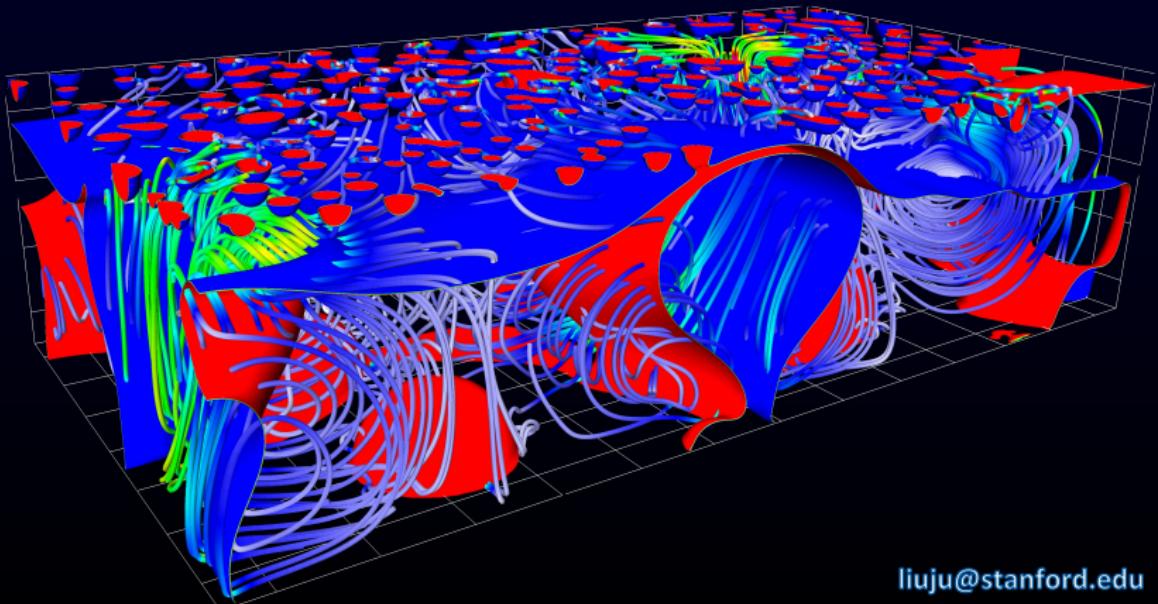


Multiphase Flows: Thermomechanical Theory, Algorithms, and Simulations

Ju Liu



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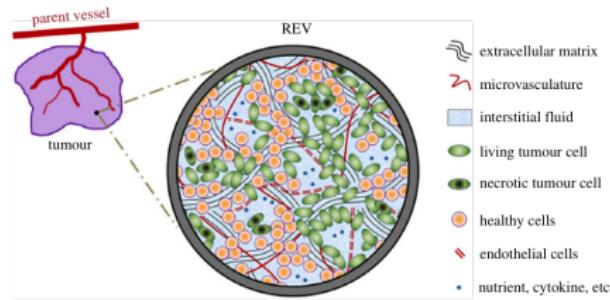
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 - Continuum theory
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- Future work

Motivation: Multiphase Flows

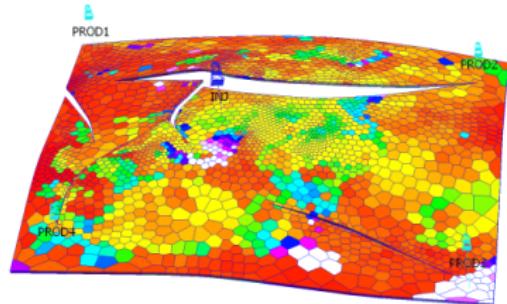
Phase: material component.



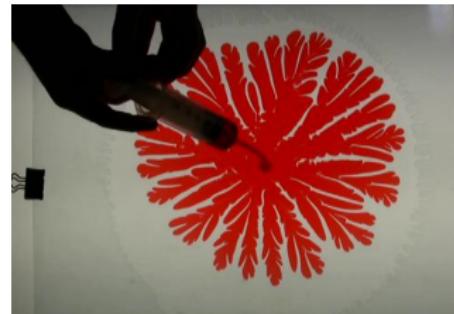
The Great Wave off Kanagawa



Tumor growth



Multicomponent flow in a reservoir



Viscous fingering

D. Richter and F. Veron, *Ocean spray: An outsized influence on weather and climate*, Physics Today, 69, 11, 34 (2016).

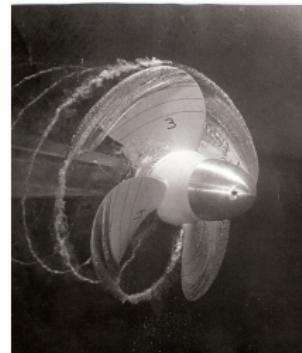
ICES Tumor Modeling Group, *Toward Predictive Multiscale Modeling of Vascular Tumor Growth: Computational and Experimental Oncology for Tumor Prediction*, ICES Report 2015.

Motivation: Multiphase Flows

Phase: state of matter.

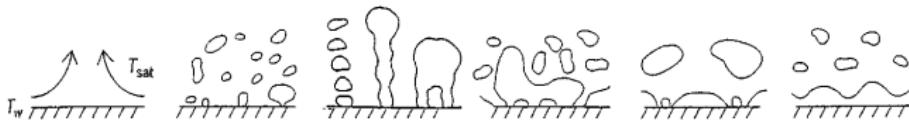


boiling heat transfer



cavitating flow

$$\rho = \rho(p, \theta) \Rightarrow \frac{1}{\rho} \frac{D\rho}{Dt} = \frac{1}{\rho} \frac{\partial \rho}{\partial p} \frac{Dp}{Dt} + \frac{1}{\rho} \frac{\partial \rho}{\partial \theta} \frac{D\theta}{Dt}$$

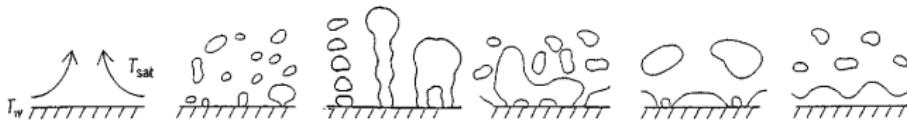


Nucleate boiling

- bubbles are released from discrete sites of the heated surface
- efficient in heat transfer
- very few numerical studies:
 - level-set method by V.K. Dhir's group
- ✗ Dhir's approach requires empirical knowledge

Film boiling

- bubbles are generated from an unstable vapor film
- dangerous for the solid surface
- amenable to analysis:
 - level-set method by V.K. Dhir's group,
 - front-tracking method by G. Tryggvason's group,
 - VOF approach by S.W. Welch et al.
- ✗ all the models start with a pre-existing thin vapor film



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"When a bubble reaches the top cold plate, it is **removed from the calculation** to model condensation and **a new bubble is introduced** at a random position on the bottom hot plate [...]"

V.K. Dhir, *Boiling heat transfer*. Annual Review of Fluid Mechanics, 1998.

R. Lakkaraju, et al. *Heat transport in bubbling turbulent convection*. PNAS, 2013.

Motivation: Diffuse-interface models

- Classical multiphase solvers (e.g. VOF, Level-set methods, Front tracking method, etc.) are based on **geometrical** description of existing interfaces.

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$$\Delta p = \tilde{\gamma} \tilde{\kappa} \rightarrow \infty \text{ as the bubble radius goes to 0.}$$

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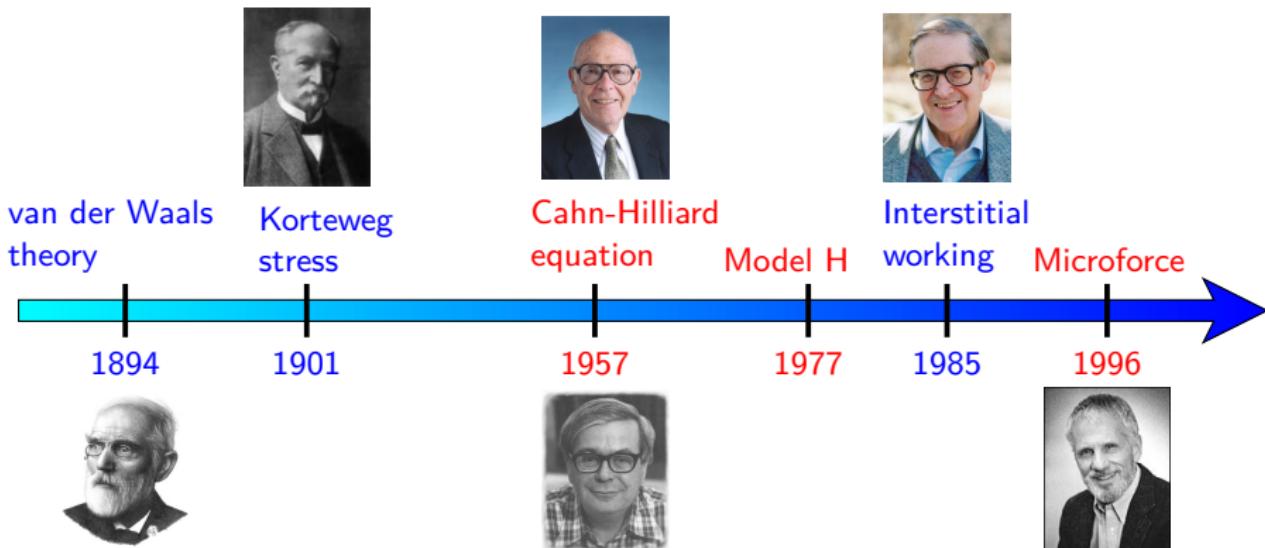
“Classical models break down when the interfacial thickness is comparable to the length scale of the phenomena being examined.”

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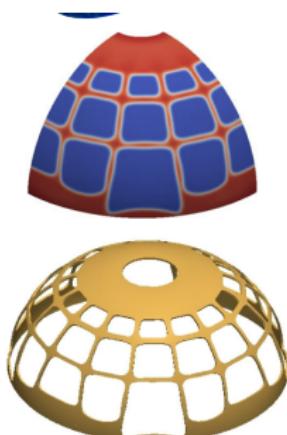
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"Classical models break down when the interfacial thickness is comparable to the length scale of the phenomena being examined."



Motivation: Numerical Analysis

- Nonlinear stability
 - Entropy stable fully discrete schemes utilizing the **convexity** of the mathematical entropy functions have been developed for the compressible Euler and Navier-Stokes equations in the 1980s.
 - For phase-field models, **convexity is lost**.
 - An appropriate notion of nonlinear stability (i.e., entropy) needs to be developed for phase-field models and new algorithms are needed.



- Isogeometric analysis
 - Exact geometric representation.
 - k -refinement.
 - Robustness.

T.J.R. Hughes, et al., *A new finite element formulation for computational fluid dynamics: I. Symmetric forms of the compressible Euler and Navier-Stokes equations and the second law of thermodynamics*. CMAME, 1986.

T.J.R. Hughes, et al., *Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement*. CMAME, 2005.

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"If someone points out to you that your pet theory of the universe is in disagreement with Maxwell's equations – then so much the worse for Maxwell's equations. If it is found to be contradicted by observation – well, these experimentalists do bungle things sometimes. But if your theory is found to be against the second law of thermodynamics I can give you no hope; there is nothing for it but to collapse in deepest humiliation."

— Sir Arthur S. Eddington, 1915

Modeling techniques

- Balance laws
- Microforce balance equations
- Truesdell equipresence principle
- Coleman-Noll approach

B.D. Coleman and W. Noll, The thermodynamics of elastic materials with heat conduction and viscosity, ARMA, 1963.

J. Liu, et al., Liquid-Vapor Phase Transition: Thermomechanical Theory, Entropy Stable Numerical Formulation, and Boiling Simulations, CMAME, 2015.

Continuum Theory: Balance Laws

- Conservation of mass

$$\frac{d}{dt} \int_{\Omega_t} \rho dV_{\mathbf{x}} = 0.$$

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$$\frac{d}{dt} \int_{\Omega_t} \rho \underbrace{c_\alpha}_{\text{mass fraction}} dV_{\mathbf{x}} = \int_{\partial\Omega_t} -\underbrace{\mathbf{h}_\alpha}_{\text{mass flux}} \cdot \mathbf{n} dA_{\mathbf{x}} + \int_{\Omega_t} \underbrace{\mathbf{m}_\alpha}_{\text{mass source}} dV_{\mathbf{x}},$$

for $\alpha = 1, \dots, N - 1$.

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for $\alpha = 1, \dots, N - 1$.

- Balance of linear momentum

$$\frac{d}{dt} \int_{\Omega_t} \rho \mathbf{u} dV_x = \int_{\partial\Omega_t} \boldsymbol{\sigma} dA_x + \int_{\Omega_t} \rho \mathbf{b} dV_x,$$
$$\boldsymbol{\sigma} = \mathbf{T}\mathbf{n}.$$

- Balance of angular momentum

$$\frac{d}{dt} \int_{\Omega_t} \mathbf{x} \times \rho \mathbf{u} dV_x = \int_{\partial\Omega_t} \mathbf{x} \times \boldsymbol{\sigma} dA_x + \int_{\Omega_t} \mathbf{x} \times \rho \mathbf{b} dV_x.$$



“ fundamental physical laws involving energy should account for the working associated with each operative kinematical process [...] and it seems plausible that there should be ‘microforces’ whose working accompanies changes in ρ .”

— M.E. Gurtin, 1996

Fundamental Postulate

There exists a set of microscopic forces that accompanies the evolution of each phase-field order parameter.

Phase-field order parameter for the transition of the state of matter $\Rightarrow \rho$.

M.E. Gurtin, Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a microforce balance. Physica D, 1996.

Continuum Theory: Balance Laws

- Balance of microforces associated with ρ

$$\int_{\partial\Omega_t} \boldsymbol{\xi} \cdot \mathbf{n} dA_{\mathbf{x}} + \int_{\Omega_t} \varrho dV_{\mathbf{x}} + \int_{\Omega_t} \mathbf{l} dV_{\mathbf{x}} = 0.$$

$\boldsymbol{\xi}$: microstress, ϱ : internal microforce, \mathbf{l} : external microforce.

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$$\int_{\partial\Omega_t} \xi \cdot \mathbf{n} dA_{\mathbf{x}} + \int_{\Omega_t} \varrho dV_{\mathbf{x}} + \int_{\Omega_t} \mathfrak{l} dV_{\mathbf{x}} = 0.$$

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- Balance of energy

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega_t} \rho E dV_{\mathbf{x}} := \frac{d}{dt} \int_{\Omega_t} \overbrace{\frac{\rho}{2} |\mathbf{u}|^2}^{\text{kinetic energy}} + \overbrace{\rho \iota}^{\text{internal energy}} dV_{\mathbf{x}} \\ &= \int_{\partial\Omega_t} \left(\mathbf{T}\mathbf{u} + \frac{d}{dt} \rho \xi - \mathbf{q} \right) \cdot \mathbf{n} dA_{\mathbf{x}} + \int_{\Omega_t} \rho \mathbf{b} \cdot \mathbf{u} + \underbrace{\iota \frac{d}{dt} \rho}_{\text{external microforce}} + \rho r dV_{\mathbf{x}}. \end{aligned}$$

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- The second law of thermodynamics

$$\int_{\Omega_t} \mathcal{D} dV_{\mathbf{x}} := \frac{d}{dt} \int_{\Omega_t} \rho s dV_{\mathbf{x}} + \int_{\partial\Omega_t} \frac{\mathbf{q} \cdot \mathbf{n}}{\theta} dA_{\mathbf{x}} - \int_{\Omega_t} \frac{\rho r}{\theta} dV_{\mathbf{x}} \geq 0.$$

M.E. Gurtin, Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a microforce balance.
Physica D, 1996.

Continuum Theory: Balance Laws

$$\left\{ \begin{array}{l} \text{Conservation of mass} \quad \frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{u} = 0, \\ \text{Balance of linear momentum} \quad \rho \frac{d\mathbf{u}}{dt} = \nabla \cdot \mathbf{T} + \rho \mathbf{b}, \\ \text{Balance of angular momentum} \quad \mathbf{T} = \mathbf{T}^T, \\ \text{Balance of microforce} \quad \nabla \cdot \boldsymbol{\xi} + \varrho + \mathfrak{l} = 0, \\ \text{Balance of energy} \quad \rho \frac{dE}{dt} = \nabla \cdot \left(\mathbf{T}\mathbf{u} + \frac{d\rho}{dt} \boldsymbol{\xi} - \mathbf{q} \right) + \rho \mathbf{b} \cdot \mathbf{u} + \mathfrak{l} \frac{d\rho}{dt} + \rho r, \\ \text{The second law} \quad \mathcal{D} := \rho \frac{ds}{dt} + \nabla \cdot \left(\frac{\mathbf{q}}{\theta} \right) - \frac{\rho r}{\theta} \geq 0. \end{array} \right.$$

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Truesdell's principle of equipresence

+

Coleman-Noll approach



B.D. Coleman and W. Noll, *The thermodynamics of elastic materials with heat conduction and viscosity*. Archive for Rational Mechanics and Analysis, 1968.

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Constitutive relations

The constitutive relations are represented in terms of the Helmholtz free energy Ψ .

- Microstresses

$$\boldsymbol{\xi} = \rho \frac{\partial \Psi}{\partial (\nabla \rho)}.$$

- Heat flux

$$\mathbf{q} = -\kappa \nabla \theta.$$

- Cauchy stress

$$\begin{aligned}\mathbf{T} = & 2\bar{\mu}\mathbf{L}^d - \frac{\rho}{2} \left(\nabla \rho \otimes \frac{\partial \Psi}{\partial (\nabla \rho)} + \frac{\partial \Psi}{\partial (\nabla \rho)} \otimes \nabla \rho \right) \\ & + \left(\rho \nabla \cdot \left(\rho \frac{\partial \Psi}{\partial (\nabla \rho)} \right) - \rho^2 \frac{\partial \Psi}{\partial \rho} + \rho \mathbf{l} + B \rho^2 \nabla \cdot \mathbf{u} \right) \mathbf{I}.\end{aligned}$$

- Entropy density per unit mass

$$s = -\partial \Psi / \partial \theta.$$

Continuum Theory: Dissipation Inequalities

Theorem (Dissipation for isolated systems)

Given the above constitutive relations, the dissipation \mathcal{D} takes the following form:

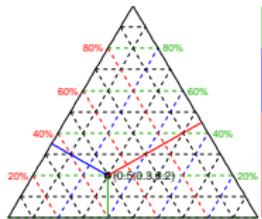
$$\rho \frac{ds}{dt} + \nabla \cdot \left(\frac{\mathbf{q}}{\theta} \right) - \frac{\rho r}{\theta} = \mathcal{D} = \frac{2\bar{\mu}}{\theta} |\mathbf{L}^d|^2 + \frac{1}{\theta} B \rho^2 (\nabla \cdot \mathbf{u})^2 + \frac{1}{\theta^2} \kappa |\nabla \theta|^2 \geq 0.$$

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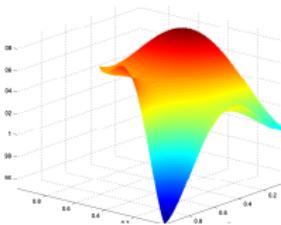
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Gibbs triangle



Free energy for a three-component system

- The perfect gas model
- The van der Waals liquid-vapor two-phase fluid model
- The Navier-Stokes-Cahn-Hilliard multicomponent fluid model
- The Navier-Stokes-Cahn-Hilliard-Korteweg multicomponent multiphase fluid model

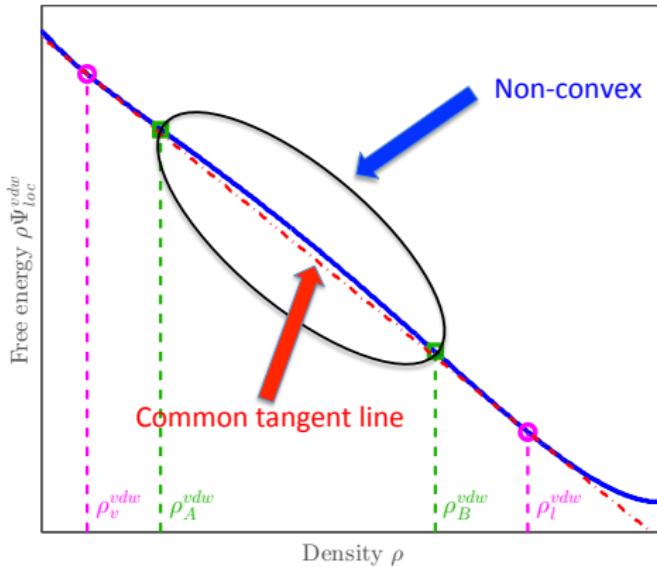
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Continuum Theory: The van der Waals Fluid Model

Thermodynamic potential

$$\Psi(\rho, \theta, \nabla \rho) = \Psi_{loc}(\rho, \theta) + \frac{\lambda}{2\rho} |\nabla \rho|^2, \Leftarrow \text{regularization}$$

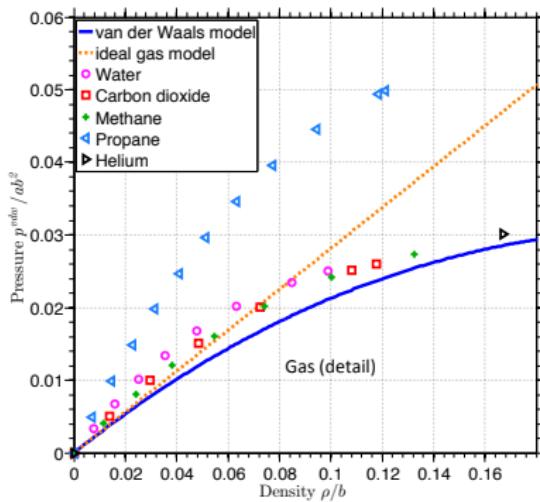
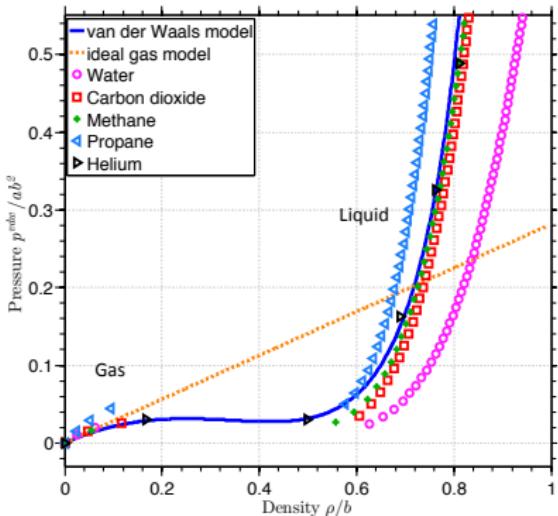
$$\Psi_{loc}(\rho, \theta) = -a\rho + R\theta \log\left(\frac{\rho}{b-\rho}\right) - C_v \theta \log\left(\frac{\theta}{\theta_{ref}}\right) + C_v \theta.$$



J.D. van der Waals, *The thermodynamic theory of capillarity under the hypothesis of a continuous variation of density*. Z. Physik. Chem., 1894.

The Navier-Stokes-Korteweg equations: the thermodynamic pressure

$$p(\rho, \theta) = \frac{8}{27} \frac{\theta \rho}{1 - \rho} - \rho^2.$$

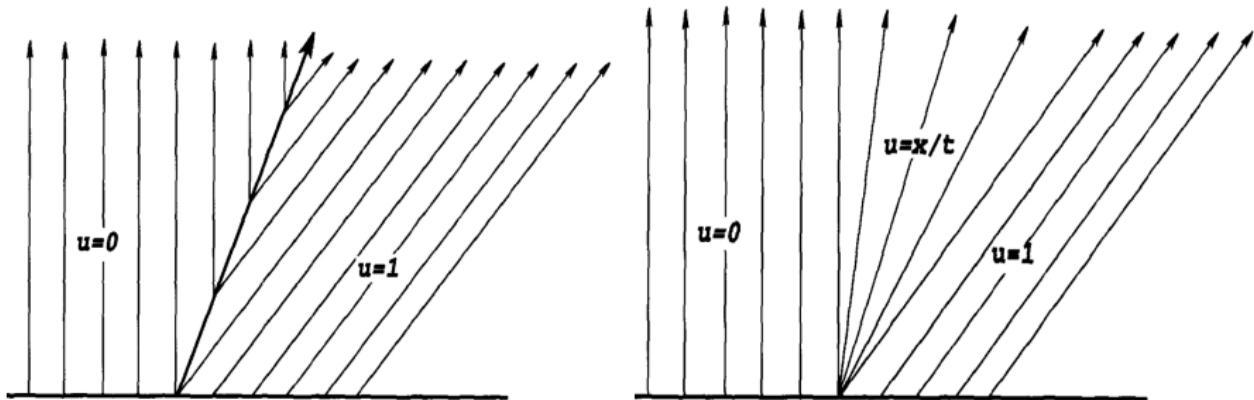


Comparison of the van der Waals equation of state with real fluids at $\theta = 0.95\theta_{crit}$.

NIST, Thermophysical Properties of Fluid Systems. [Online; accessed 11-February-2016].

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Thermodynamically Consistent Algorithm



Non-physical shock

Physical shock

Weak solutions of the conservation law



The second law of thermodynamics

Thermodynamically Consistent Algorithm: Spatial Discretization

Given the conservation variables $\mathbf{U} = \{\rho; \rho\mathbf{u}^T; \rho E\}^T$, and the mathematical entropy function $H := -\rho s$, the entropy variables are defined as $\mathbf{V} = \partial H / \partial \mathbf{U}$.

A. Harten, On the symmetric form of systems of conservation laws with entropy. JCP, 1983.

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$$\int_{\Omega} \underbrace{\mathbf{V}}_{\text{test function}} \cdot (\text{Balance Equations}) d\mathbf{x} = 0 \quad \Leftrightarrow \quad \text{Clausius-Duhem inequality.}$$

\Updownarrow

\mathbf{V} lives in the test function spaces.

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\Updownarrow
 \mathbf{V} lives in the test function spaces.

\Updownarrow
Solve the equations in terms of \mathbf{V} ,
if there is a **well-defined** algebraic change-of-variables between \mathbf{U} and \mathbf{V} .

\Updownarrow
There is a **well-defined** algebraic change-of-variables for ideal gas.

\Updownarrow
Aerodynamists are lucky.

Thermodynamically Consistent Algorithm: Spatial Discretization

Given the conservation variables $\mathbf{U} = \{\rho; \rho\mathbf{u}^T; \rho E\}^T$, and the mathematical entropy function $H := -\rho s$, the entropy variables are defined as $\mathbf{V} = \partial H / \partial \mathbf{U}$.

$$\int_{\Omega} \underbrace{\mathbf{V}}_{\text{test function}} \cdot (\text{Balance Equations}) d\mathbf{x} = 0 \Leftrightarrow \text{Clausius-Duhem inequality.}$$

↑
V lives in the test function spaces.

↑
Solve the equations in terms of V,
if there is a **well-defined** algebraic change-of-variables between U and V.

↑
There is a **well-defined** algebraic change-of-variables for ideal gas.

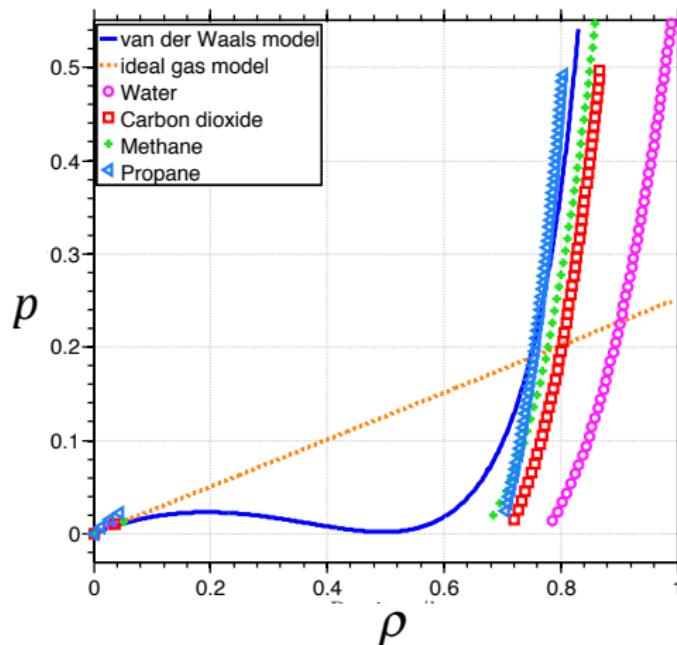
↑
Aerodynamists are lucky.

For the Navier-Stokes-Korteweg equations (in fact, all phase-field models), the mapping from \mathbf{U} to \mathbf{V} is **not** invertible!

A. Harten, On the symmetric form of systems of conservation laws with entropy. JCP, 1983.

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$$p(\rho, \theta) = \frac{8}{27} \frac{\theta \rho}{1 - \rho} - \rho^2.$$



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Thermodynamically Consistent Algorithm: Spatial Discretization

Mathematical entropy function

$$H := -\rho s = \frac{8}{27} \rho \log \left(\frac{\rho}{1-\rho} \right) - \frac{8}{27(1-\gamma)} \rho \log (\theta),$$
$$\theta = \theta(\rho, \rho \mathbf{u}, \rho E, \nabla \rho).$$

$$\mathbf{V} := \frac{\delta H}{\delta \mathbf{U}} = [V_1; V_2; V_3; V_4; V_5]^T.$$

$$V_1[\delta v_1] = \frac{1}{\theta} \left(-2\rho + \frac{8}{27} \theta \log \left(\frac{\rho}{1-\rho} \right) - \frac{8}{27(\gamma-1)} \theta \log (\theta) + \frac{8}{27(\gamma-1)} \theta \right. \\ \left. + \frac{8\theta}{27(1-\rho)} - \frac{|\mathbf{u}|^2}{2} \right) \delta v_1 + \frac{1}{\text{We}} \frac{1}{\theta} \nabla \rho \cdot \nabla \delta v_1,$$

$$V_2[\delta v_2] = \frac{u_1}{\theta} \delta v_2, \quad V_3[\delta v_3] = \frac{u_2}{\theta} \delta v_3, \quad V_4[\delta v_4] = \frac{u_3}{\theta} \delta v_4,$$

$$V_5[\delta v_5] = -\frac{1}{\theta} \delta v_5.$$

J. Liu, et al., Functional Entropy Variables: A New Methodology for Deriving Thermodynamically Consistent Algorithms for Complex Fluids, with Particular Reference to the Isothermal Navier-Stokes-Korteweg Equations. JCP, 2013.

Stability of the weak formulation

The solutions of the *semi-discrete* finite element formulation based on the *functional* entropy variables \mathbf{V} satisfy

$$\begin{aligned} \int_{\Omega} \left(\frac{\partial H(\rho^h, \theta^h)}{\partial t} + \nabla \cdot (H(\rho^h, \theta^h) \mathbf{u}^h) - \nabla \cdot \left(\frac{\mathbf{q}^h}{\theta^h} \right) + \frac{\rho^h r}{\theta^h} \right) d\mathbf{x} \\ = - \int_{\Omega} \frac{1}{\theta^h} \boldsymbol{\tau}^h : \nabla \mathbf{u}^h d\mathbf{x} - \int_{\Omega} \frac{\kappa |\nabla \theta^h|^2}{\theta^2} d\mathbf{x}. \end{aligned}$$

The *spatial* discretization is stable. Now we need to design a *time-stepping* algorithm that preserves this stability.

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Thermodynamically Consistent Algorithm: Temporal Discretization

- Runge-Kutta : no stability proof for nonlinear problems;
- Generalized- α method : no stability proof for nonlinear problems;
- Space-time formulation : stability requires convexity of the energy.

1. D.J. Eyre, *An unconditionally stable one-step scheme for gradient systems*. published on line.
2. H. Gomez and T.J.R. Hughes, *Provably Unconditionally Stable, Second-order Time-accurate, Mixed Variational Methods for Phase-field Models*. JCP, 2011.
3. J. Liu, et al. *Functional Entropy Variables: A New Methodology for Deriving Thermodynamically Consistent Algorithms for Complex Fluids, with Particular Reference to the Isothermal Navier-Stokes-Korteweg Equations*. JCP 2013.
4. G. Tierra and F. Guillen-Gonzalez. *Numerical Methods for Solving the Cahn-Hilliard Equation and Its Applicability to Related Energy-Based Models*. Archives of Computational Methods in Engineering, 2015.
5. J. Liu, et al., *Liquid-Vapor Phase Transition: Thermomechanical Theory, Entropy Stable Numerical Formulation, and Boiling Simulations*, CMAME, 2015.

Thermodynamically Consistent Algorithm: Temporal Discretization

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A suite of new time integration schemes is developed.

- Rectangular quadrature rules^{1,3} \Leftrightarrow Eyre's method;
- Perturbed trapezoidal rules² \Leftrightarrow Gomez-Hughes method;
- Perturbed mid-point rules³: Second-order accurate, less numerical dissipation;
- ...^{4,5}

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Thermodynamically Consistent Algorithm: Temporal Discretization

Discrete entropy dissipation and time accuracy

1. The fully discrete scheme is *unconditionally entropy-stable* in the following sense.

$$\begin{aligned}
 & \int_{\Omega} \left(\frac{H(\rho_{n+1}^h, \theta_{n+1}^h) - H(\rho_n^h, \theta_n^h)}{\Delta t_n} + \nabla \cdot \left(H(\rho_{n+\frac{1}{2}}^h, \theta_{n+\frac{1}{2}}^h) \mathbf{u}_{n+\frac{1}{2}}^h \right) \right. \\
 & \quad \left. - \nabla \cdot \left(\mathbf{q}_{n+\frac{1}{2}}^h / \theta_{n+\frac{1}{2}}^h \right) + \rho_{n+\frac{1}{2}}^h r / \theta_{n+\frac{1}{2}}^h \right) d\mathbf{x} \\
 = & - \underbrace{\int_{\Omega} \frac{1}{\theta_{n+\frac{1}{2}}^h} \boldsymbol{\tau}_{n+\frac{1}{2}}^h : \nabla \mathbf{u}_{n+\frac{1}{2}}^h d\mathbf{x} - \int_{\Omega} \frac{\kappa |\nabla \theta_{n+\frac{1}{2}}^h|^2}{\left(\theta_{n+\frac{1}{2}}^h \right)^2} d\mathbf{x}}_{\text{physical dissipation}} \\
 & - \underbrace{\int_{\Omega} \frac{1}{\theta_{n+\frac{1}{2}}^h \Delta t_n} \left(\frac{\llbracket \rho_n^h \rrbracket^4}{24} \frac{\partial^3 \nu_{loc}}{\partial \rho^3}(\rho_{n+\xi_1}^h, \theta_{n+\frac{1}{2}}^h) - \frac{\llbracket \theta_n^h \rrbracket^4}{24} \frac{\partial^3 H}{\partial \theta^3}(\rho_{n+\frac{1}{2}}^h, \theta_{n+\xi_2}^h) \right) d\mathbf{x}}_{\text{numerical dissipation}} \leq 0.
 \end{aligned}$$

2. The local truncation error in time $\Theta(t)$ may be bounded by $|\Theta(t_n)| \leq K \Delta t_n^2 \mathbf{1}_5$ for all $t_n \in [0, T]$, where K is a constant independent of Δt_n . and $\mathbf{1}_5 = (1; 1; 1; 1; 1)^T$.

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Isogeometric Analysis and Software Design



METIS

TetGen

PETSc

hype

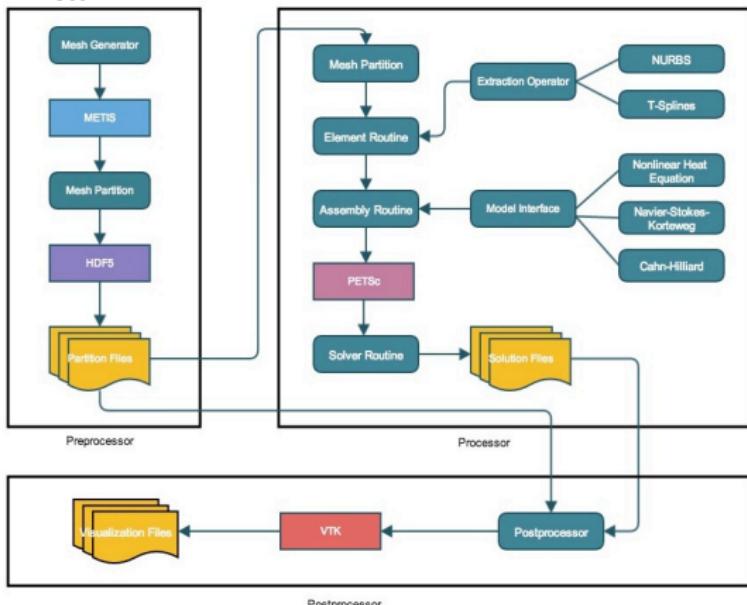


VTK

Paraview

PERIGEE: an object-oriented C++ code for parallel FEM/IGA multiscale multiphysics simulations:

- Cahn-Hilliard equation;
- Navier-Stokes-Korteweg equation;
- Incompressible Navier-Stokes equation;
- Fluid-structure interaction (ongoing);
- etc.



Isogeometric Analysis and Software Design



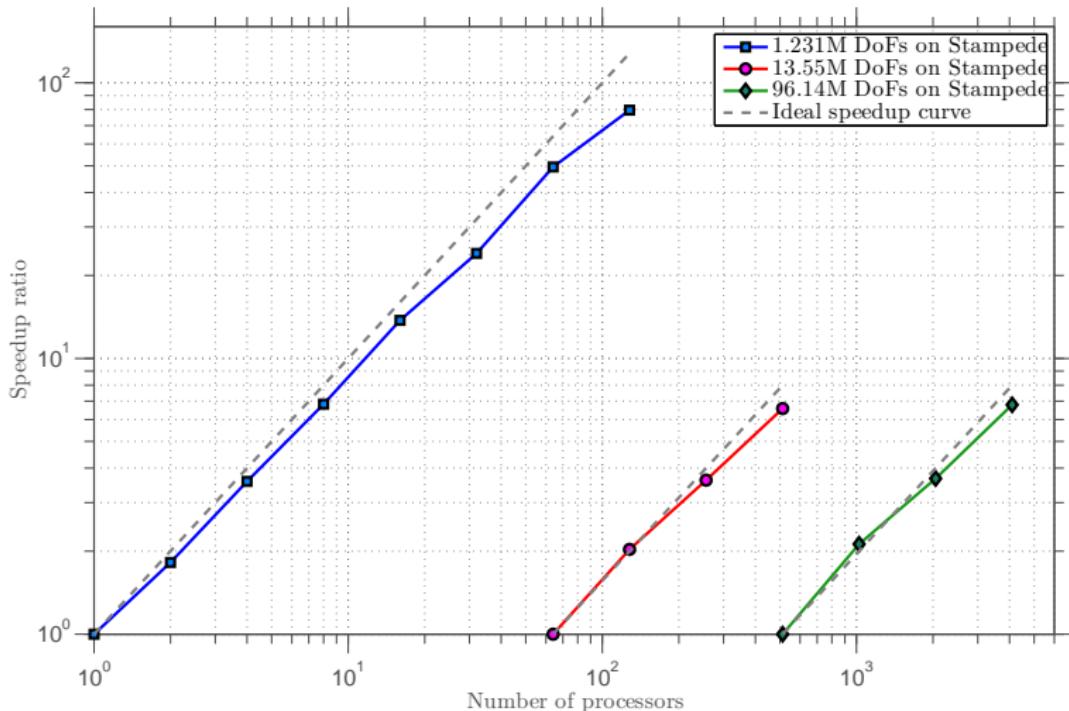
Stampede
A 10 PFLOPS (PF) Dell Linux Cluster at TACC;
The 10th fastest supercomputer in the world.



Maverick
An HP/NVIDIA Interactive Visualization
and Data Analytics System.

Top500 Supercomputer Sites, www.top500.org.

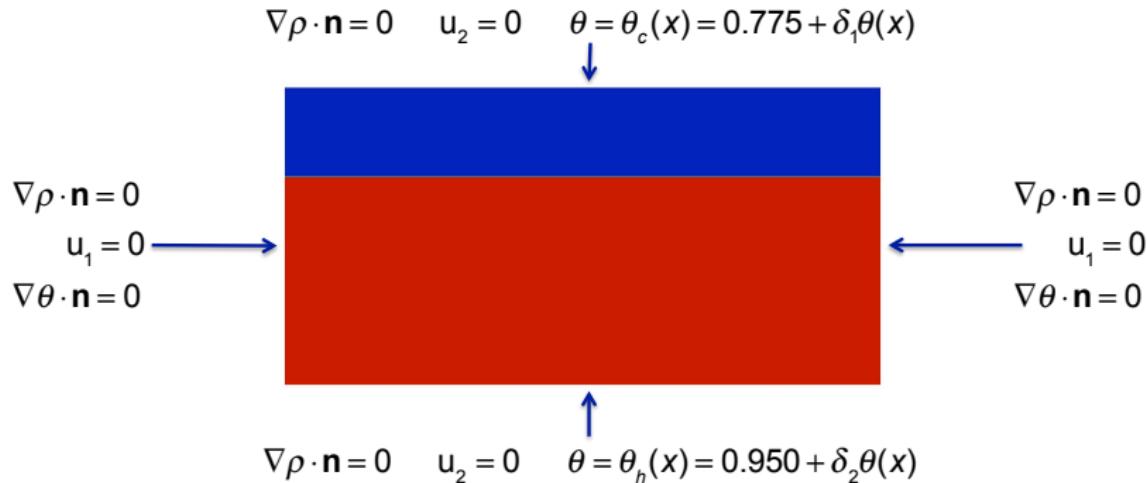
Isogeometric Analysis and Software Design



J. Liu, *Thermodynamically Consistent Modeling and Simulation of Multiphase Flows*. Ph.D. Dissertation, The University of Texas at Austin, 2014.

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Applications: Nucleate Boiling



- $\Omega = (0, 1) \times (0, 0.5)$ and $\mathbf{b} = (0; -0.025)^T$
- $\bar{\mu} = C_\mu \rho$ and $\kappa = C_\kappa \rho$
- $C_\mu = 1.15 \times 10^{-4}$, $C_\kappa = 1.725 \times 10^{-5}$, $\text{We} = 8.401 \times 10^6$, and $\gamma = 1.333$
- 2048×1024 uniform quadratic NURBS, $\Delta t = 5.0 \times 10^{-4}$, and $T = 100.0$

Applications: Nucleate Boiling



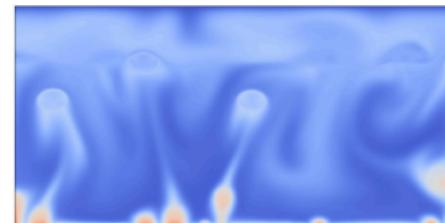
$t = 0.0$



$t = 1.25$



$t = 18.75$



$t = 62.5$

Applications: Nucleate Boiling

Applications: Film Boiling

$$\nabla \rho \cdot \mathbf{n} = 0 \quad u_2 = 0 \quad \theta = \theta_c(x) = 0.775 + \delta_1 \theta(x)$$



$$\nabla \rho \cdot \mathbf{n} = 0$$

$$u_1 = 0 \longrightarrow$$

$$\nabla \theta \cdot \mathbf{n} = 0$$



$$\nabla \rho \cdot \mathbf{n} = 0$$

$$u_1 = 0 \longleftarrow$$

$$\nabla \theta \cdot \mathbf{n} = 0$$

$$\nabla \rho \cdot \mathbf{n} = 0 \quad u_2 = 0 \quad \theta = \theta_h(x) = 0.950 + \delta_2 \theta(x)$$



- $\Omega = (0, 1) \times (0, 0.5)$ and $\mathbf{b} = (0; -0.025)^T$
- $\bar{\mu} = C_\mu \rho$ and $\kappa = C_\kappa \rho$
- $C_\mu = 4.60 \times 10^{-4}$, $C_\kappa = 1.725 \times 10^{-5}$, $\text{We} = 8.401 \times 10^6$, and $\gamma = 1.333$
- 2048×1024 uniform quadratic NURBS, $\Delta t = 5.0 \times 10^{-4}$, and $T = 500.0$

Applications: Film Boiling



$t = 0.0$



$t = 100.0$



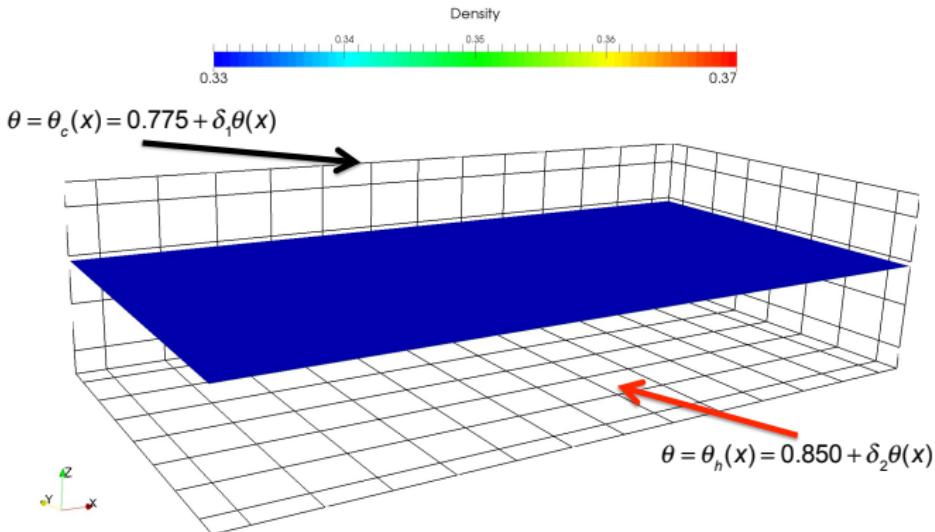
$t = 200.0$



$t = 225.0$

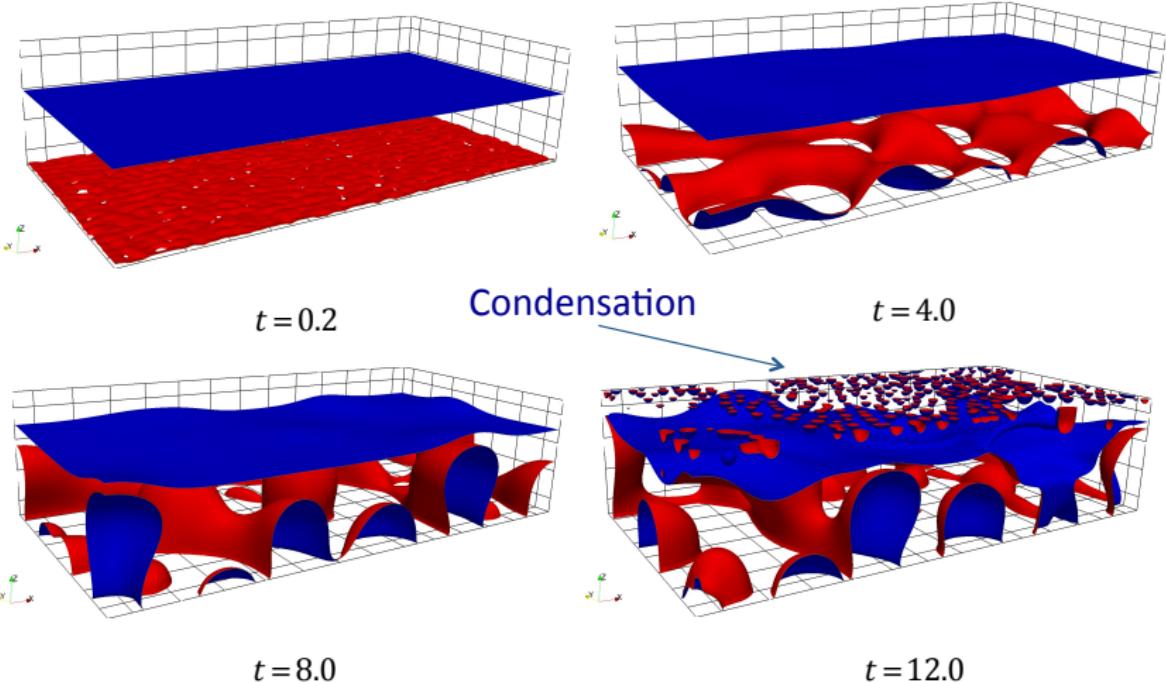
Applications: Film Boiling

Applications: Three-dimensional boiling



- $\Omega = (0, 1) \times (0, 0.5) \times (0, 0.25)$
- $\bar{\mu} = C_\mu \rho$ and $\kappa = C_\kappa \rho$
- $C_\mu = 1.289 \times 10^{-4}$, $C_\kappa = 7.732 \times 10^{-5}$, $\text{We} = 6.533 \times 10^5$, and $\gamma = 1.333$
- $600 \times 300 \times 150$ uniform quadratic NURBS and $\Delta t = 2.0 \times 10^{-3}$
- $\nabla \rho \cdot \mathbf{n} = 0$ and slip boundary condition for \mathbf{u} on $\partial\Omega$

Applications: Three-dimensional boiling



Applications: Three-dimensional Boiling

Applications: Three-dimensional Boiling

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Conclusions

- ✓ A thermodynamically consistent **modeling framework** for multiphase flows is developed based on the concept of microforces.
 - The interstitial working flux of Dunn and Serrin is derived from fundamental hypothesis.
- ✓ The notion of **entropy variables** is generalized to the **functional** setting and is applied to the Navier-Stokes-Korteweg equations to construct an entropy-stable spatial discretization.
- ✓ A second-order accurate, unconditionally entropy-stable, time-stepping method is developed based on **special quadrature rules**.
 - There are no convexity requirements.
- ✓ The formulation constitutes a new approach to simulate **boiling**.
 - Two-dimensional nucleate boiling
 - Two-dimensional film boiling
 - Three-dimensional boiling

Conclusions

- ✓ A thermodynamically consistent modeling framework for multiphase flows is developed based on the concept of microforces.
 - The interstitial working flux of Dunn and Serrin is derived from fundamental hypothesis.
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"When a bubble reaches the top cold plate, it is removed from the calculation to model condensation and a new bubble is introduced at a random position on the bottom hot plate [...]"