Modelling and Simulation of Liquid-Vapor Phase Transition

A Boiling Crisis Study Contribution

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Boiling Crisis

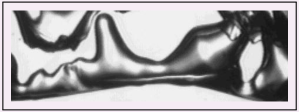
Phenomenon

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.

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

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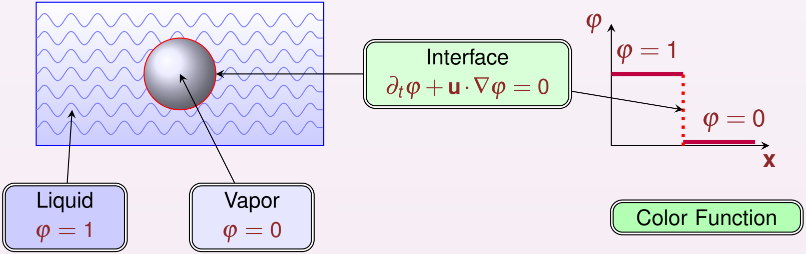
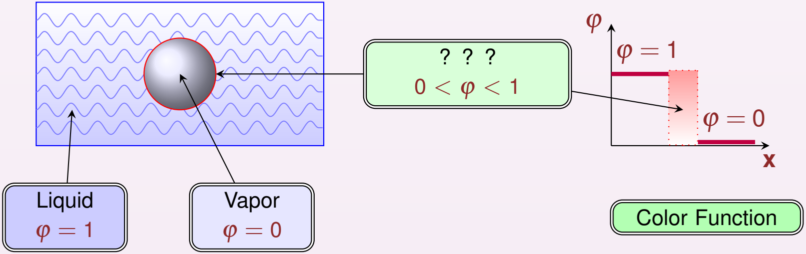
Liquid-Vapor Interface



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

Liquid-Vapor Interface



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

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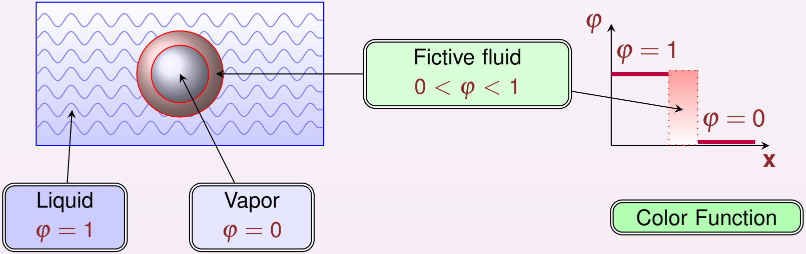

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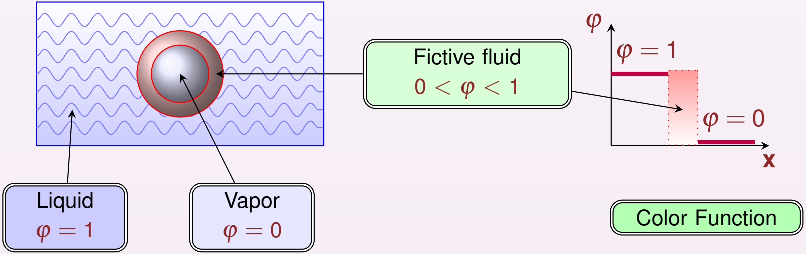

Goal: define a global pressure law such that

- $(\rho, \varepsilon, \mathbf{u}, P)$ are continuous (3 zones)
- the interface position and the phase change are implicit ($\leadsto \cancel{\varphi}$)
- 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.);

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

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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

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

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EOS WITH PHASE CHANGE

ENTROPY WITHOUT PH.CH.

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

ENTROPY AT EQUILIBRIUM

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

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

Optimization Problem:

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

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

Solution: (z^*, y^*, ψ^*)

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Entropy at equilibrium

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

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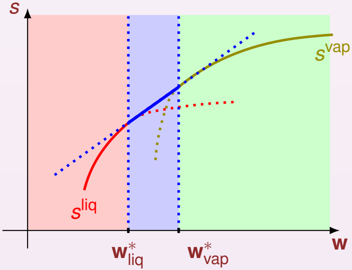

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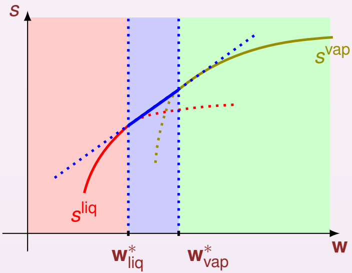

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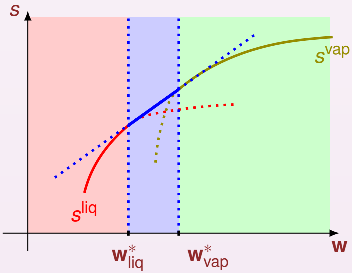

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Properties [G. Allaire, G. Faccanoni, S. Kokh]

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]
- Viscuous Solver (the Liu solution is the only solution that has a viscuous 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

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

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

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In the interface

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

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

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

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

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

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

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

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

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

Numerical Scheme

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

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

❶ $\mu_j = +\infty$

$\Downarrow$

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

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

❷ $\mu_j = 0$

$\Downarrow$

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

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

Numerical Scheme

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

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NUMERICAL SCHEME

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

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

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Numerical Scheme

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

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

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

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

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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

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

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

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

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

T SOLUTION OF

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

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

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

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

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

TABULATED EOS

Water Examples

(τ,ε) fixed

T SOLUTION OF

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

$$\wr\wr$$

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

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

TABULATED EOS

Water Examples

(τ, ε) fixed

T SOLUTION OF

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

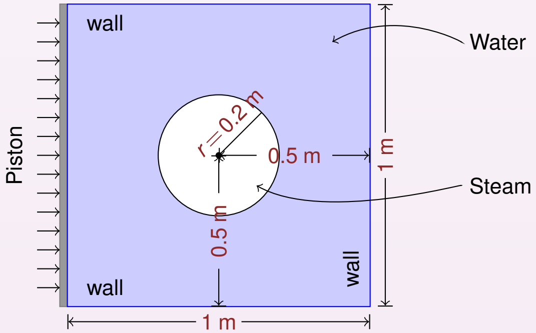
$$\wr\wr$$

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

least square approximations

OUTLINE

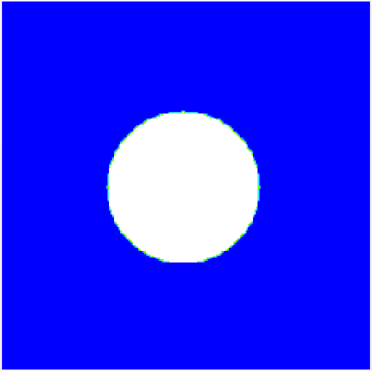
Compression of a Vapor Bubble



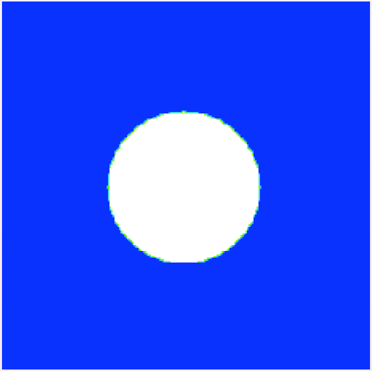
Compression of a 2D Vapor Bubble involving two Stiffened Gases for water and steam.
The piston moves towards right at constant speed $u_p = 30$ m/s.

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

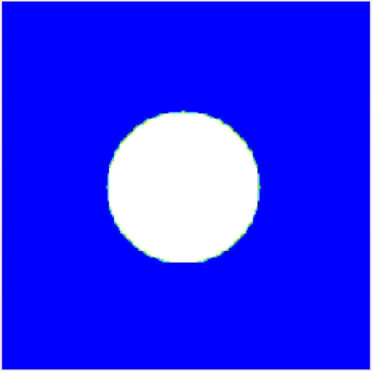


$t = 0.00$ ms

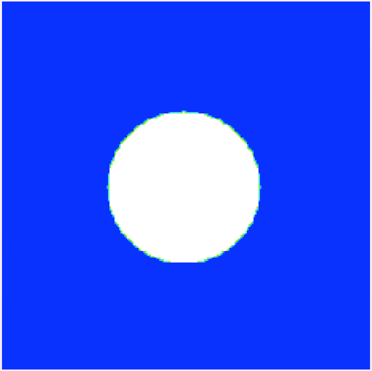
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



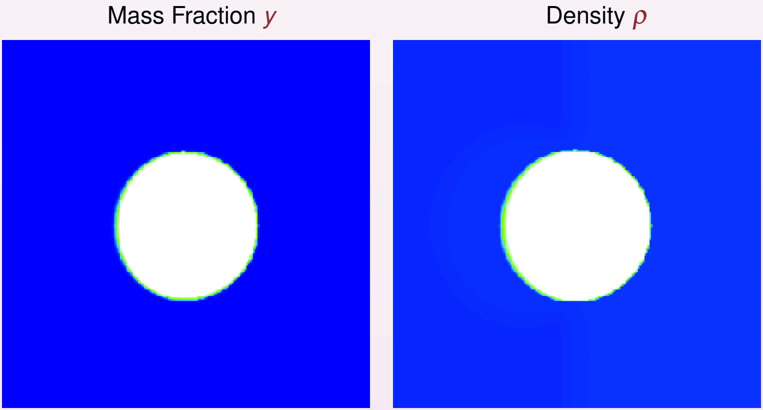
Density ρ



$t = 0.00$ ms

Geometry Play Skip

Compression of a Vapor Bubble

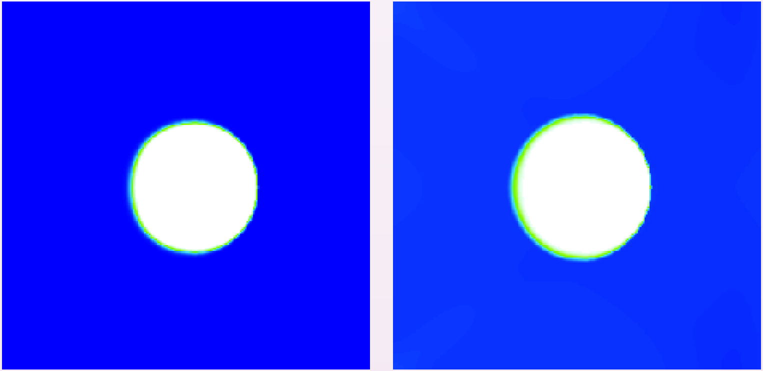


$t = 0.89$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ

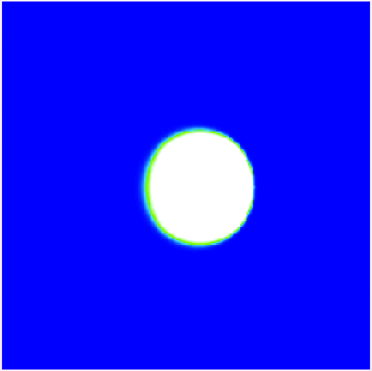


$t = 1.49$ ms

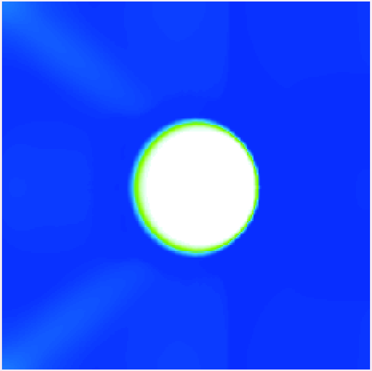
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

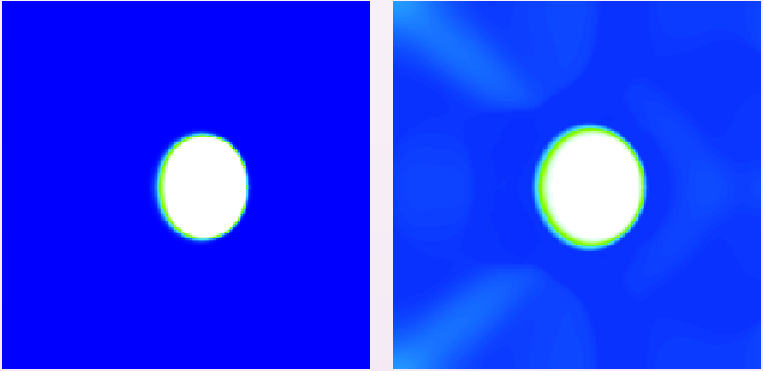


$t = 2.09$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ

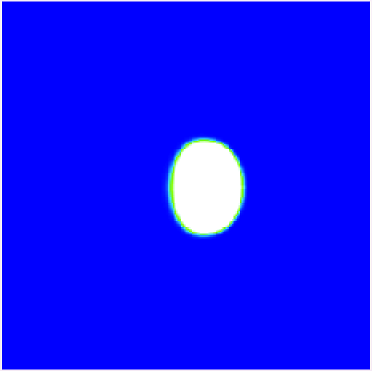


$t = 2.69$ ms

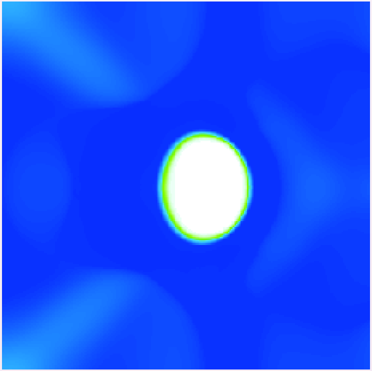
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

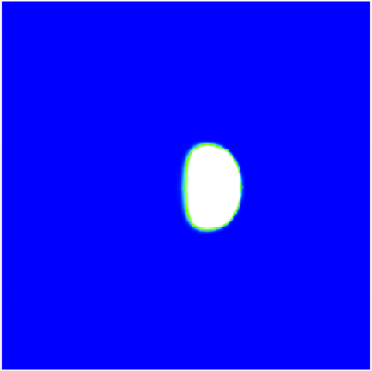


$t = 3.30$ ms

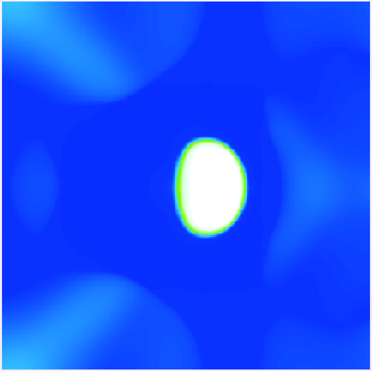
Geometry Play Skip

COMPRESSION OF A VAPOR BUBBLE

Mass Fraction y



Density ρ

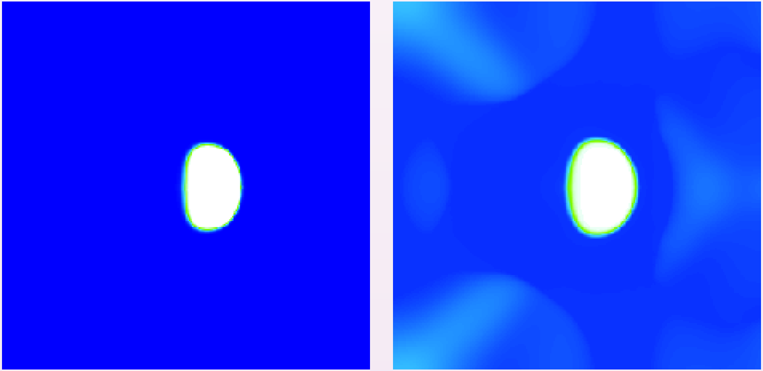


$t = 3.60$ ms

Geometry Play Skip

Compression of a Vapor Bubble

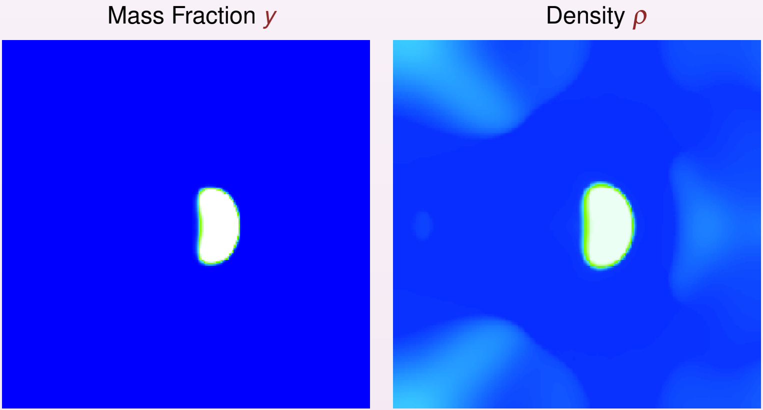
Mass Fraction y Density ρ



$t = 3.60$ ms

Geometry Play Skip

Compression of a Vapor Bubble

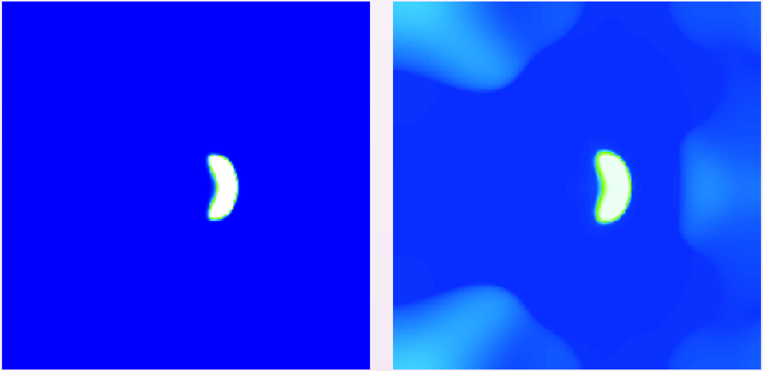


$t = ?$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ

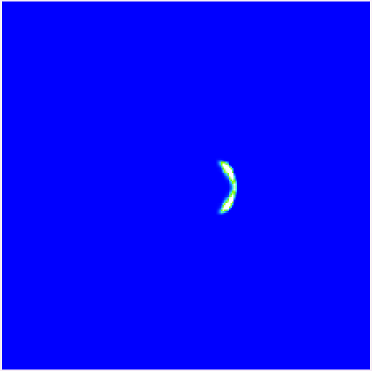


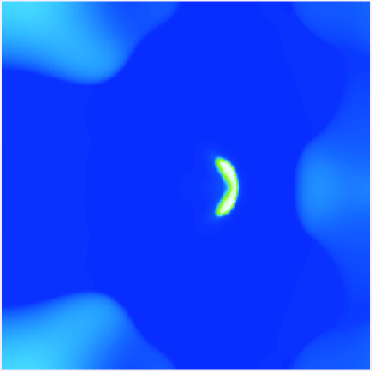
$t = ?$ ms

Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y Density ρ



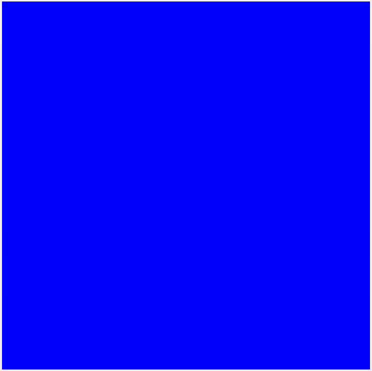


$t = ?$ ms

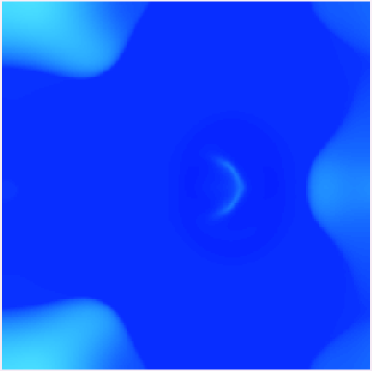
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

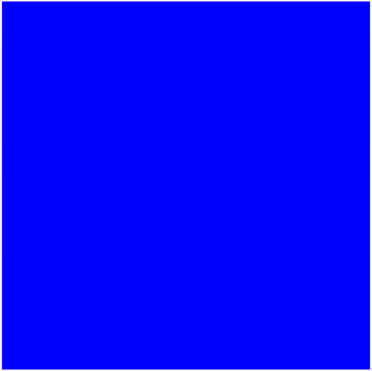


$t = ?$ ms

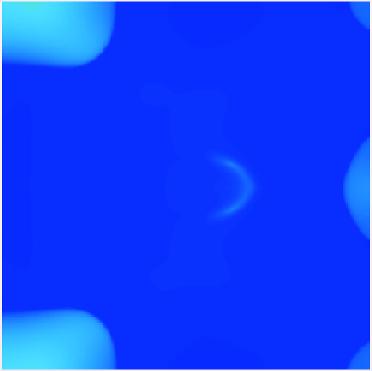
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

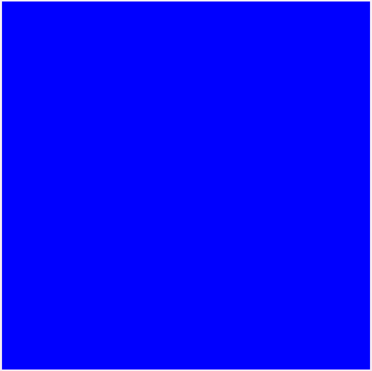


$t = ?$ ms

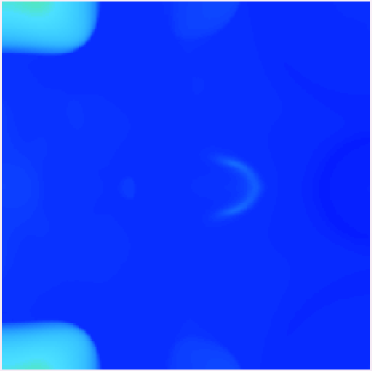
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



Density ρ

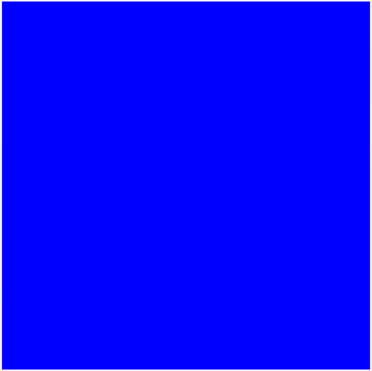


$t = ?$ ms

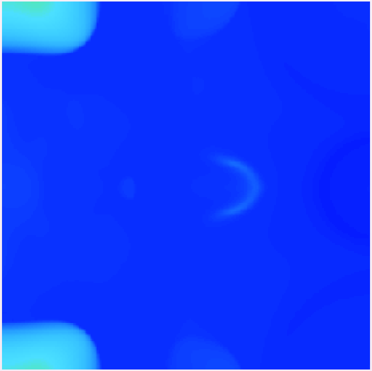
Geometry Play Skip

Compression of a Vapor Bubble

Mass Fraction y



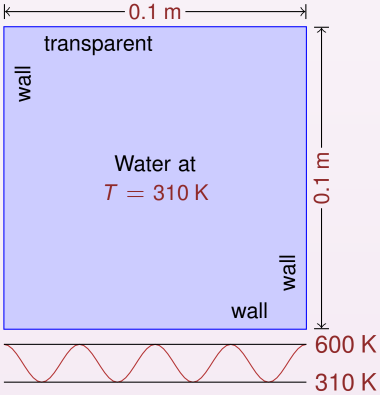
Density ρ



$t = ?$ ms

Geometry Play Skip

NUCLEATING BUBBLES

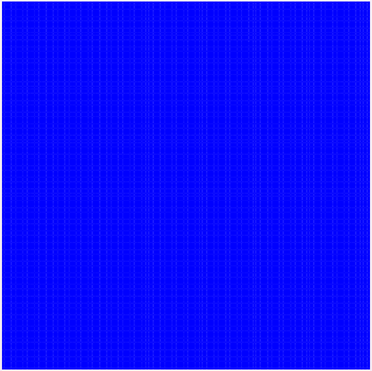


Nucleation of a 2D Vapor Bubbles involving two Stiffened Gases for water and steam. The temperature of the south wall is fixed at

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

NUCLEATING BUBBLES

Mass Fraction y

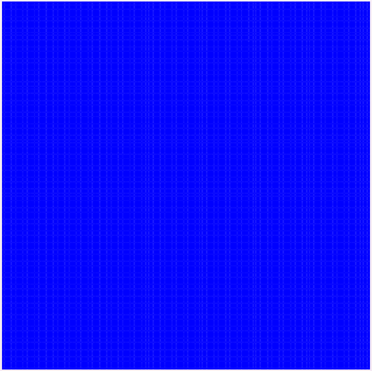


Temperature T

Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

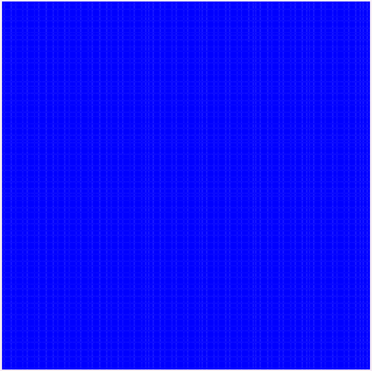


Temperature T

◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y

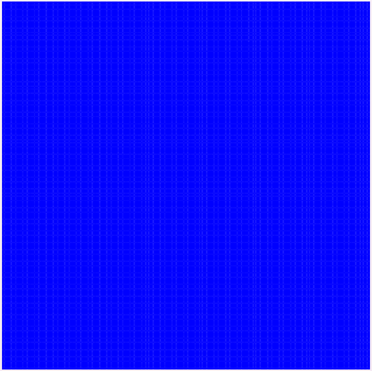


Temperature T

Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y

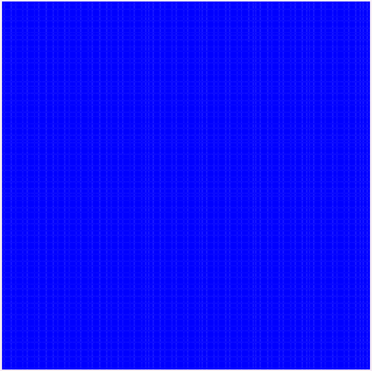


Temperature T

Geometry Play Skip

Nucleating Bubbles

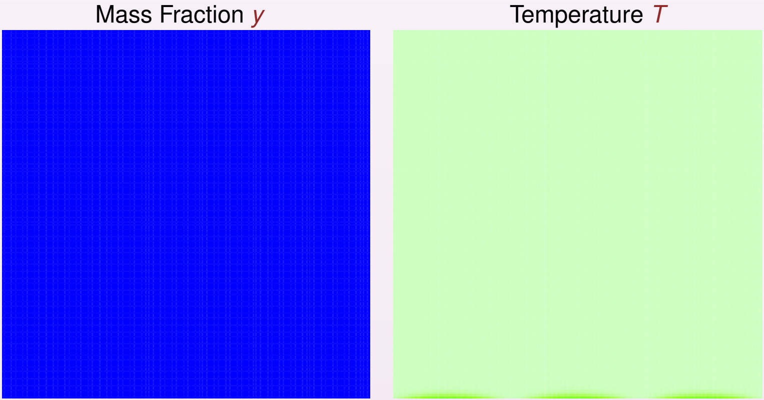
Mass Fraction y



Temperature T

Geometry Play Skip

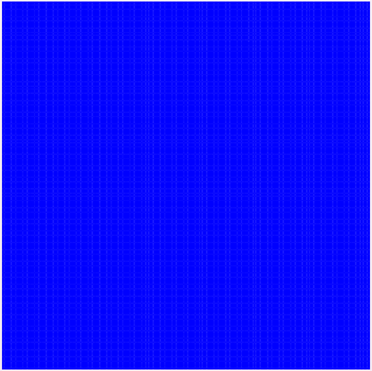
NUCLEATING BUBBLES



Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

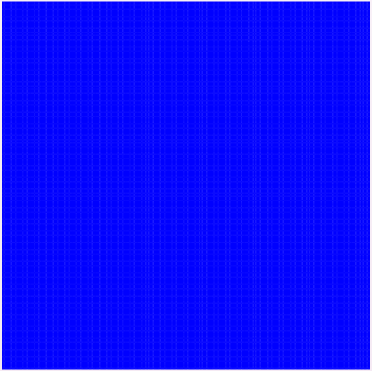


Temperature T

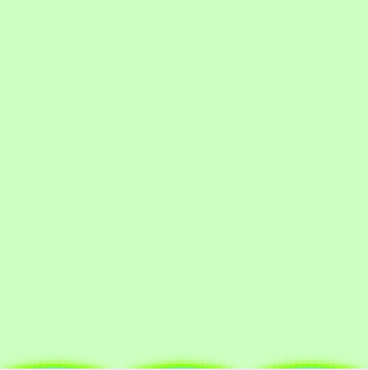
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



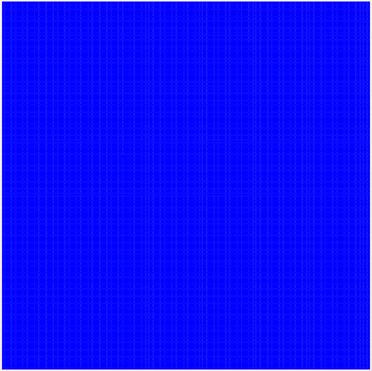
Temperature T



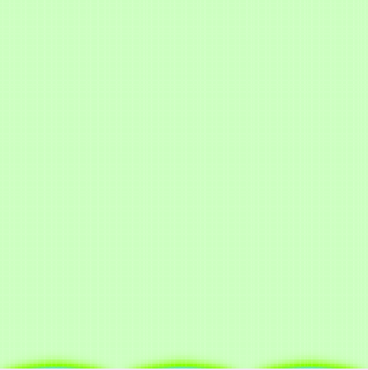
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y

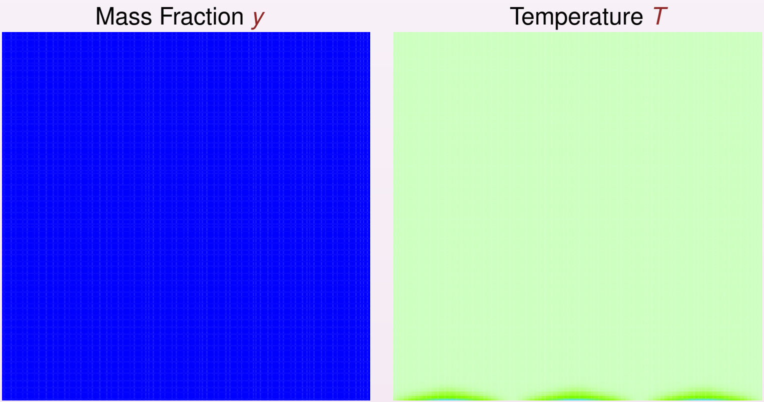


Temperature T



◂ Geometry ▸ Play ▸▸ Skip

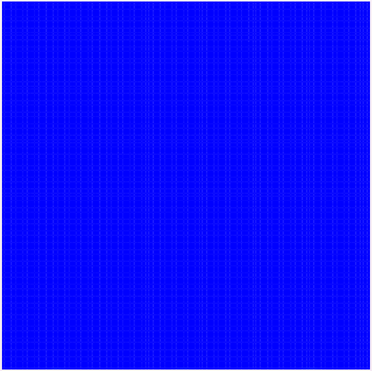
Nucleating Bubbles



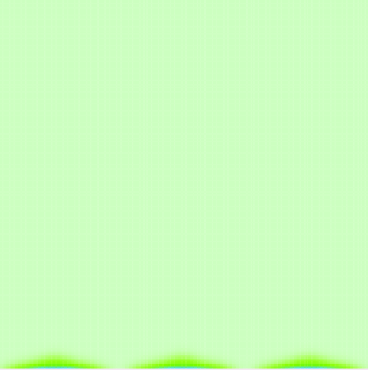
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



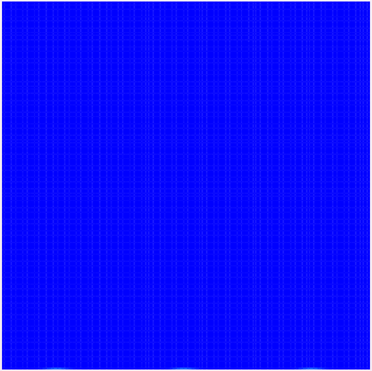
Temperature T



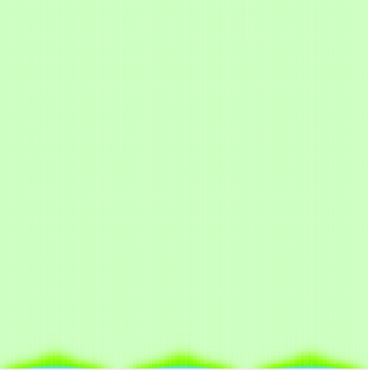
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y



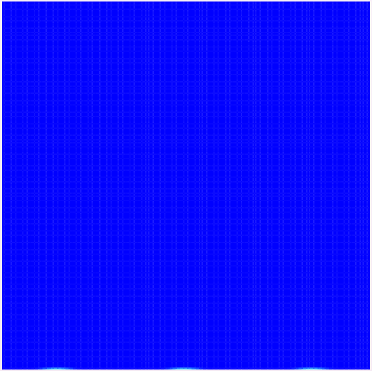
Temperature T



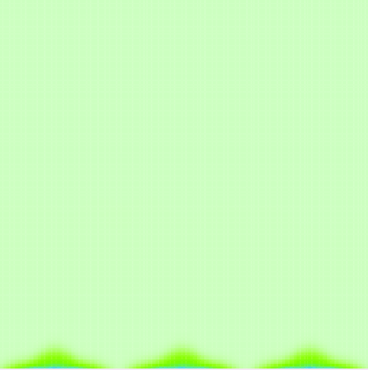
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



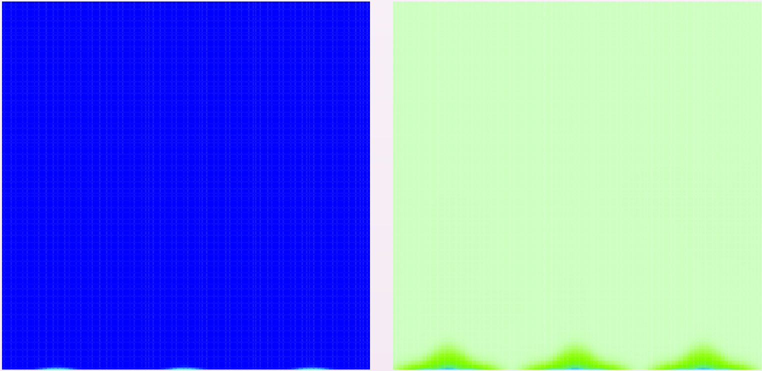
Temperature T



Geometry Play Skip

Nucleating Bubbles

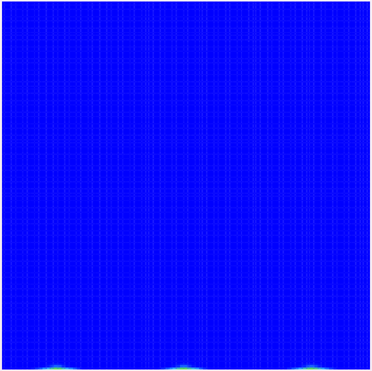
Mass Fraction y Temperature T



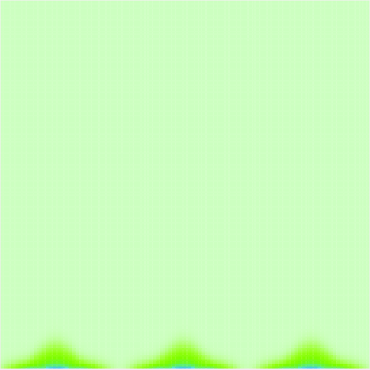
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



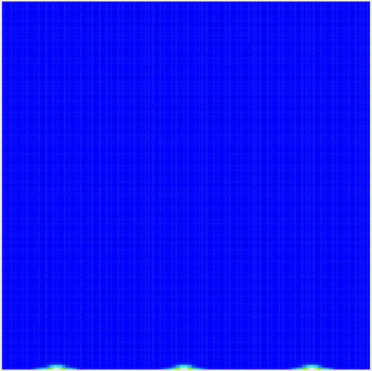
Temperature T



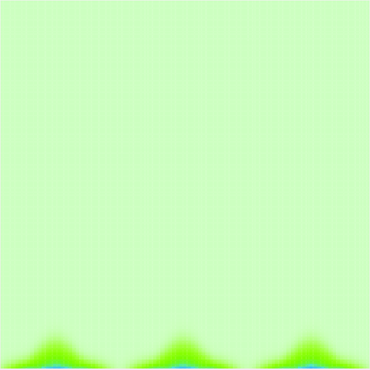
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



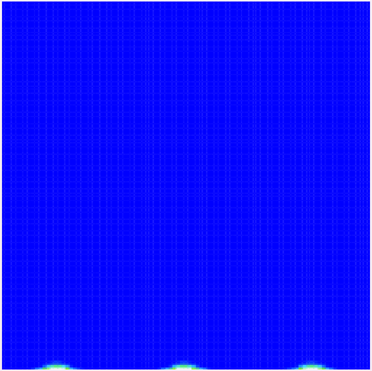
Temperature T



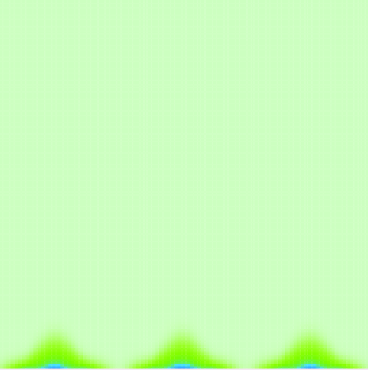
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



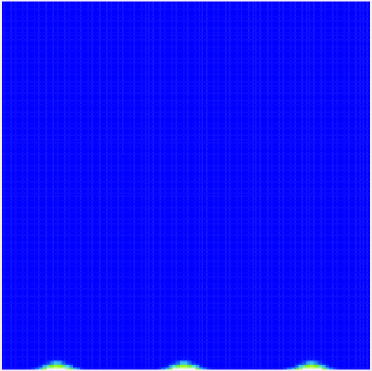
Temperature T



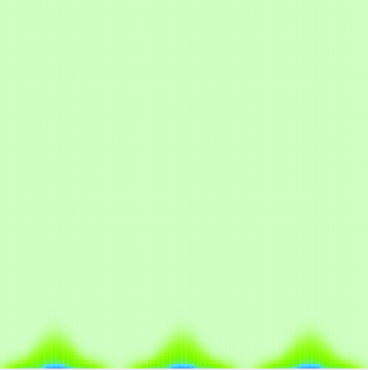
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



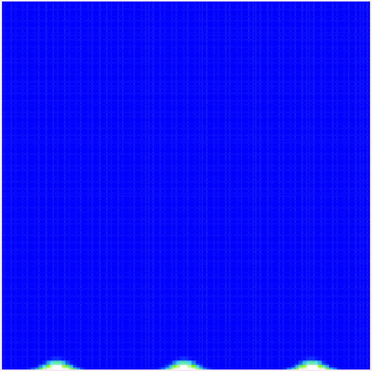
Temperature T



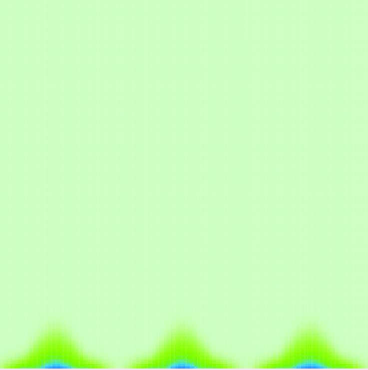
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



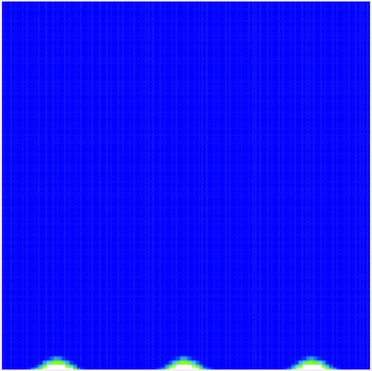
Temperature T



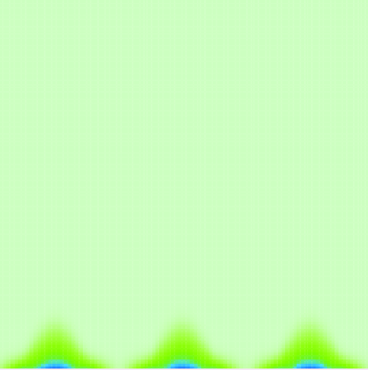
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



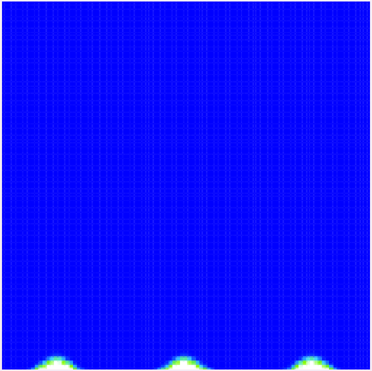
Temperature T



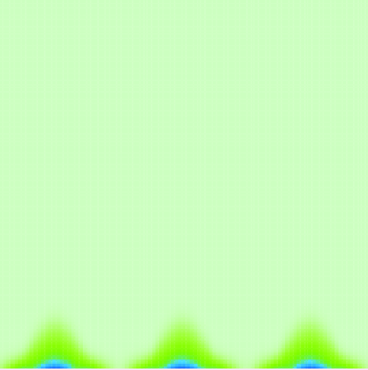
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



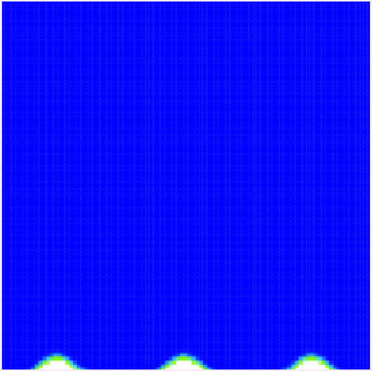
Temperature T



◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y



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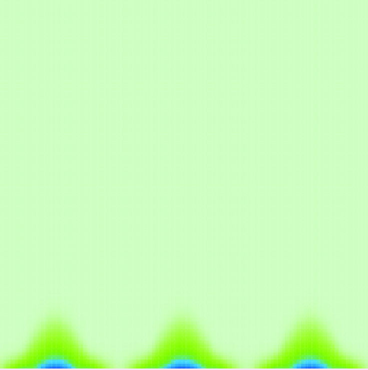
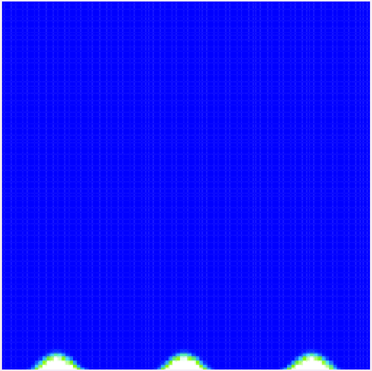


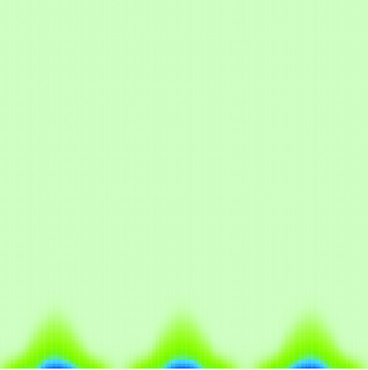
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



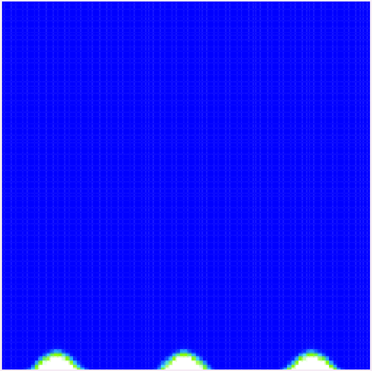
Temperature T



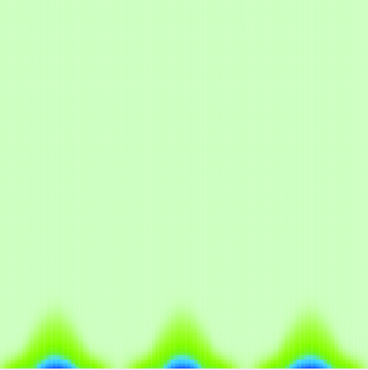
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y



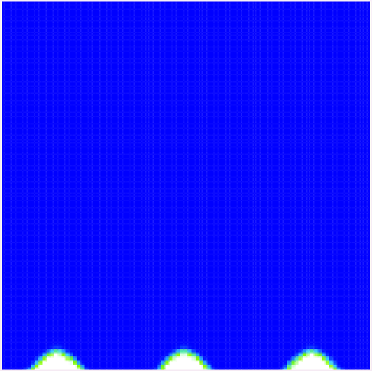
Temperature T



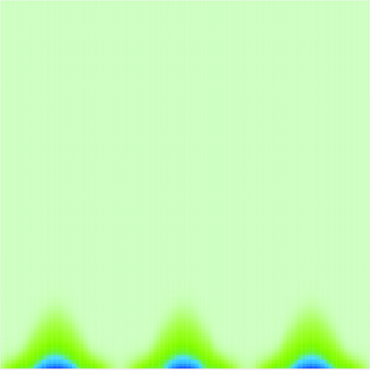
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y

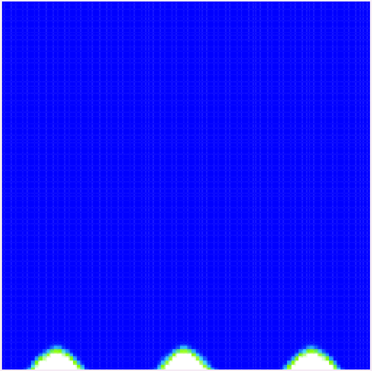


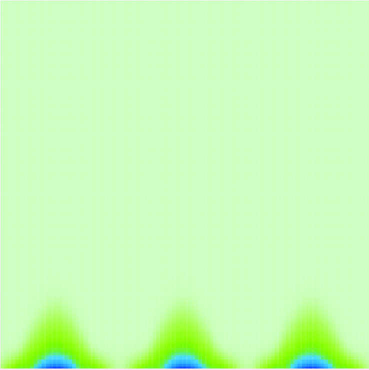
Temperature T



Geometry Play Skip

Nucleating Bubbles

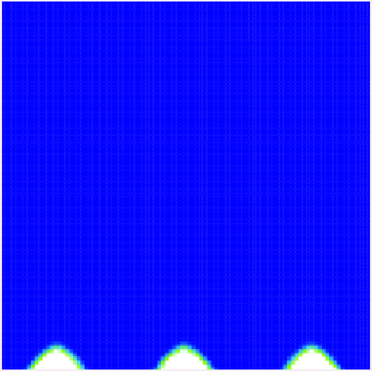




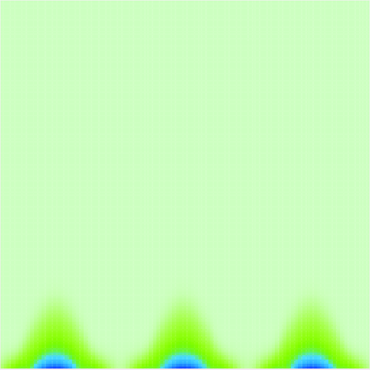
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



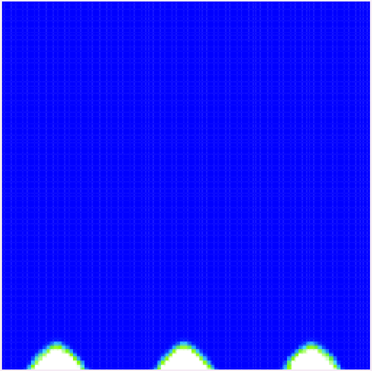
Temperature T



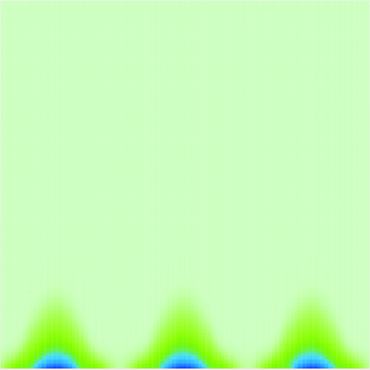
◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLES

Mass Fraction y



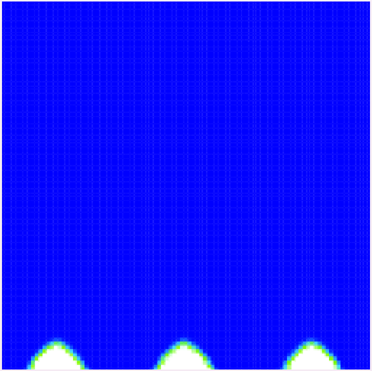
Temperature T



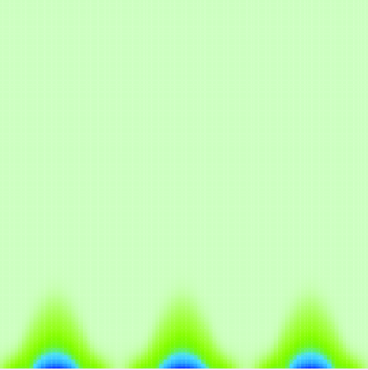
◂ Geometry ▸ Play ▸▸ Skip

Nucleating Bubbles

Mass Fraction y

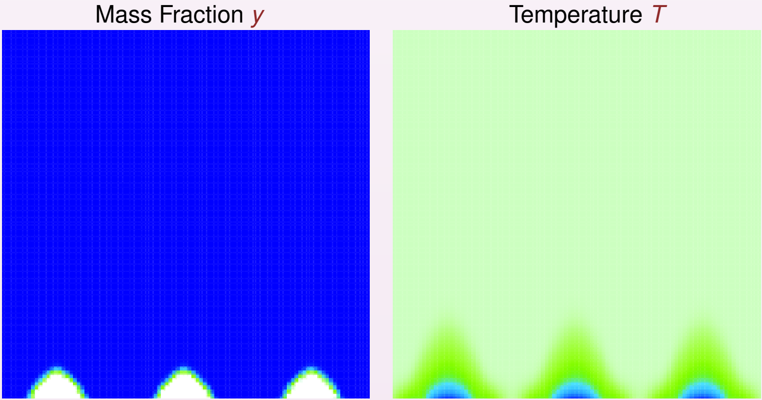


Temperature T



Geometry Play Skip

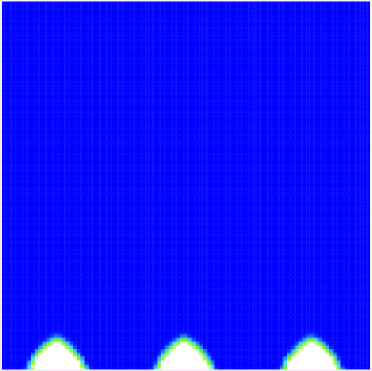
Nucleating Bubbles



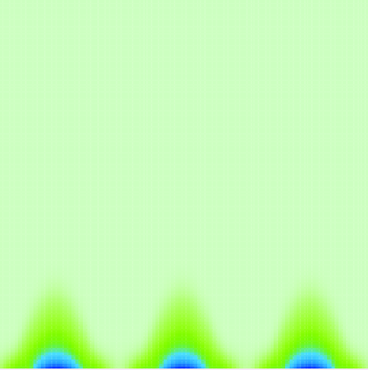
◂ Geometry ▸ Play ▸▸ Skip

NUCLEATING BUBBLES

Mass Fraction y



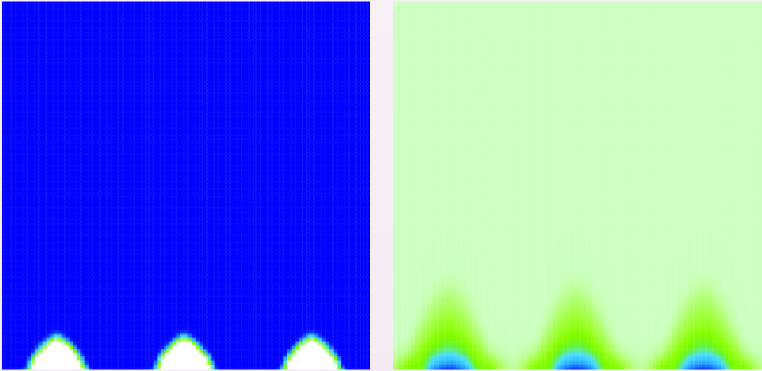
Temperature T



Geometry Play Skip

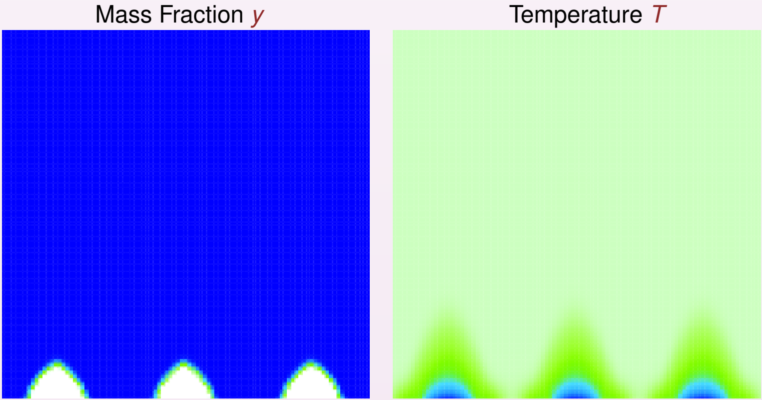
Nucleating Bubbles

Mass Fraction y Temperature T



Geometry Play Skip

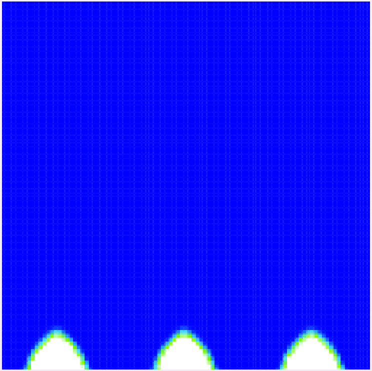
Nucleating Bubbles



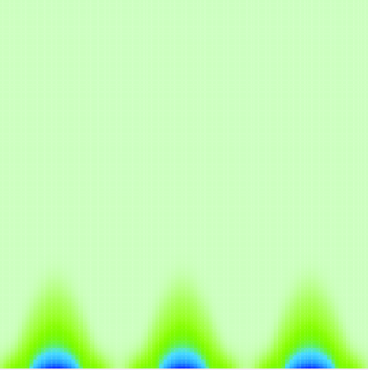
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



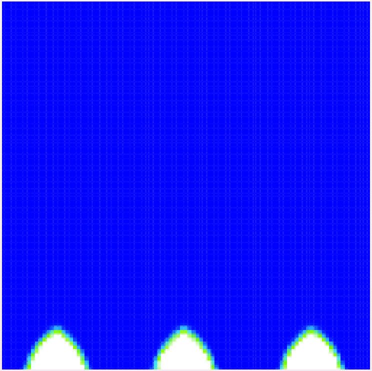
Temperature T



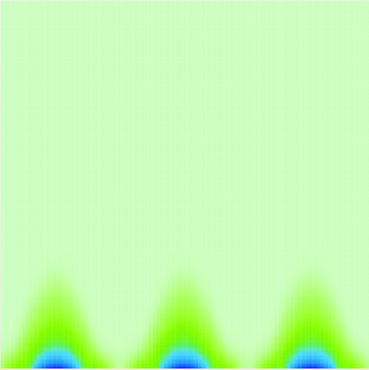
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



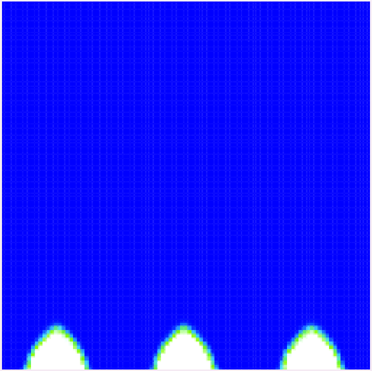
Temperature T



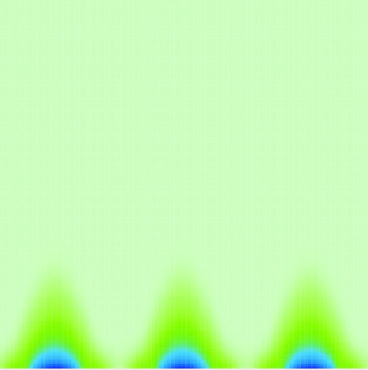
◀ Geometry ▶ Play ▶▶ Skip

Nucleating Bubbles

Mass Fraction y

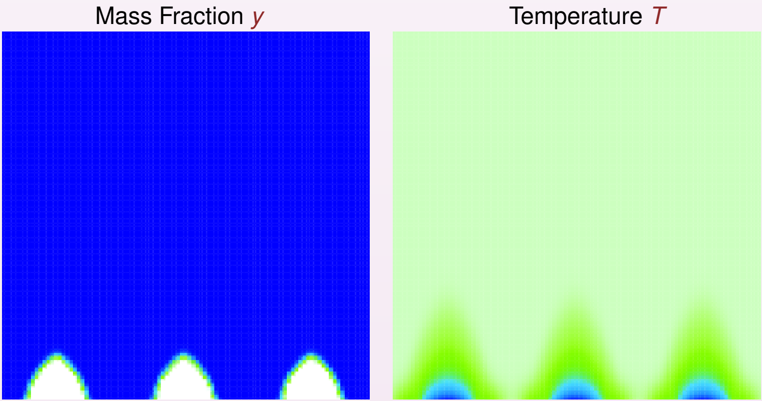


Temperature T



Geometry Play Skip

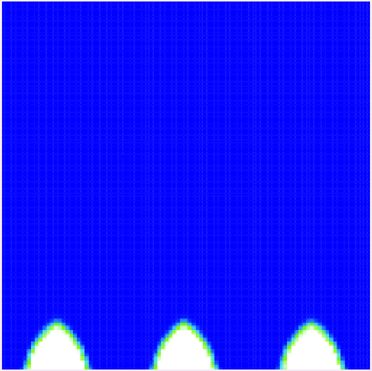
Nucleating Bubbles



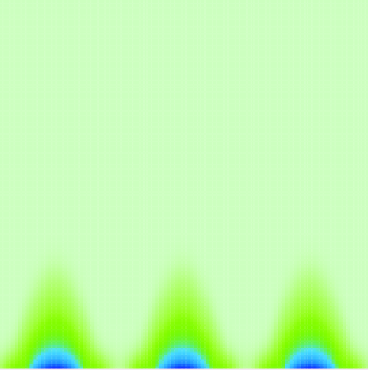
◀ Geometry ▶ Play ▶▶ Skip

Nucleating Bubbles

Mass Fraction y



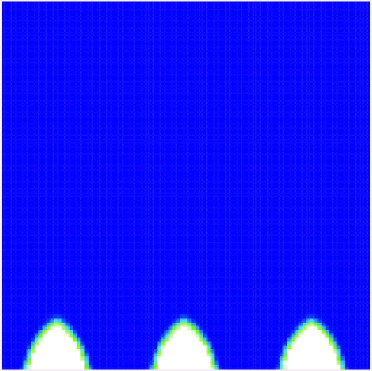
Temperature T



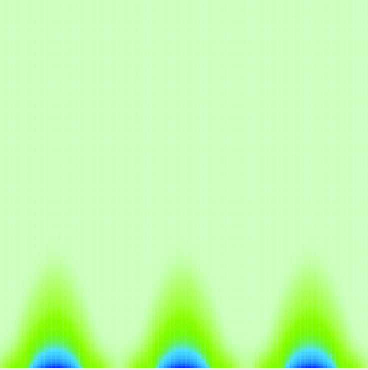
Geometry Play Skip

NUCLEATING BUBBLES

Mass Fraction y



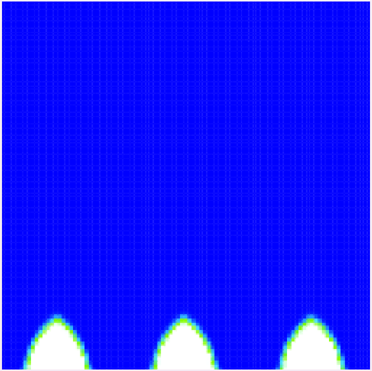
Temperature T



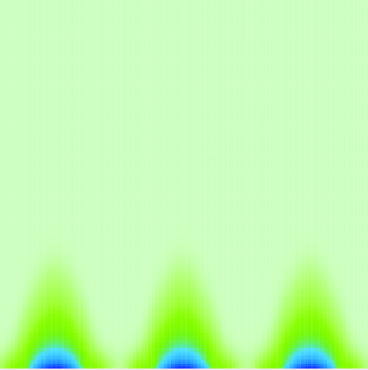
Geometry Play Skip

Nucleating Bubbles

Mass Fraction y



Temperature T



Geometry Play Skip

NUCLEATING BUBBLES

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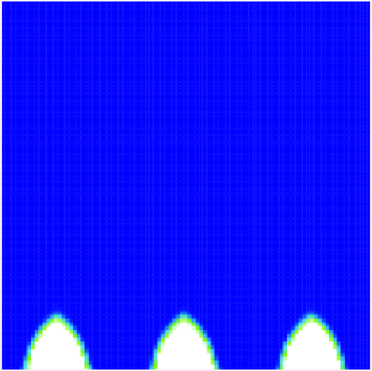
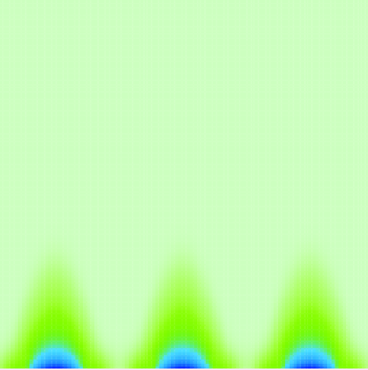


Temperature T



Geometry Play Skip

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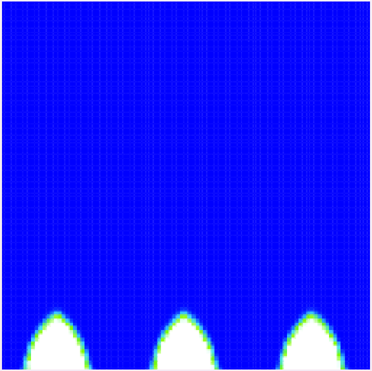
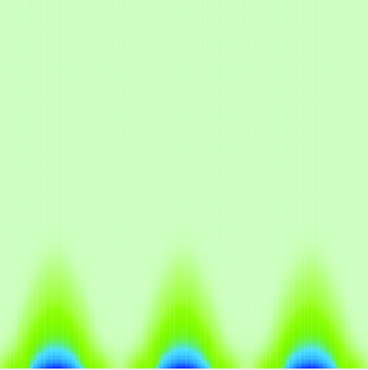


Temperature T



Geometry Play Skip

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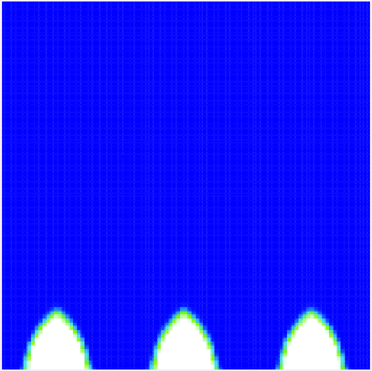

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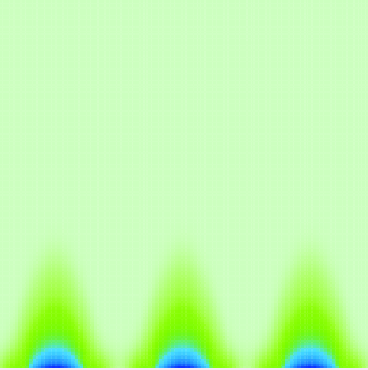

Geometry Play Skip

NUCLEATING BUBBLES

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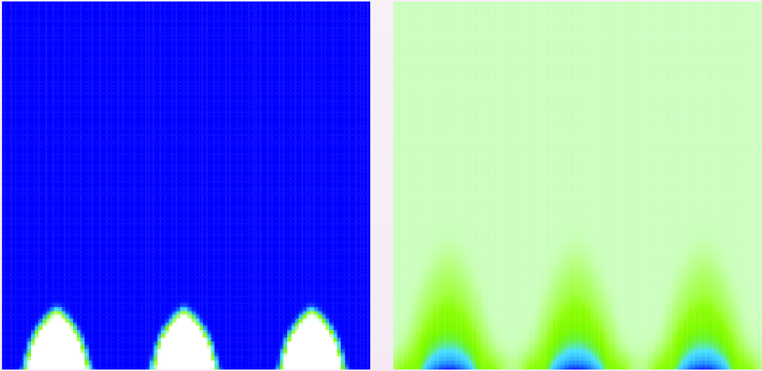

◂ Geometry ▸ Play ▸▸ Skip

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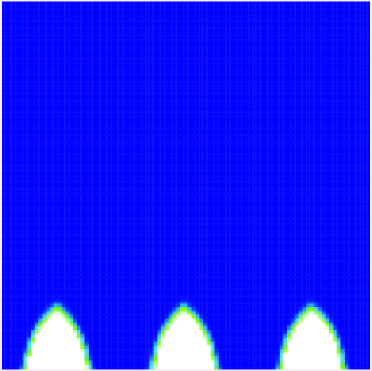

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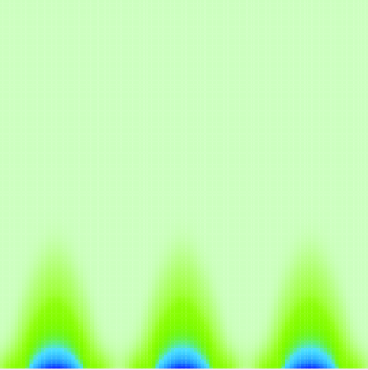

Geometry Play Skip

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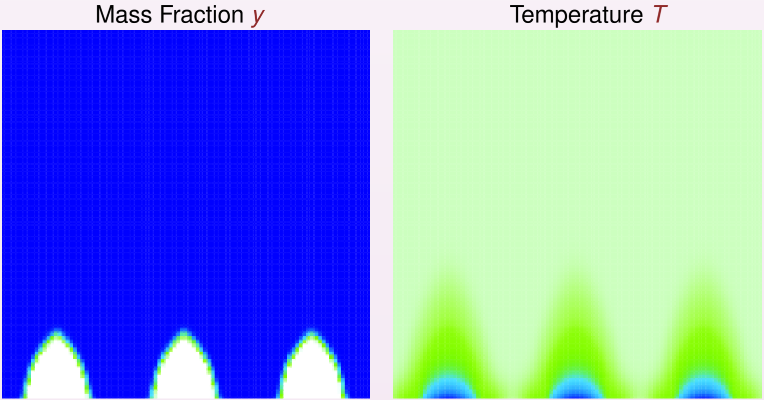

Geometry Play Skip

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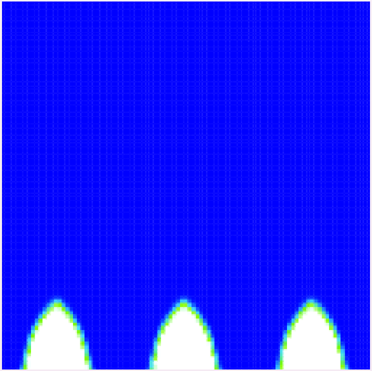

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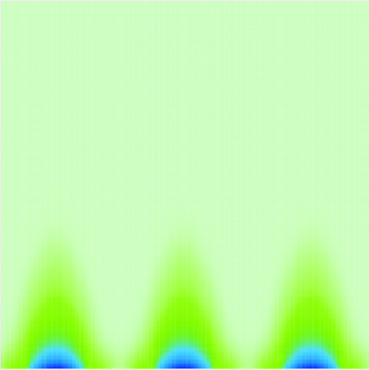

◀ Geometry ▶ Play ▶▶ Skip

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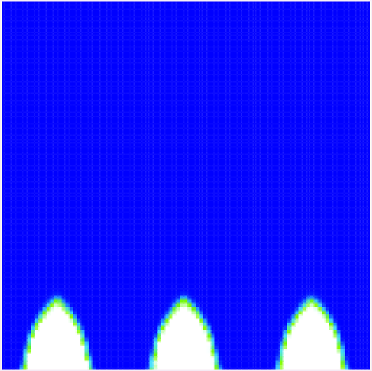

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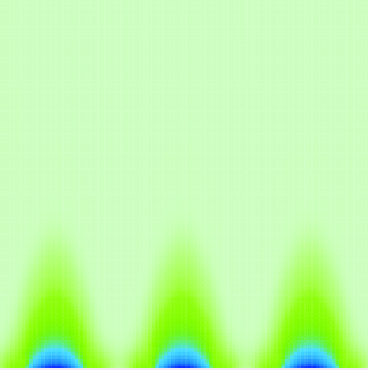

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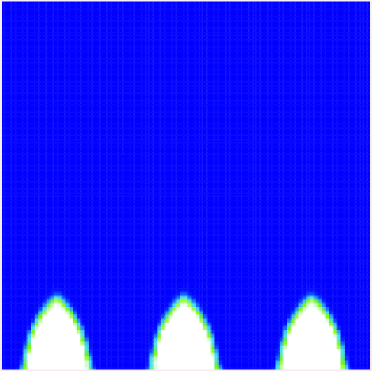

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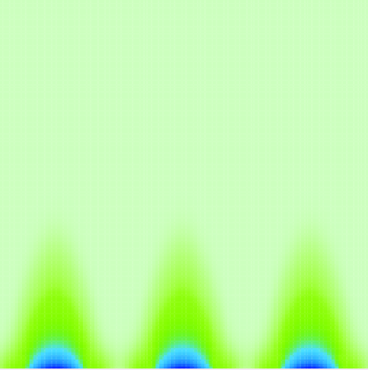

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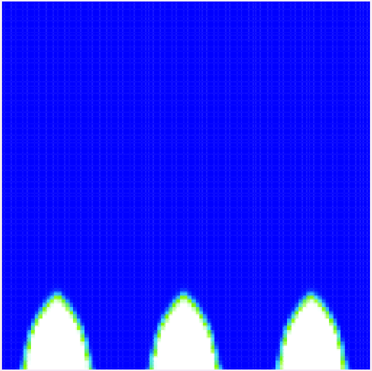

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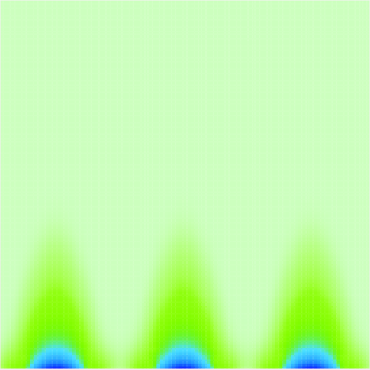

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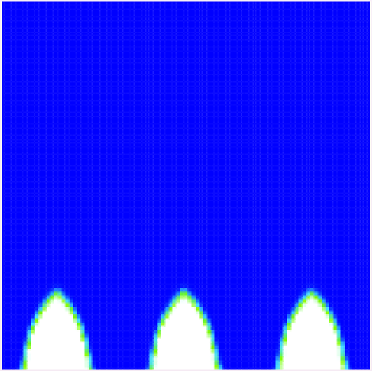

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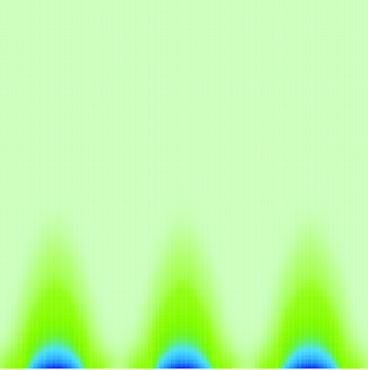

Geometry Play Skip

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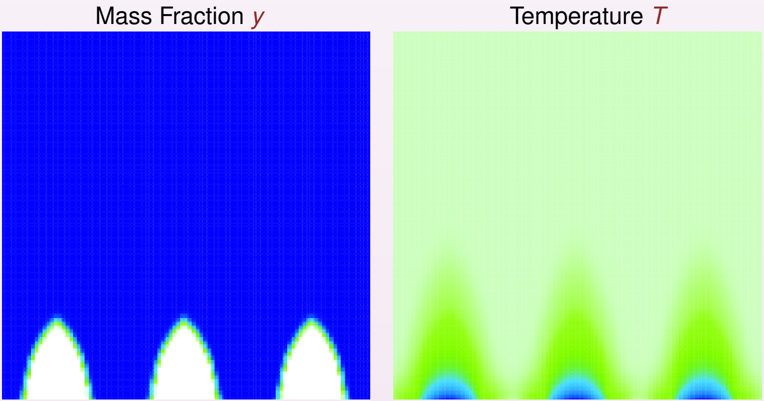

Geometry Play Skip

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,
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Stiffened Gas for Water

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

Phase	c_v [J/(kg·K)]	γ	π [Pa]	q [J/kg]	m [J/(kg·K)]
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.

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

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Return

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Water Tabulated EOS

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

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

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

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