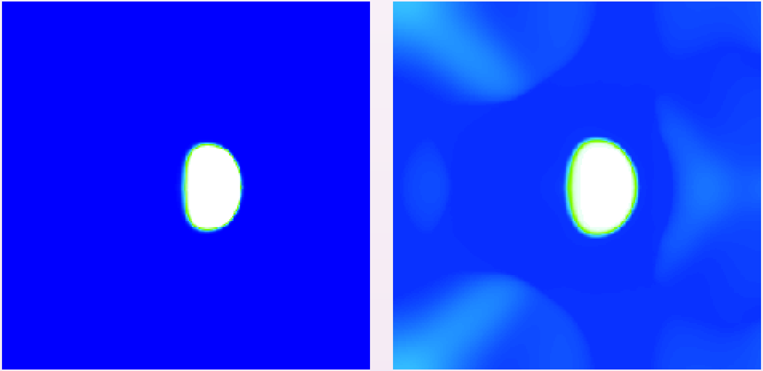


$t = 2.39$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y | Density ρ

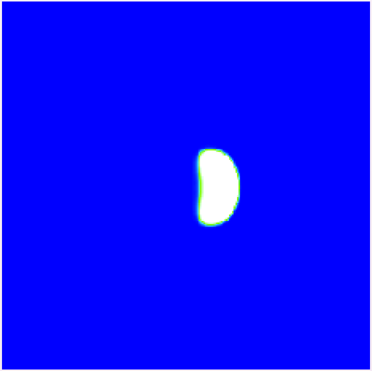


$t = 2.69$ ms

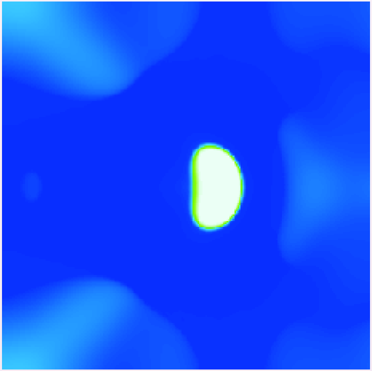
Geometry | Play | Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

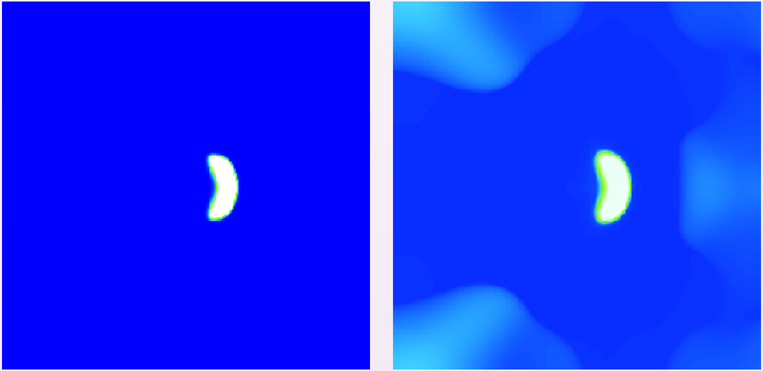


$t = 2.99$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ

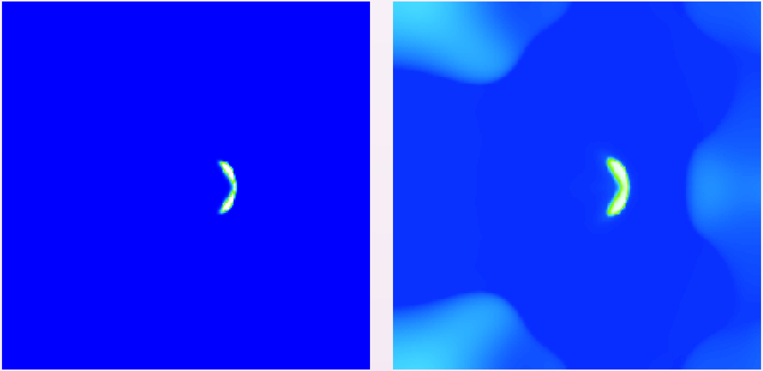


$t = 3.29$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ

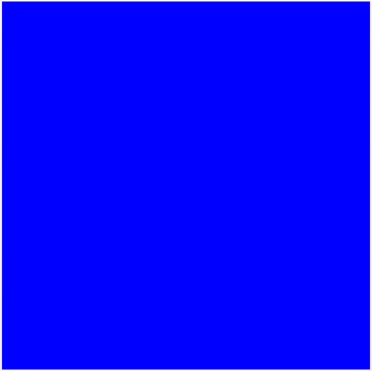


$t = 3.49$ ms

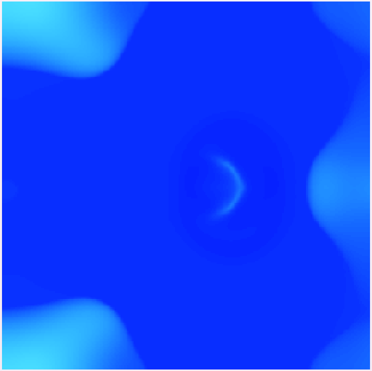
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

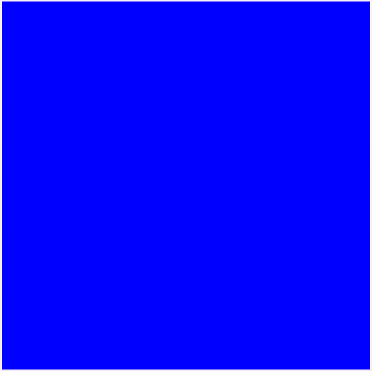


$t = 3.60$ ms

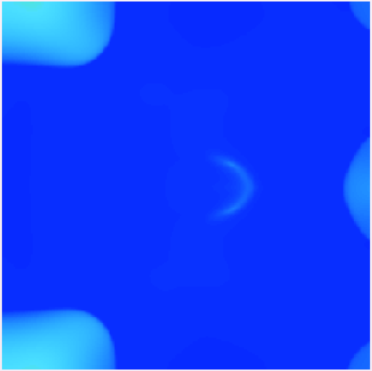
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



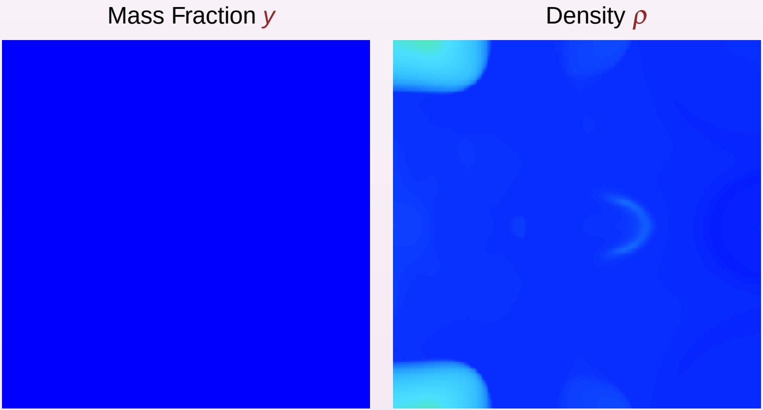
Density ρ



$t = 3.80$ ms

Geometry Play Skip

Compression of a Vapor Bubble

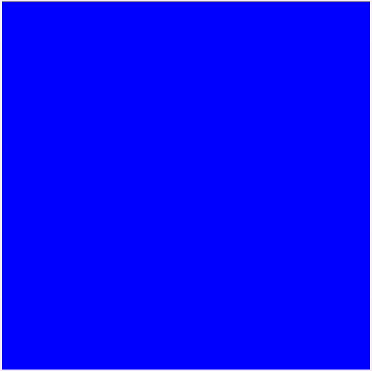


$t = 3.99$ ms

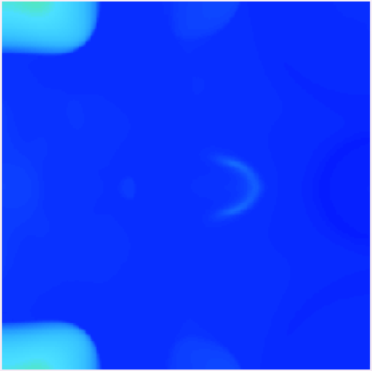
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



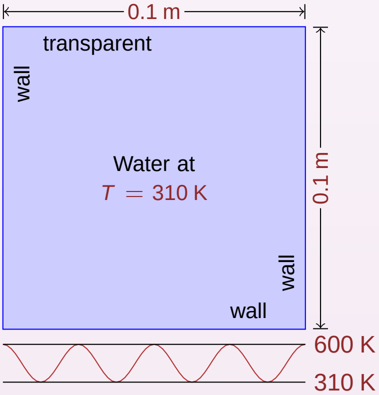
Density ρ



$t = 4.10$ ms

◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLES

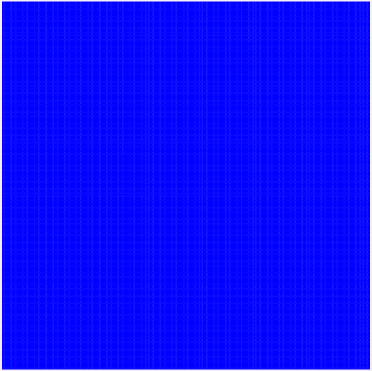


Nucleation of a 2D Vapor Bubbles involving two Stiffened Gases for water and steam. The temperature of the south wall is fixed at

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

Nucleating Bubbles

Mass Fraction y

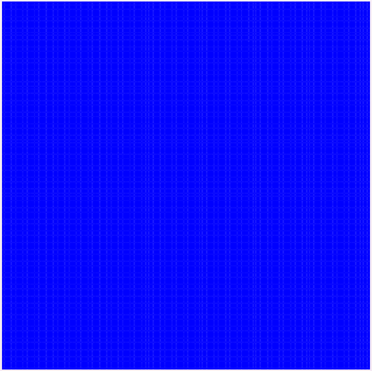


Temperature T

Geometry Play Skip

Nucleating Bubbles

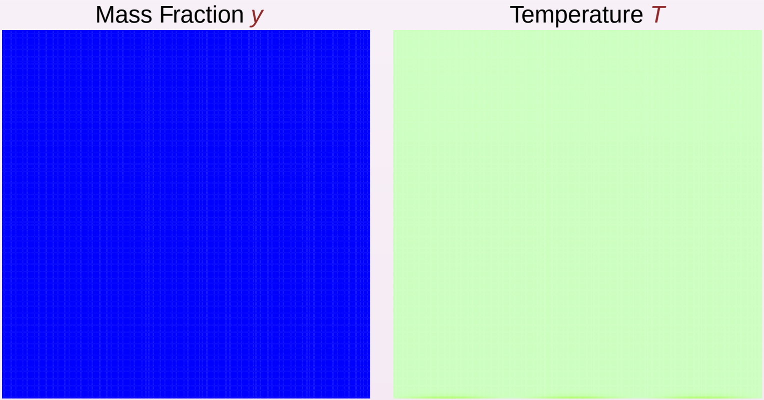
Mass Fraction y



Temperature T

Geometry Play Skip

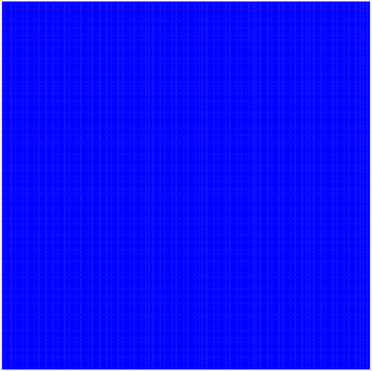
Nucleating Bubbles



Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

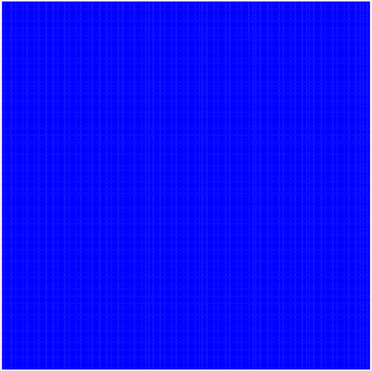


Temperature T

Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

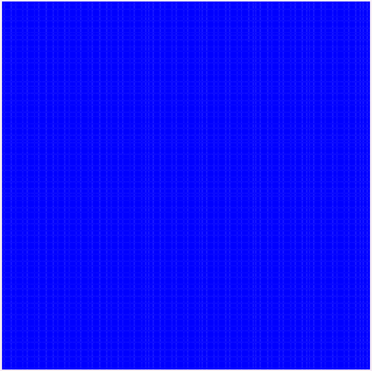


Temperature T

Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

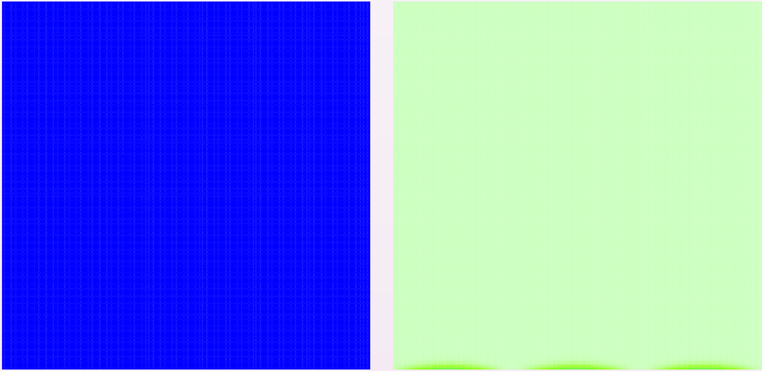


Temperature T

◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

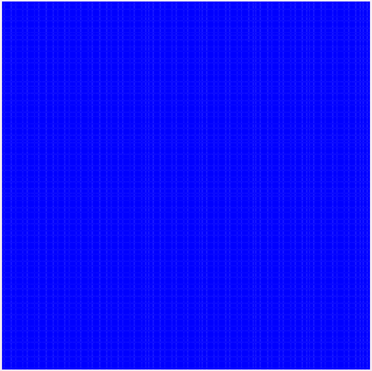
Mass Fraction y Temperature T



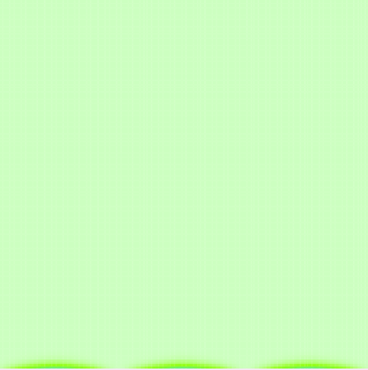
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y

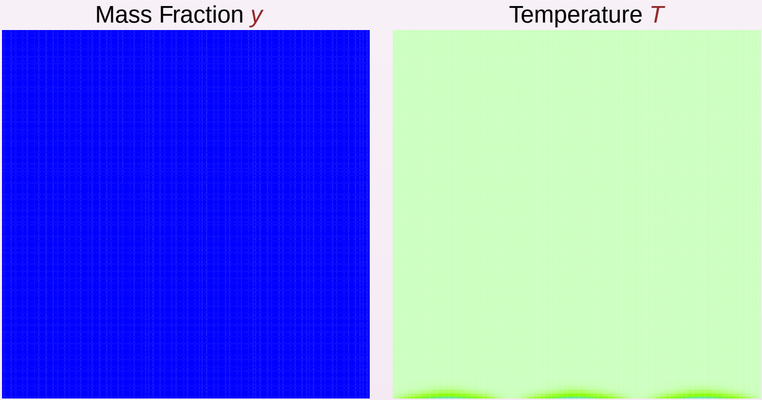


Temperature T



Geometry Play Skip

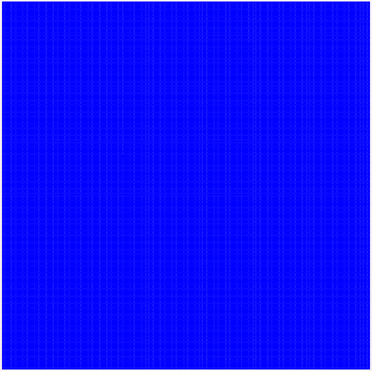
Nucleating Bubbles



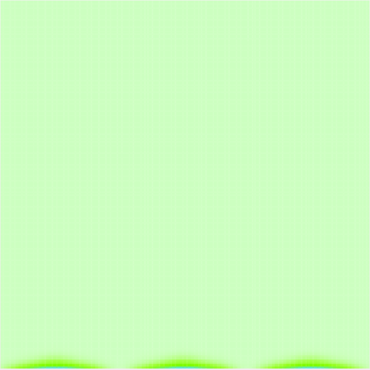
◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLES

Mass Fraction y



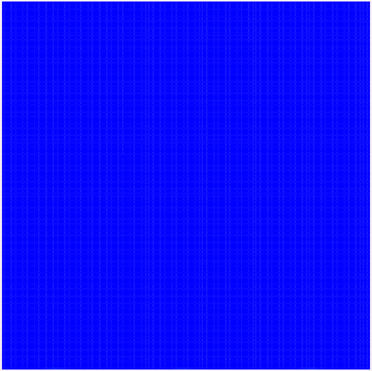
Temperature T



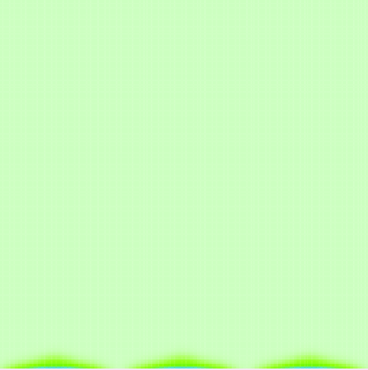
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



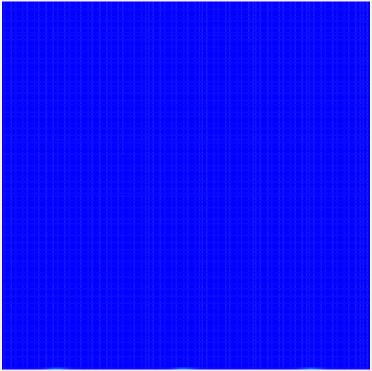
Temperature T



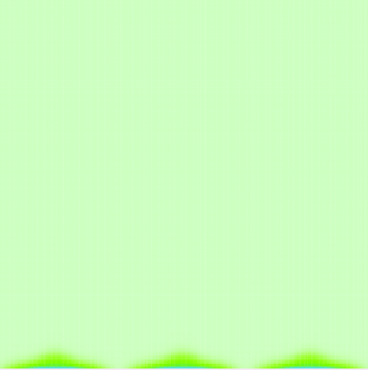
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



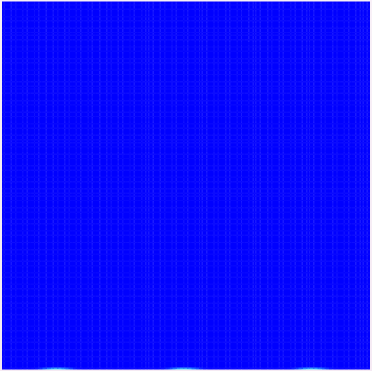
Temperature T



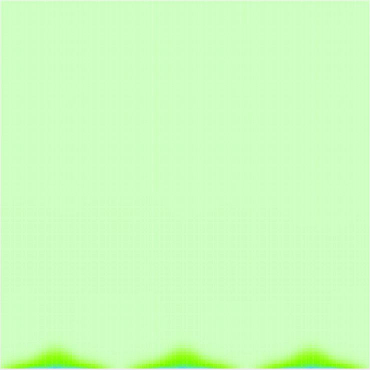
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



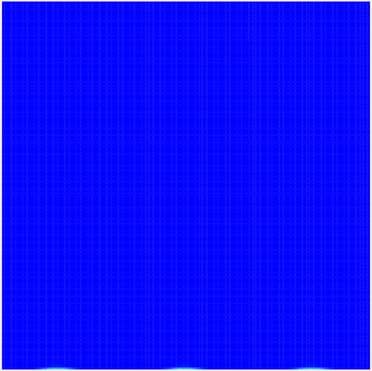
Temperature T



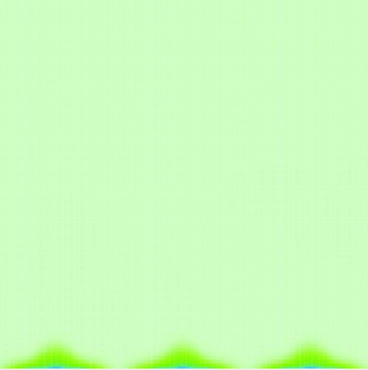
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

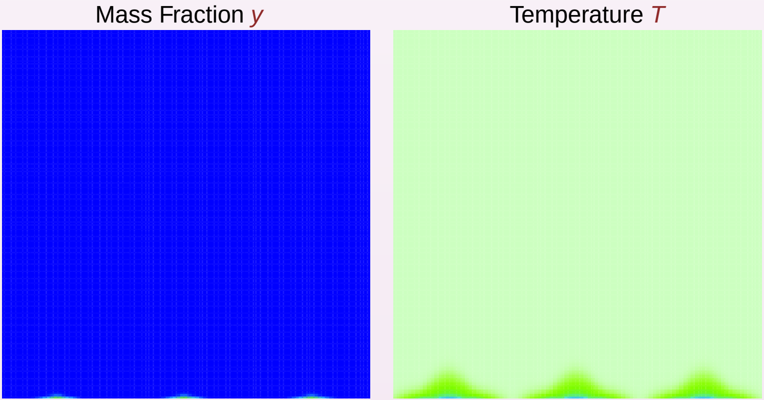


Temperature T



◂ Geometry ▸ Play ▸▸ Skip

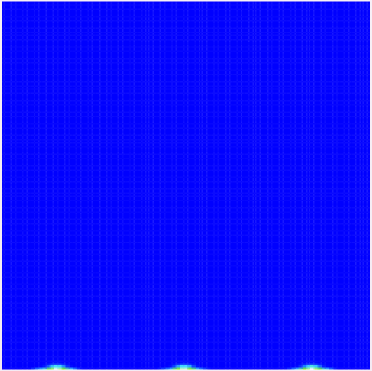
Nucleating Bubbles



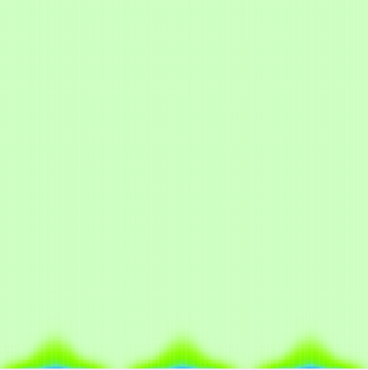
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y



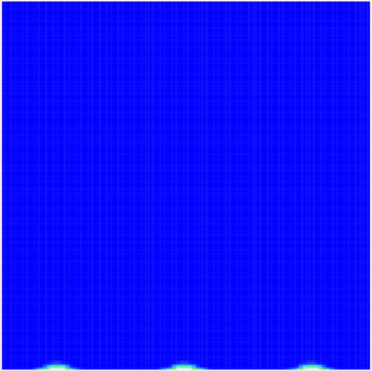
Temperature T



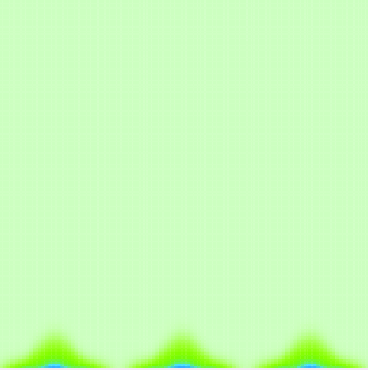
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

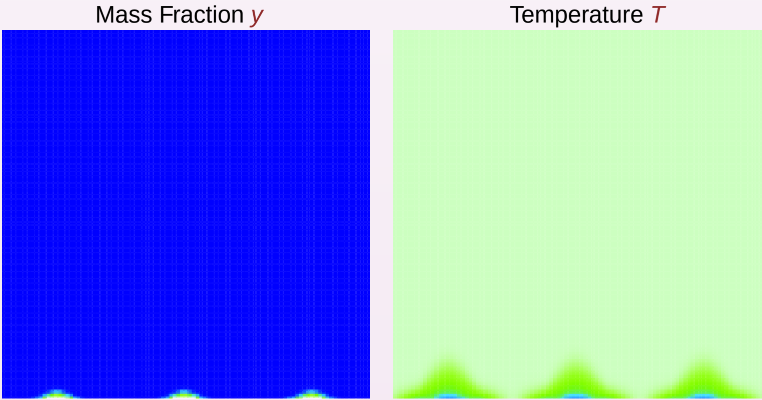


Temperature T



Geometry Play Skip

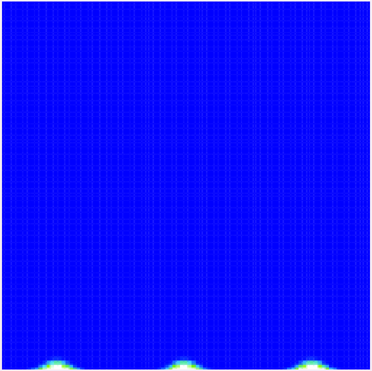
Nucleating Bubbles



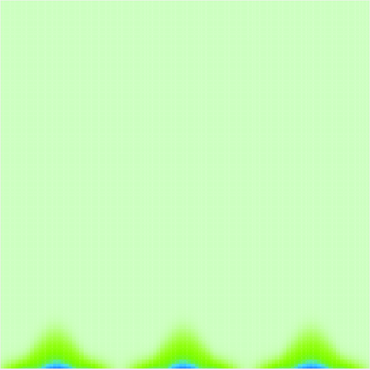
◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLES

Mass Fraction y



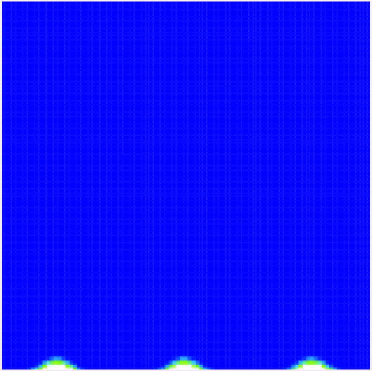
Temperature T



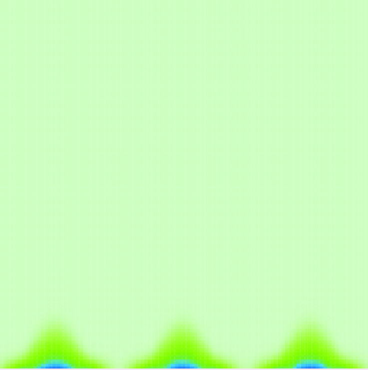
◀ Geometry ▶ Play ▶▶ Skip

Nucleating Bubbles

Mass Fraction y



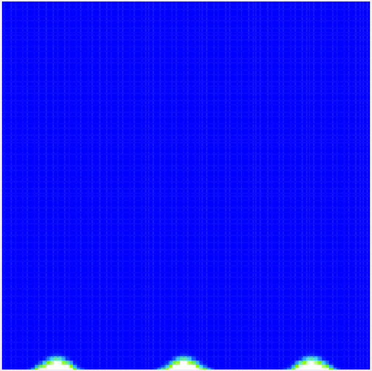
Temperature T



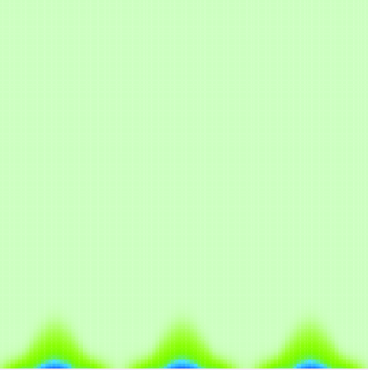
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



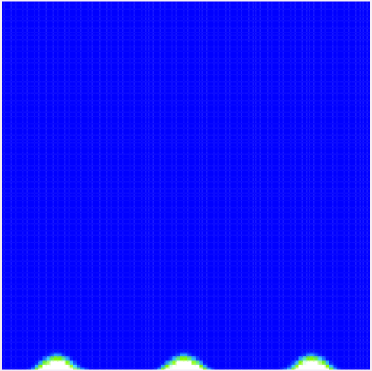
Temperature T



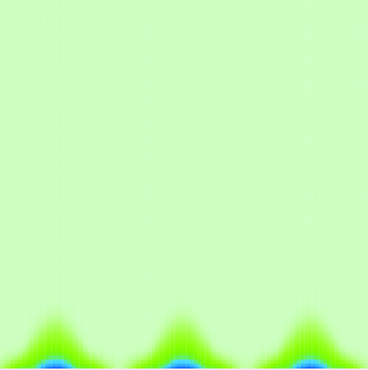
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



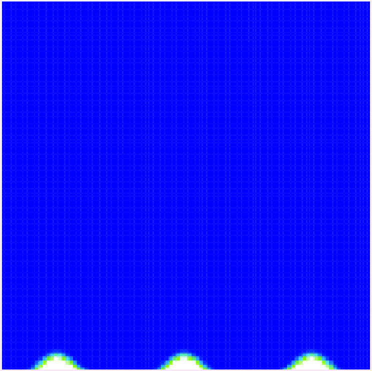
Temperature T



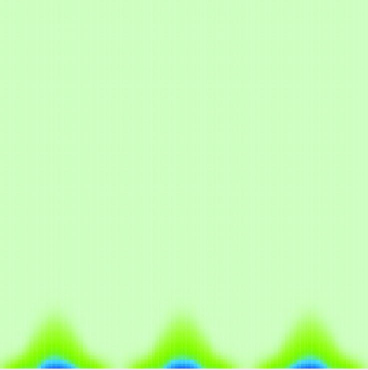
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



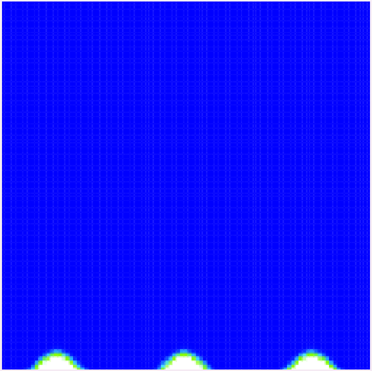
Temperature T



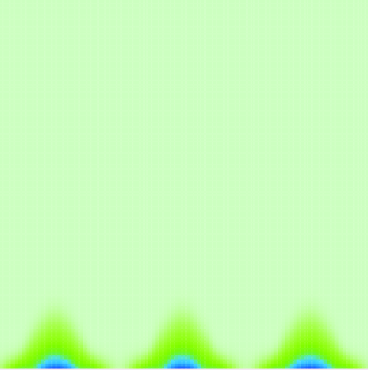
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



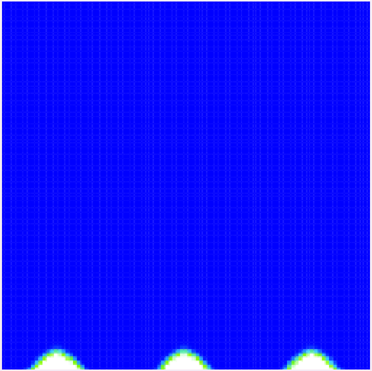
Temperature T



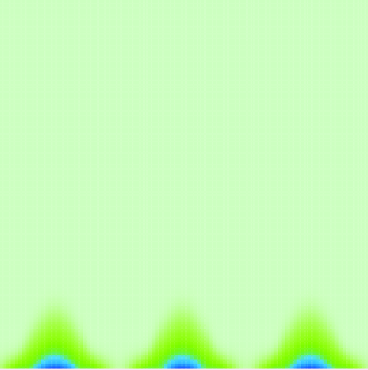
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



Temperature T



◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

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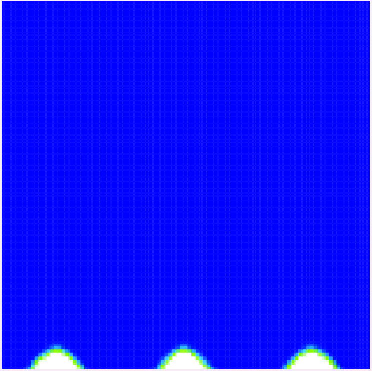
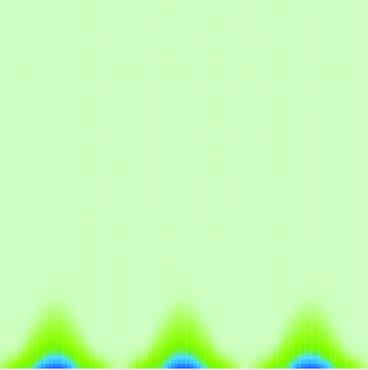
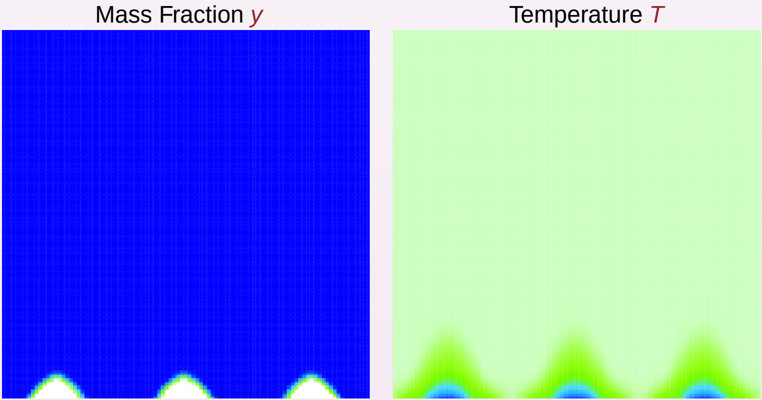


Temperature T



Geometry Play Skip

Nucleating Bubbles



Geometry Play Skip

Nucleating Bubbles

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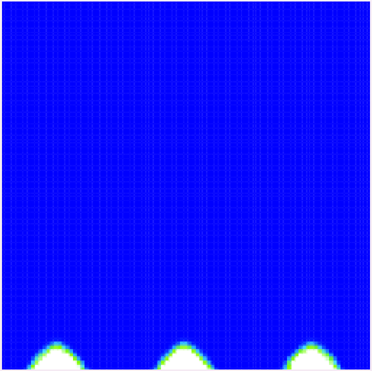
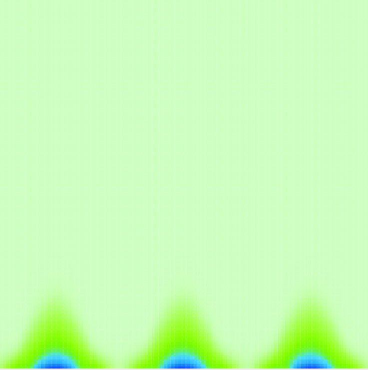


Temperature T



Geometry Play Skip

Nucleating Bubbles

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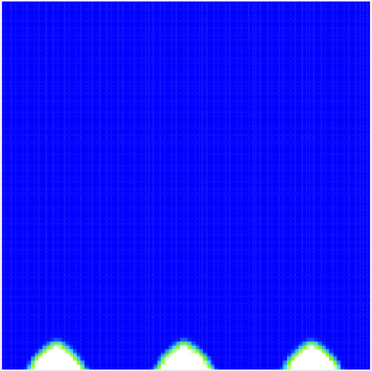
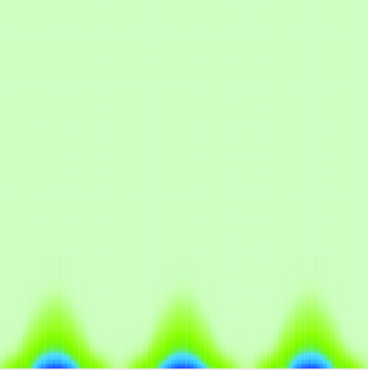


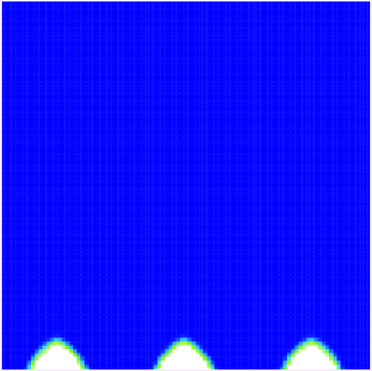
Temperature T



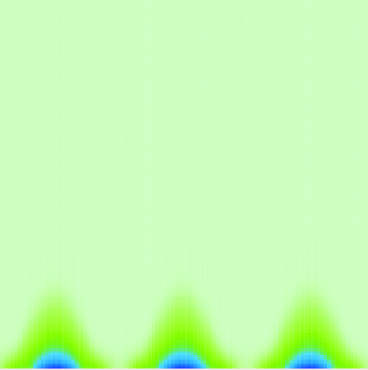
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



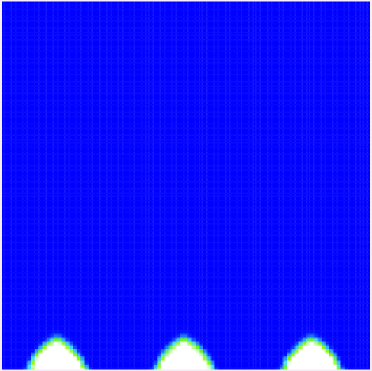
Temperature T



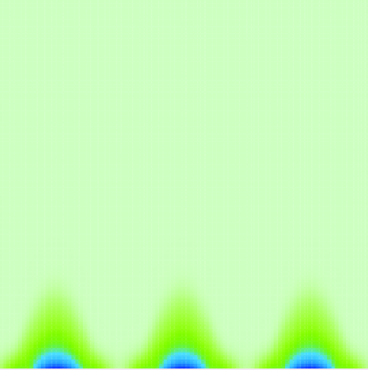
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



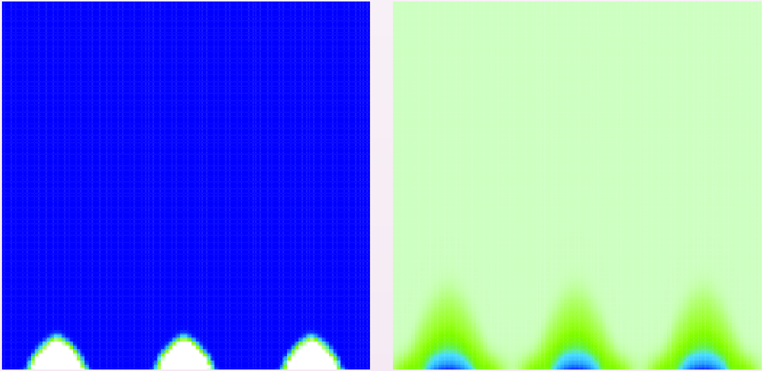
Temperature T



Geometry Play Skip

Nucleating Bubbles

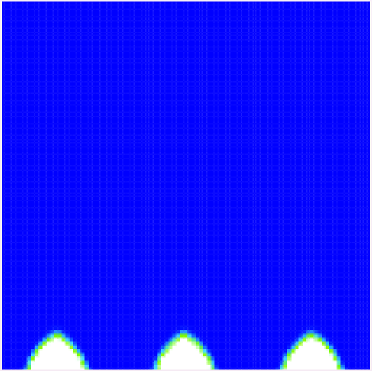
Mass Fraction y Temperature T



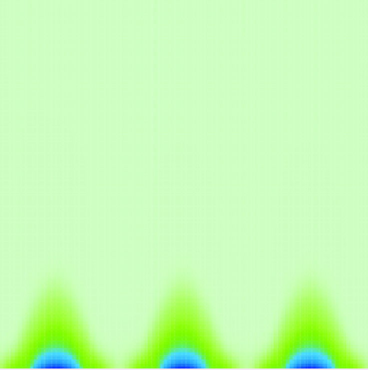
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



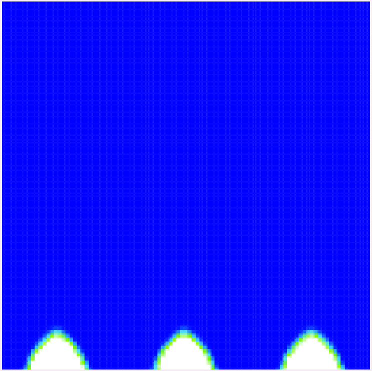
Temperature T



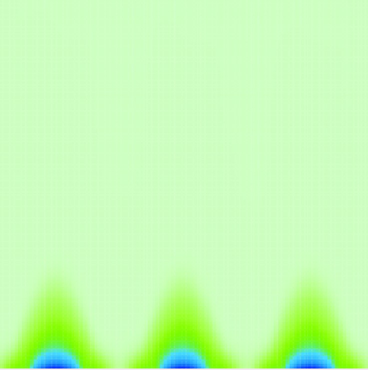
Geometry Play Skip

Nucleating Bubbles

Mass Fraction *y*

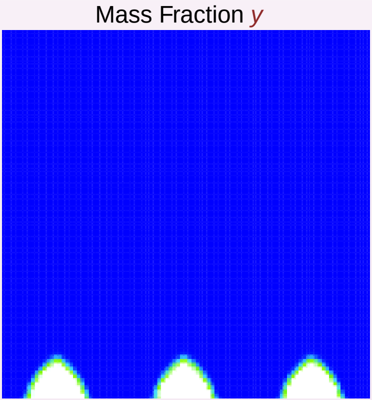


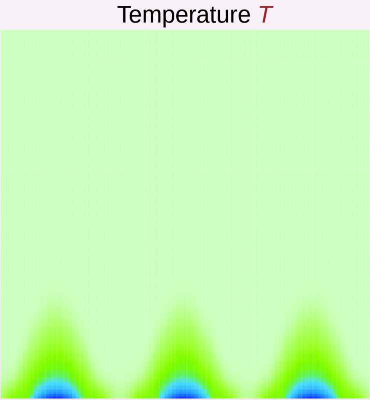
Temperature *T*



Geometry Play Skip

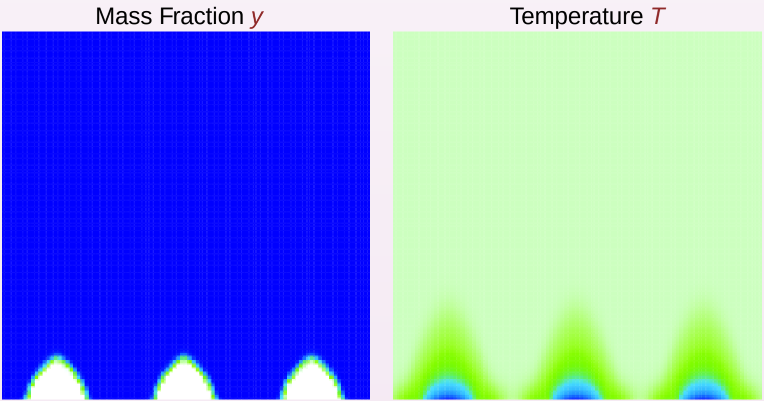
NUCLEATING BUBBLES





Geometry Play Skip

Nucleating Bubbles



◂ Geometry ▸ Play ▸▸ Skip

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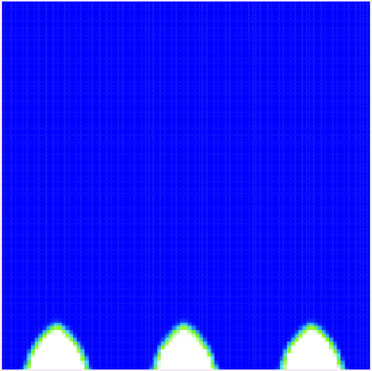
Mass Fraction y



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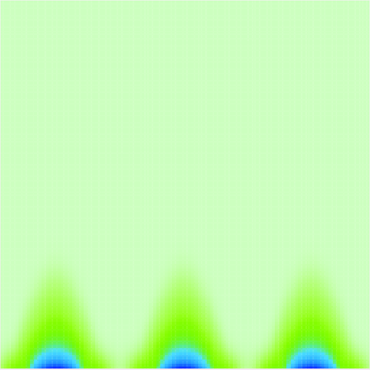

◂ Geometry ▸ Play ▸▸ Skip

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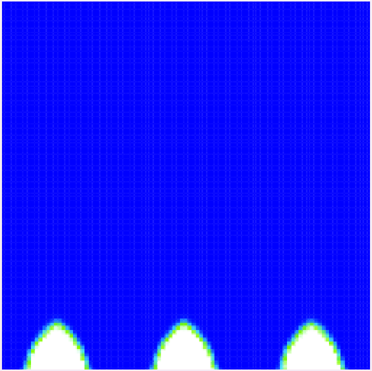
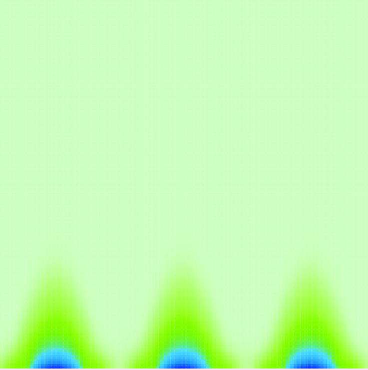


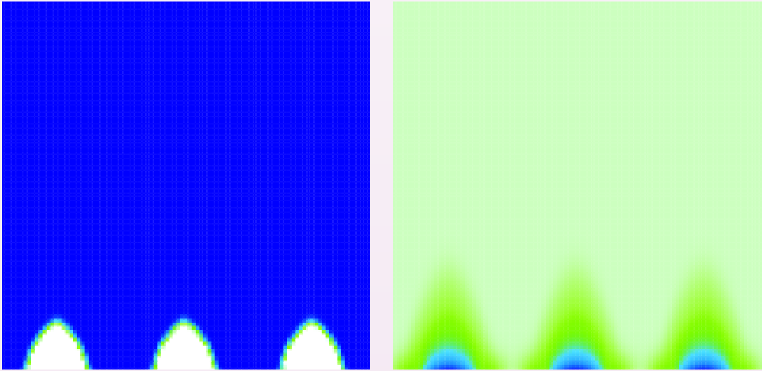
Temperature T



Geometry Play Skip

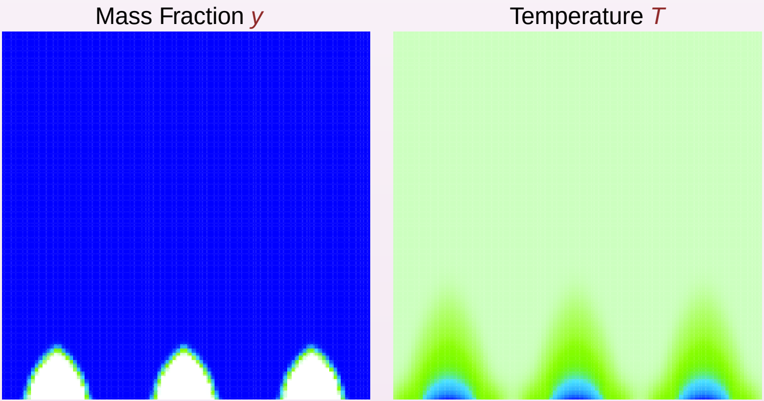
Nucleating Bubbles

Mass Fraction y | Temperature T



◂ Geometry ▸ Play ▸▸ Skip

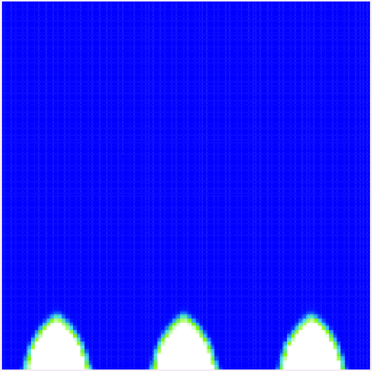
Nucleating Bubbles



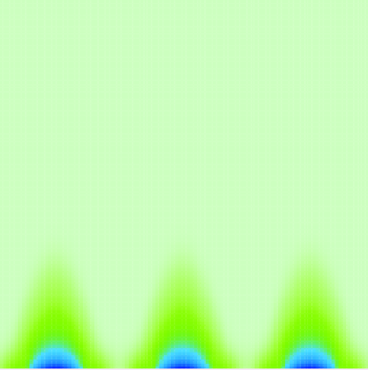
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



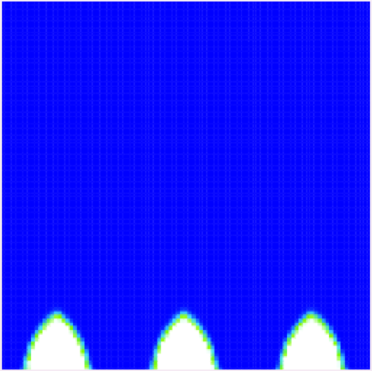
Temperature T



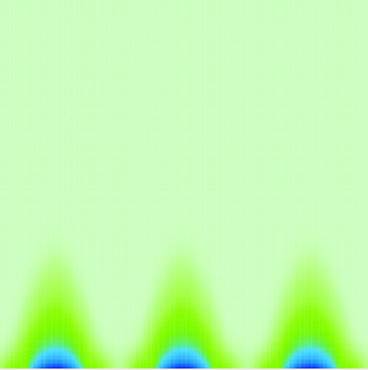
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



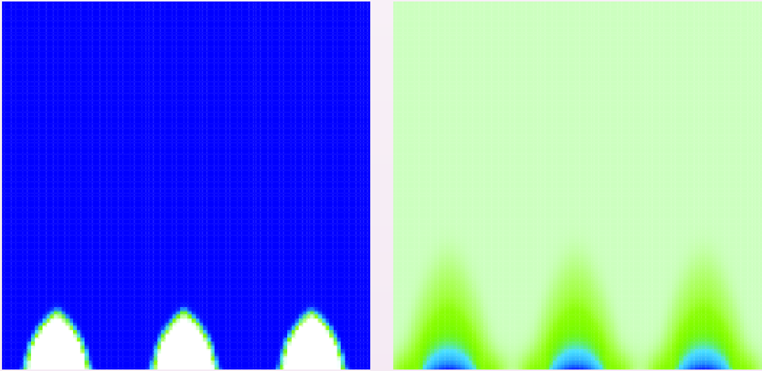
Temperature T



Geometry Play Skip

Nucleating Bubbles

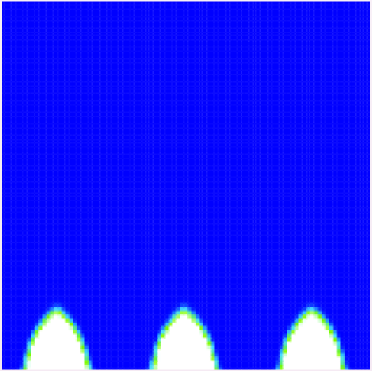
Mass Fraction y Temperature T



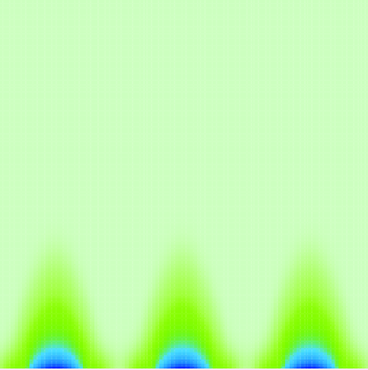
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y



Temperature T



◂ Geometry ▸ Play ▸▸ Skip

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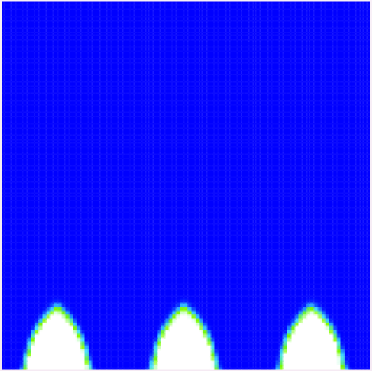
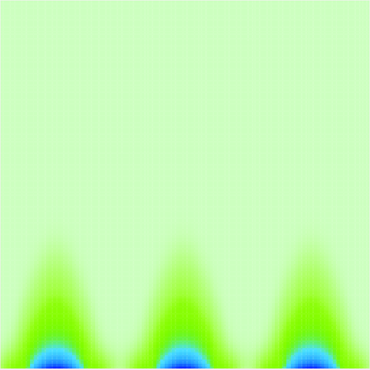


Temperature T



Geometry Play Skip

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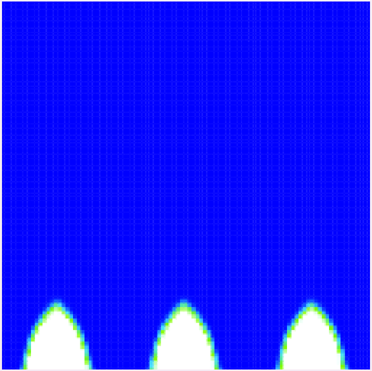

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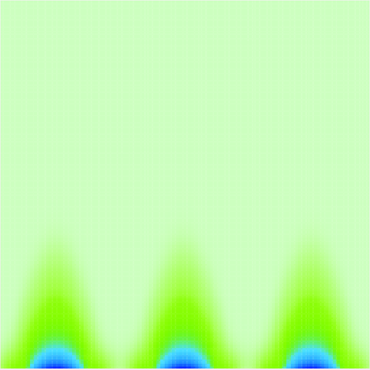

◂ Geometry ▸ Play ▸▸ Skip

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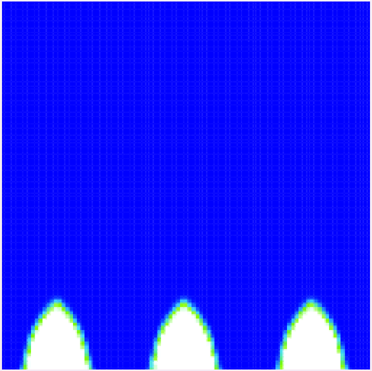
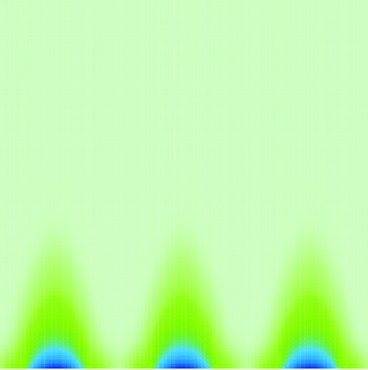
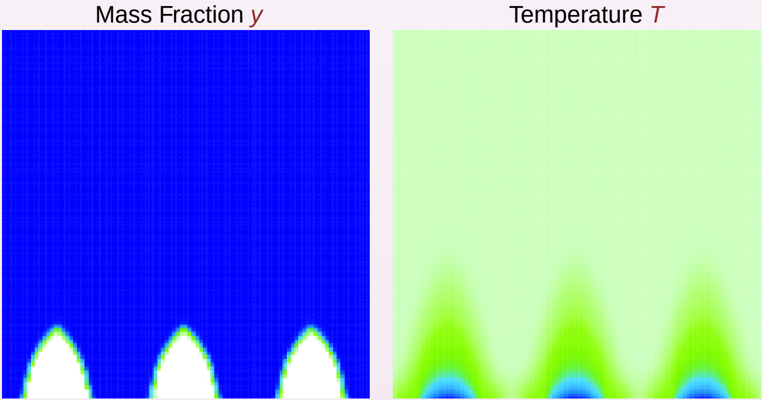


Temperature T



Geometry Play Skip

Nucleating Bubbles



Geometry Play Skip

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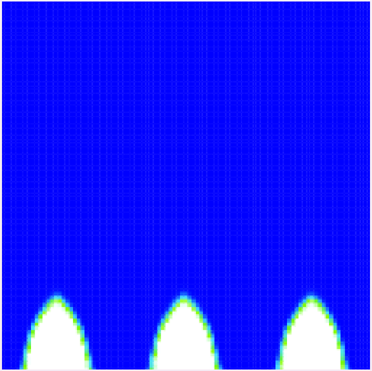

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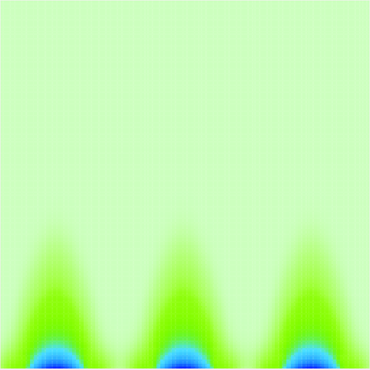

Geometry Play Skip

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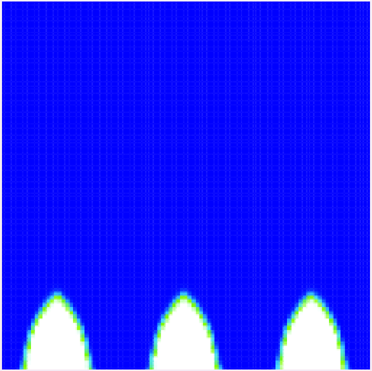

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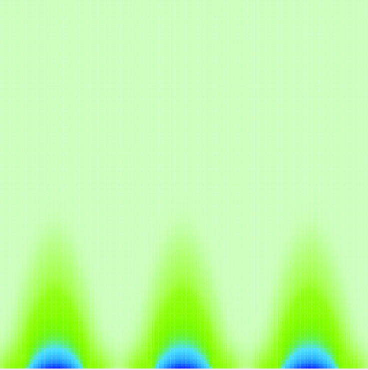

Geometry Play Skip

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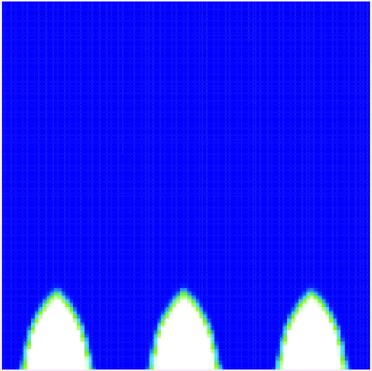

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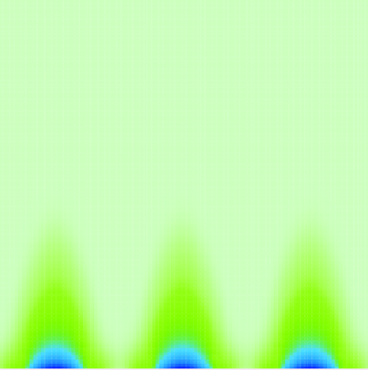

Geometry Play Skip

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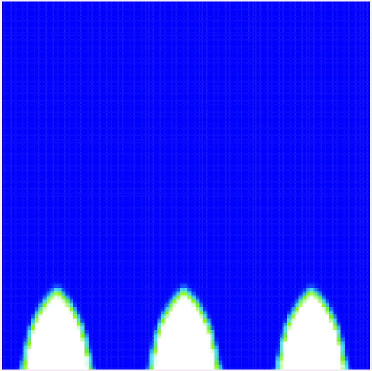
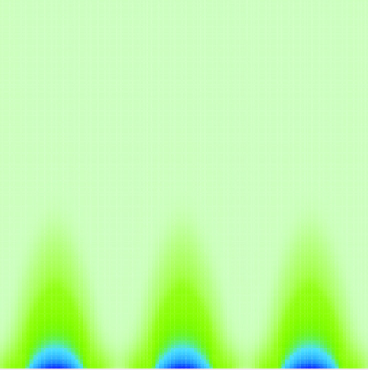


Temperature T



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).

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Speed of sound

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

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

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

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

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

Return

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

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

Speed of sound

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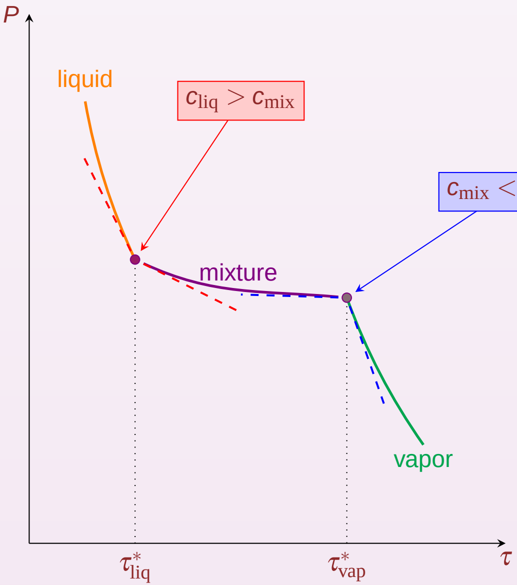
$\forall \mathbf{w}$ equilibrium mixture state, $\mathbf{v}(\mathbf{w}) \stackrel{?}{\not\asymp} [P^{eq}(\mathbf{w}), -1]$

Isentropic curves



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.

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

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

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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)]
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Stiffened Gas for Water

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

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

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

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