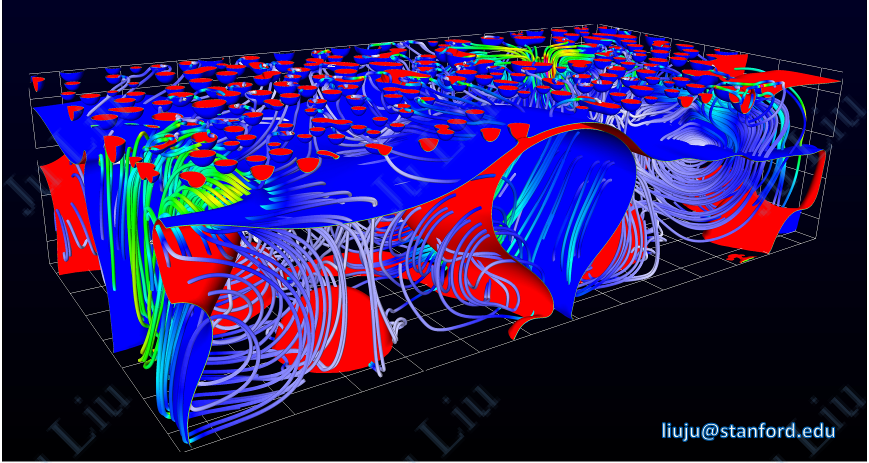
Multiphase Flows: Thermomechanical Theory, Algorithms, and Simulations

Ju Liu



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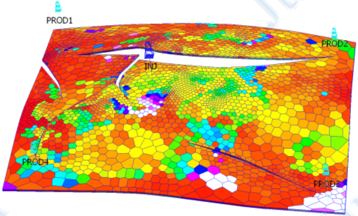
Outline

- Motivation
- Thermomechanical Theory
  - Continuum theory
  - Thermodynamics of the van der Waals model
- Algorithms
  - Entropy variables and spatial discretization
  - Quadrature rules and temporal discretization
  - Parallel code development and code verification
- Boiling simulations
- Conclusions
- Future work

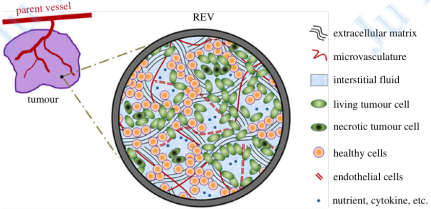
Motivation: Multiphase Flows

Phase: material component.

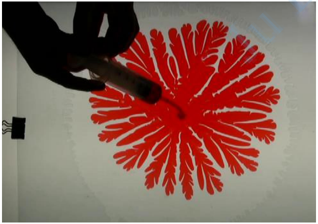
The Great Wave off Kanagawa



Multicomponent flow in a reservoir



Tumor growth

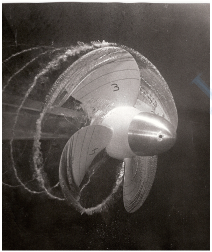


Viscous fingering

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.

Phase: state of matter.

boiling heat transfer



cavitating flow

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

Motivation: Boiling Models

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

V.K. Dhir, Boiling heat transfer. Annual Review of Fluid Mechanics, 1998.
R. Lakkaraju, et al. Heat transport in bubbling turbulent convection. PNAS, 2013.

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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.

D.M. Anderson, et al. Diffuse-interface methods in fluid mechanics. Annu. Rev. Fluid Mech., 1998.

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.
- Interfacial physics are described by phenomenological relations, such as the Young-Laplace law.

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

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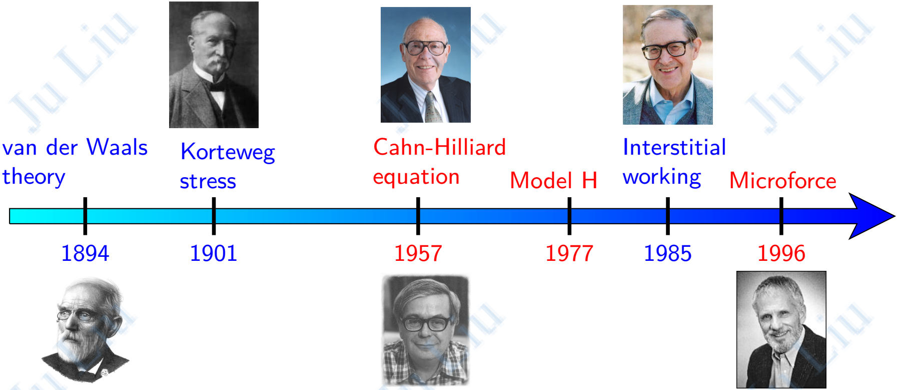

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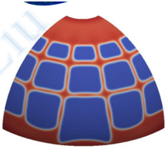
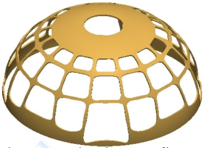
Motivation: Numerical Analysis





- 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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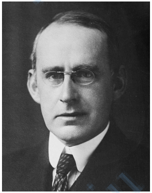
Continuum Theory: Balance Laws



"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.

- Conservation of mass

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

Continuum Theory: Balance Laws

- Conservation of mass

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

- Balance of components

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

$$\text{for } \alpha = 1, \cdots, \mathbf{N} - 1.$$

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for $\alpha = 1, \cdots, \mathrm{N} - 1.$

- Balance of linear momentum

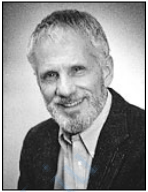
$$\frac{d}{dt}\int_{\Omega_t} \rho\mathbf{u} dV_{\mathbf{x}} = \int_{\partial\Omega_t} \boldsymbol{\sigma} dA_{\mathbf{x}} + \int_{\Omega_t} \rho\mathbf{b} dV_{\mathbf{x}},$$

$$\boldsymbol{\sigma} = \mathbf{Tn}.$$

- Balance of angular momentum

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

Continuum Theory: Balance Laws



" 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.

- Balance of microforces associated with ρ

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

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

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- Balance of energy

$$\frac{d}{dt}\int_{\Omega_t} \rho E\,dV_{\mathbf{x}} := \frac{d}{dt}\int_{\Omega_t} \overbrace{\frac{\rho}{2}|\mathbf{u}|^2}^{\text{kinetic energy}} + \overbrace{\rho\iota}^{\text{internal energy}}\,dV_{\mathbf{x}}$$

$$= \int_{\partial\Omega_t} \left(\mathbf{T}\mathbf{u} + \frac{d}{dt}\rho\boldsymbol{\xi} - \mathbf{q}\right)\cdot\mathbf{n}\,dA_{\mathbf{x}} + \int_{\Omega_t} \rho\mathbf{b}\cdot\mathbf{u} + \mathfrak{l}\frac{d}{dt}\rho + \rho r\,dV_{\mathbf{x}}.$$

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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

$$
\begin{cases}
\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{cases}
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B.D. Coleman and W. Noll, The thermodynamics of elastic materials with heat conduction and viscosity. Archive for Rational Mechanics and Analysis, 1968.
J. Liu, et al., Liquid-Vapor Phase Transition: Thermomechanical Theory, Entropy Stable Numerical Formulation, and Boiling Simulations, CMAME 2015.

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Truesdell's principle of equipresence $+$ Coleman-Noll approach

$$\Downarrow$$

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

Constitutive relations

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

- Microstresses

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

- Heat flux $$\mathbf{q} = -\kappa \nabla \theta.$$
- Cauchy stress

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

- Entropy density per unit mass

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

Theorem (Dissipation for isolated systems)

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

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

J. Lowengrub and L. Truskinovsky, Quasi-incompressible Cahn-Hilliard fluids and topological transitions, Proceedings of the Royal Society of London

Continuum Theory: Dissipation Inequalities

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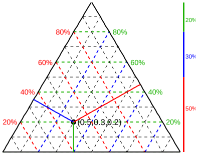
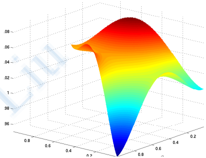


Gibbs triangle



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

J. Lowengrub and L. Truskinovsky, Quasi-incompressible Cahn-Hilliard fluids and topological transitions, Proceedings of the Royal Society of London

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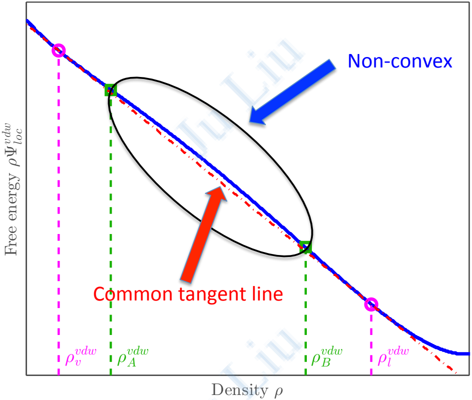
Continuum Theory: The van der Waals Fluid Model

Thermodynamic potential

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

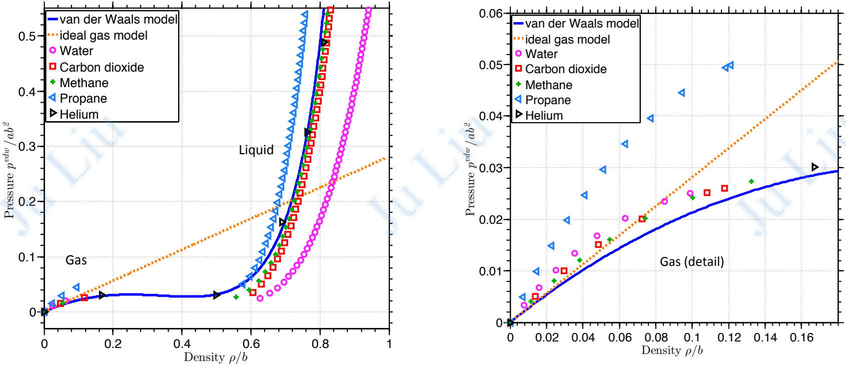
$$\Psi_{loc}(\rho,\theta) = -a\rho + R\theta\log\left(\frac{\rho}{b-\rho}\right) - C_v\theta\log\left(\frac{\theta}{\theta_{ref}}\right) + C_v\theta.$$



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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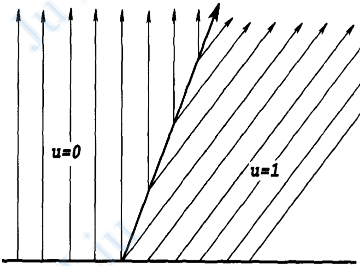
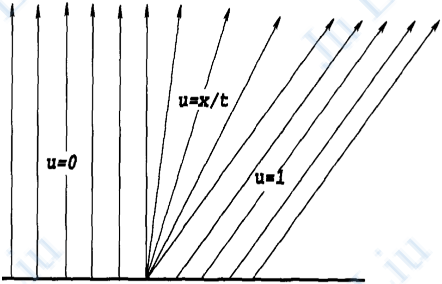
Thermodynamically Consistent Algorithm



Non-physical shock



Physical shock

✗ Weak solutions of the conservation law ✓

The second law of thermodynamics

L.C. Evans, Partial Differential Equations.

Thermodynamically Consistent Algorithm: Spatial Discretization

Given the conservation variables $\mathbf{U} = \{\rho; \rho\mathbf{u}^T; \rho E\}^T$, and the mathermatical 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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$\mathbf{V}$ lives in the test function spaces.

$\Uparrow$

Solve the equations in terms of $\mathbf{V}$,

if there is a well-defined algebraic change-of-variables between $\mathbf{U}$ and $\mathbf{V}$.

$\Uparrow$

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

$\Uparrow$

Aerodynamists are lucky.

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

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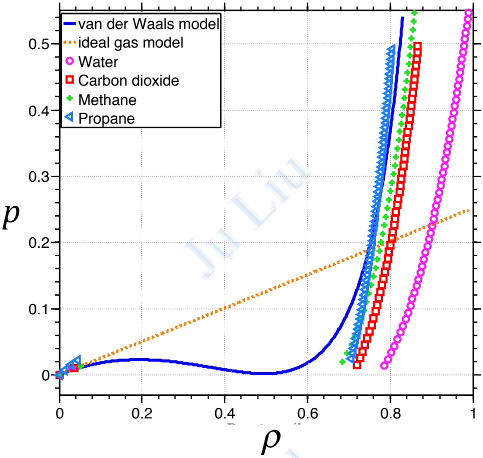
Aerodynamists are lucky.

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.

Thermodynamically Consistent Algorithm: Spatial Discretization

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



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

Thermodynamically Consistent Algorithm: Spatial Discretization

Mathematical entropy function

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

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

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

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

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

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.

Thermodynamically Consistent Algorithm: Spatial Discretization

Stability of the weak formulation

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

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

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

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

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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

- 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.

A suite of new time integration schemes is developed.

- Rectangular quadrature rules[1,3] $\Leftrightarrow$ Eyre's method;
- Perturbed trapezoidal rules[2] $\Leftrightarrow$ Gomez-Hughes method;
- Perturbed mid-point rules[3]: Second-order accurate, less numerical dissipation;
- ...[4,5]

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Discrete entropy dissipation and time accuracy

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

$$\int_\Omega \left(\frac{H(\rho^h_{n+1}, \theta^h_{n+1}) - H(\rho^h_n, \theta^h_n)}{\Delta t_n} + \nabla \cdot \left(H(\rho^h_{n+\frac{1}{2}}, \theta^h_{n+\frac{1}{2}}) \mathbf{u}^h_{n+\frac{1}{2}} \right) \right.$$

$$\left. - \nabla \cdot \left(\mathbf{q}^h_{n+\frac{1}{2}} / \theta^h_{n+\frac{1}{2}} \right) + \rho^h_{n+\frac{1}{2}} r / \theta^h_{n+\frac{1}{2}} \right) d\mathbf{x}$$

$$= \underbrace{- \int_\Omega \frac{1}{\theta^h_{n+\frac{1}{2}}} \boldsymbol{\tau}^h_{n+\frac{1}{2}} : \nabla \mathbf{u}^h_{n+\frac{1}{2}} \, d\mathbf{x} - \int_\Omega \frac{\kappa |\nabla \theta^h_{n+\frac{1}{2}}|^2}{\left(\theta^h_{n+\frac{1}{2}}\right)^2} d\mathbf{x}}_{\text{physical dissipation}}$$

$$\underbrace{- \int_\Omega \frac{1}{\theta^h_{n+\frac{1}{2}} \Delta t_n} \left(\frac{[\![\rho^h_n]\!]^4}{24} \frac{\partial^3 \nu_{loc}}{\partial \rho^3} (\rho^h_{n+\xi_1}, \theta^h_{n+\frac{1}{2}}) - \frac{[\![\theta^h_n]\!]^4}{24} \frac{\partial^3 H}{\partial \theta^3} (\rho^h_{n+\frac{1}{2}}, \theta^h_{n+\xi_2}) \right) d\mathbf{x}}_{\text{numerical dissipation}} \leq 0.$$

2. The local truncation error in time $\boldsymbol{\Theta}(t)$ may be bounded by $|\boldsymbol{\Theta}(t_n)| \leq K \Delta t_n^2 \mathbf{1}_5$ 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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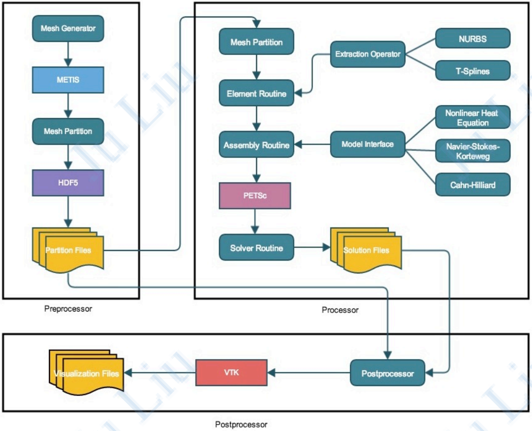
Isogeometric Analysis and Software Design

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.



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

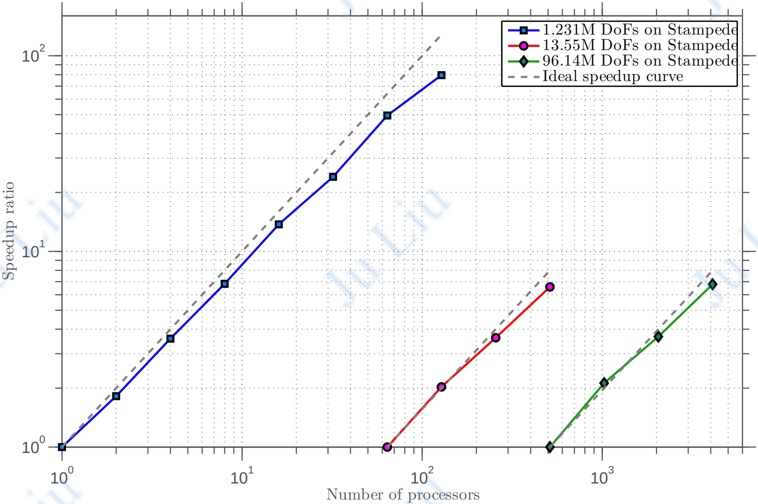
Isogeometric Analysis and Software Design

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



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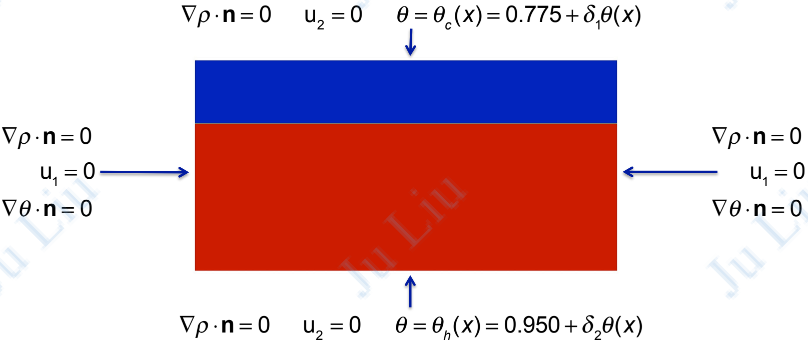
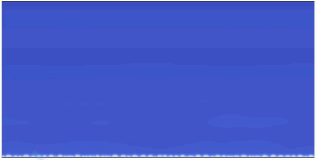


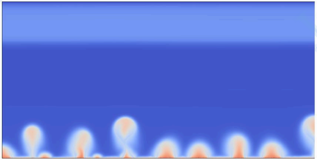
- $\Omega = (0,1)\times(0,0.5)$ and $\mathbf{b} = (0; -0.025)^T$
- $\bar{\mu} = C_\mu \rho$ and $\kappa = C_\kappa \rho$
- $C_\mu = 1.15\times 10^{-4}$, $C_\kappa = 1.725\times 10^{-5}$, $\mathrm{We} = 8.401\times 10^{6}$, and $\gamma = 1.333$
- 2048×1024 uniform quadratic NURBS, $\Delta t = 5.0\times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

Applications: Nucleate Boiling

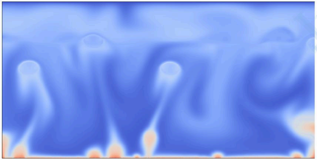
$t = 0.0$



$t = 1.25$

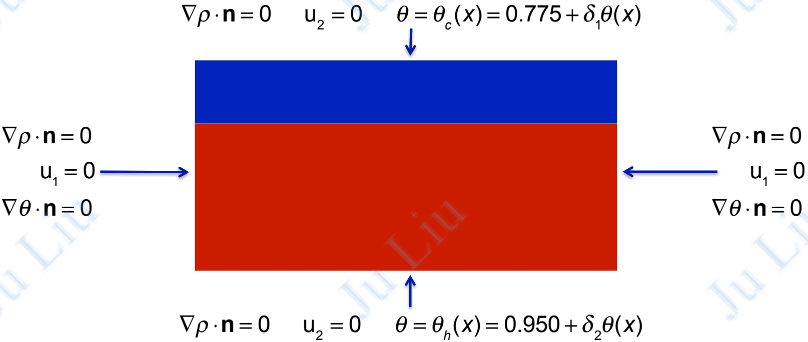


$t = 18.75$



$t = 62.5$

Applications: Nucleate Boiling

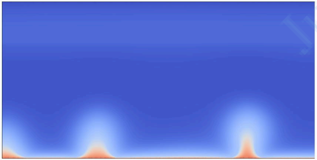


- $\Omega = (0,1)\times(0,0.5)$ and $\mathbf{b} = (0; -0.025)^T$
- $\bar{\mu} = C_\mu \rho$ and $\kappa = C_\kappa \rho$
- $C_\mu = 4.60\times10^{-4}$, $C_\kappa = 1.725\times10^{-5}$, $\mathrm{We} = 8.401\times10^{6}$, and $\gamma = 1.333$
- 2048×1024 uniform quadratic NURBS, $\Delta t = 5.0\times10^{-4}$, and $T = 500.0$

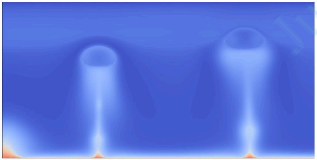
Applications: Film Boiling

$t = 0.0$

$t = 100.0$

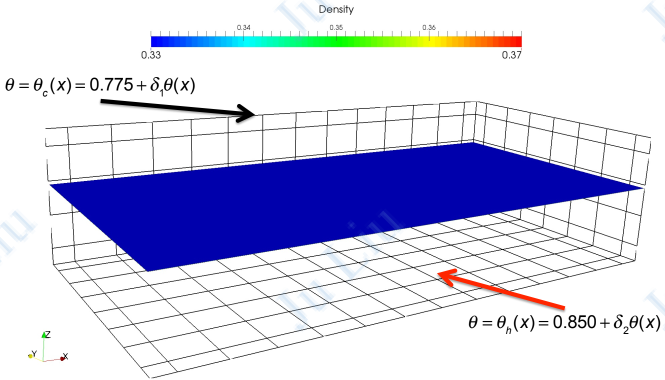


$t = 200.0$



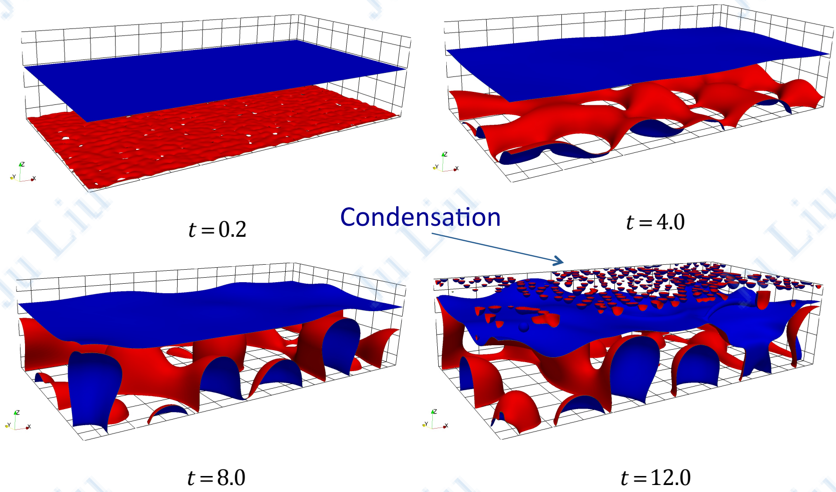
$t = 225.0$

Applications: Film Boiling



- $\Omega = (0, 1) \times (0, 0.5) \times (0, 0.25)$
- $\bar{\mu} = C_\mu \rho$ and $\kappa = C_\kappa \rho$
- $C_\mu = 1.289 \times 10^{-4}$, $C_\kappa = 7.732 \times 10^{-5}$, $\mathrm{We} = 6.533 \times 10^5$, 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

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Conclusions and Future Work

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

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

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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 [...]"

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