Computational Phase-Field Modeling

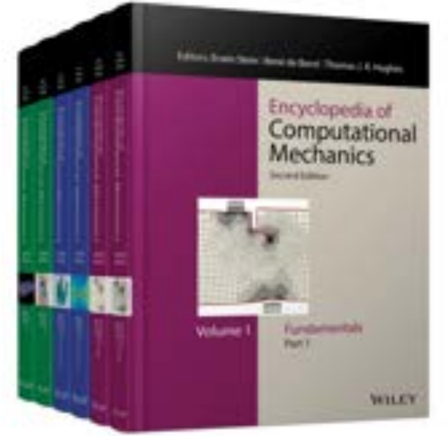
—— UKACM 2022 *School*, University of Nottingham, 20–22 April 2022 ——

Kris van der Zee

School of Mathematical Sciences

Main reference

H. Gomez and K.G. van der Zee.
Computational phase-field modeling.
in Encyclopedia of Computational Mechanics, Second Edition,
E. Stein, R. de Borst and T.J.R. Hughes, eds., John Wiley & Sons, (2017)



Abstract
Phase-field modeling is emerging as a promising tool for the treatment of problems with interfaces. . . .

Main reference

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Who am I?

- PhD (Delft), Postdoc (Austin, Texas)
  Assistant/Associate Prof (Eindhoven) (Nottingham)
- Research areas:
  Fluid–structure interaction, multi-phase flow, cancer tumour growth, finite element methods, adaptive methods, approximation of PDEs machine learning for scientific computation

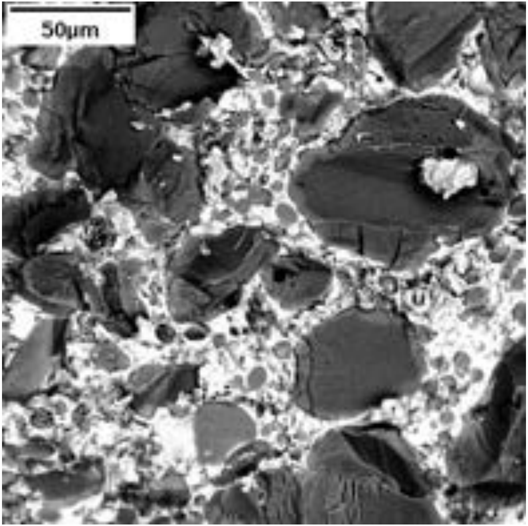
Who are you? http://menti.com

- "What is your research area?"
- "Have you heard of phase-field modeling (before today)?"

1. Two-phase fluid flow

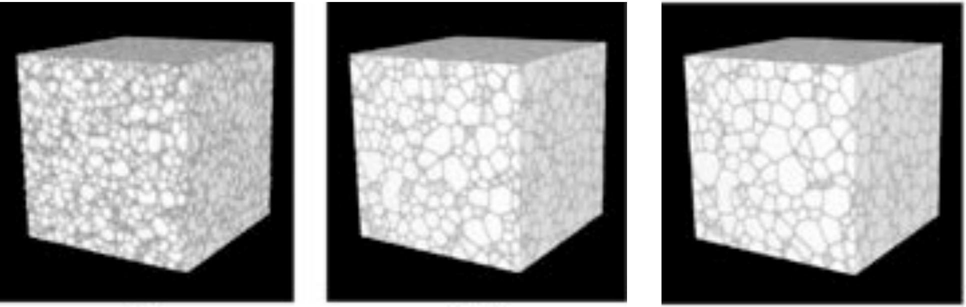
Motivation: Evolving-interface phenomena

2. Phase separation in alloys / phase transition in metals

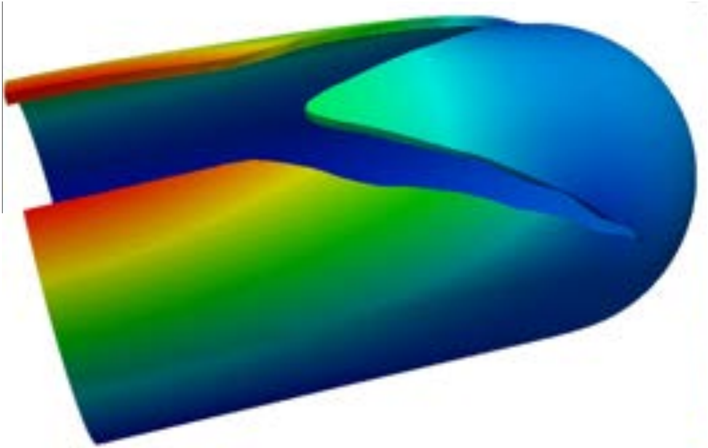


Motivation: Evolving-interface phenomena

2. Phase separation in alloys / phase transition in metals



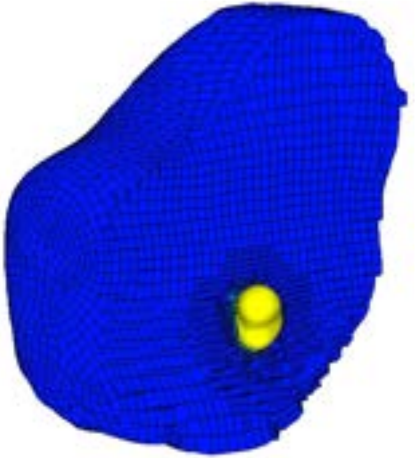
3. Crack propagation



(Borden, Verhoosel, Scott, Hughes, Landis, CMAME 2012)

4. **Solidification, melting, crystal growth**

5. Biological growth phenomena, e.g. tumors



(Hawkins-Daarud, van der Zee, Oden, IJNMBE 2012)

Motivation: Phase-field modeling

Definition: Phase-field model [1] (Wikipedia)

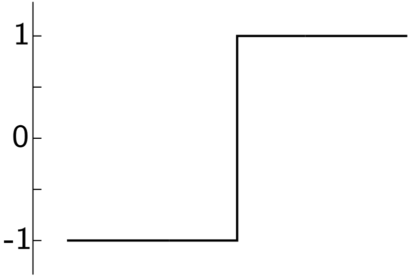
A mathematical model for solving interfacial problems.

The phase field takes distinct values in each of the phases, with a smooth change between both values around the interface.

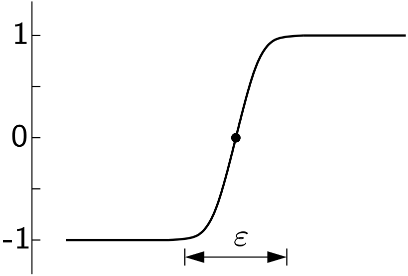
[1] Also referred to as: **Diffuse-interface model**

Motivation: Phase-field modeling

Sharp **interface vs** ***diffuse*** **interface (phase-field model)**

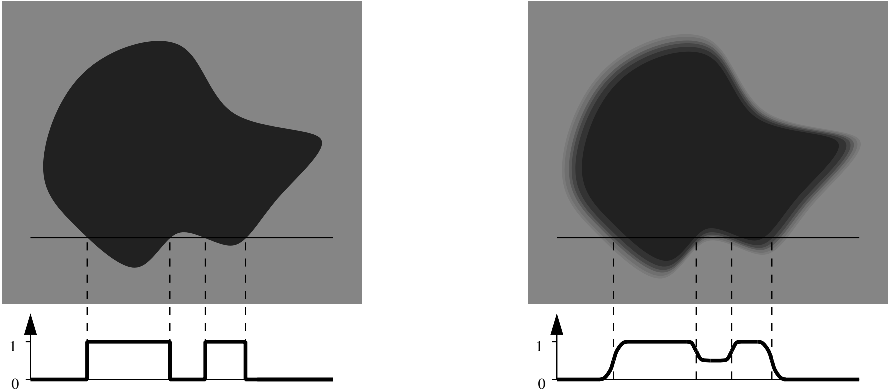


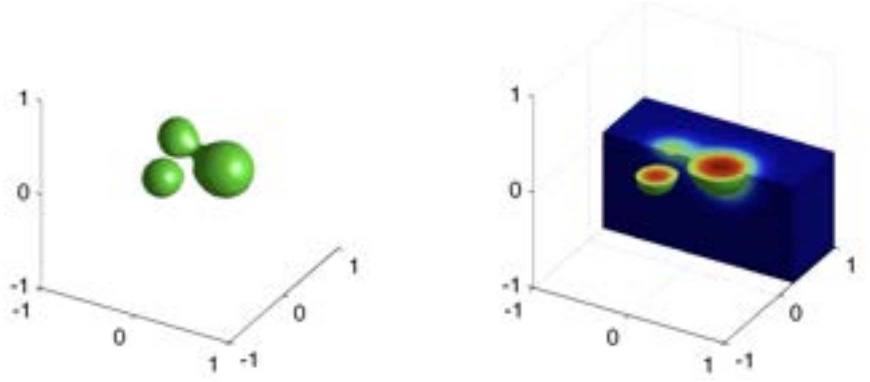
"Pure" phases {-1,1}



Diffuse interface (thickness ε)

Sharp interface vs _diffuse_ interface (phase-field model)

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Learning objectives

Computational Phase-Field Modeling

I. What are the phase-field models?
II. Why do they work?
III. How do you solve them numerically?
IV. Where do they actually come from?

Learning objectives

Computational Phase-Field Modeling

I. Examples of phase-field models

II. Main principle: Energy dissipation

III. Numerics: Energy-stable methods

IV. Foundations: Thermomechanics and mixture theory

I. Examples of phase-field models

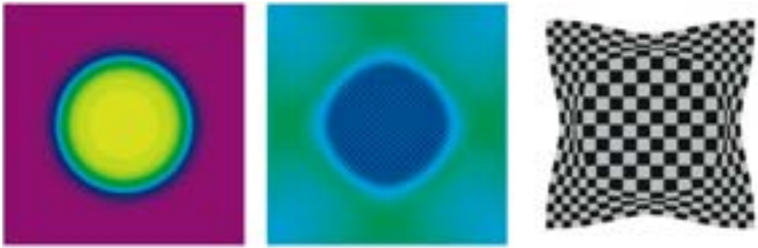
1. Navier–Stokes–Cahn–Hilliard (two-phase flow)
2. Cahn–Larché (phase separation in elastic solids)
3. Phase-field fracture
4. The phase-field model of solidification
5. Diffuse-interface tumor-growth model

I. Examples of phase-field models

1.

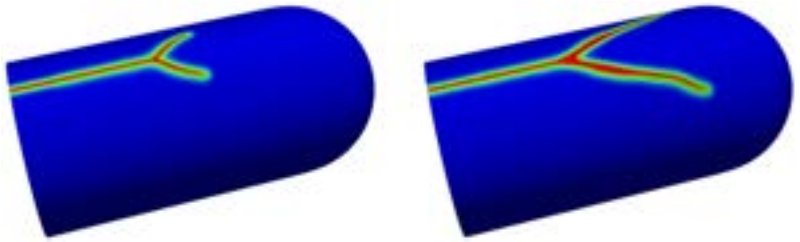
I. Examples of phase-field models

2.



I. Examples of phase-field models

3.



I. Examples of phase-field models

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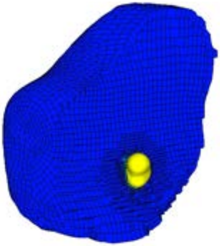


I. Examples of phase-field models

"Phase"?

- Concentration in a mixture: φ, c

  Example: volume fraction φ, mass fraction c
- State of matter (phase): ϕ

  Example: gas, liquid, solid
- Order parameter (measure of the degree of order in a system): ϕ

  Example: crystal lattice configuration

I. Examples of phase-field models

Viewpoints on phase-field models

- Computational
  Regularization of a sharp-interface.
  Complex interactions are included; no need to track interfaces.
- Physics / Mechanics
  New (!) meso-scale continuum thermo-mechanics models.
- Mathematics
  Nonlinear, higher-order, singularly perturbed, parabolic (dissipative) PDEs.

Two elementary phase-field models

- Cahn–Hilliard equation

$$\boxed{\frac{\partial \varphi}{\partial t} = \Delta\Big(\frac{1}{\varepsilon} f'(\varphi) - \varepsilon \Delta \varphi\Big)}$$

- Allen–Cahn equation

$$\boxed{\frac{\partial \varphi}{\partial t} = -\frac{1}{\varepsilon} f'(\varphi) + \varepsilon \Delta \varphi}$$

Outline

I. What are the phase-field models?
II. Why do they work?
III. How do you solve them numerically?
IV. Where do they actually come from?

Outline

I. What are the phase-field models?

II. **Why do they work?**
Main principle: Energy dissipation

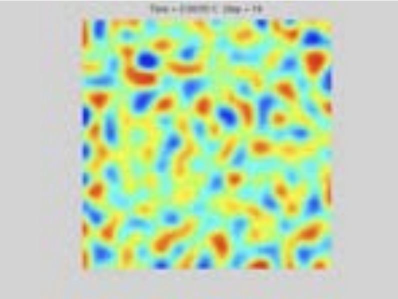
III How do you solve them numerically?

IV Where do they actually come from?

Two elementary phase-field models

- Cahn–Hilliard equation

$$\boxed{\frac{\partial \varphi}{\partial t} = \Delta\left(\frac{1}{\varepsilon} f'(\varphi) - \varepsilon \Delta \varphi\right)}$$



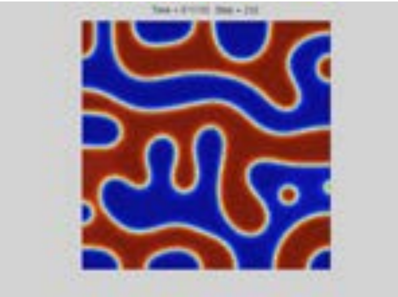
Short time scales

II. Main principle: Energy dissipation

Two elementary phase-field models

- Cahn–Hilliard equation

$$\boxed{\frac{\partial\varphi}{\partial t} = \Delta\Big(\frac{1}{\varepsilon}f'(\varphi) - \varepsilon\Delta\varphi\Big)}$$



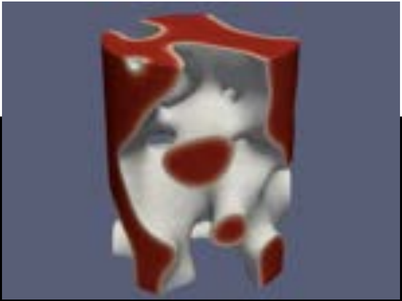
Long time scales (2-D)

II. Main principle: Energy dissipation

Two elementary phase-field models

- Cahn–Hilliard equation

$$\frac{\partial \varphi}{\partial t} = \Delta\Big(\frac{1}{\varepsilon} f'(\varphi) - \varepsilon \Delta \varphi\Big)$$



Long time scales (3-D)

II. Main principle: Energy dissipation

Cahn–Hilliard model
$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = \Delta \mu & \text{in } \Omega \\ \mu = \frac{1}{\varepsilon} f'(\varphi) - \varepsilon \Delta \varphi & \text{in } \Omega \\ \partial_n \varphi = 0 & \text{on } \partial\Omega \\ \partial_n \mu = 0 & \text{on } \partial\Omega \end{cases}$$

Energy dissipation (Cahn–Hilliard eq.)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(\varphi) \leq 0 \quad \text{where} \quad \mathcal{E}(\varphi) = \int_\Omega \left(\frac{1}{\varepsilon} f(\varphi) + \frac{\varepsilon}{2} |\nabla \varphi|^2 \right) \mathrm{d}x$$

Outline

I. What are the phase-field models?

II. Why do they work?

III. **How do you solve them numerically?**
Numerics: Energy-stable methods

IV. Where do they actually come from?

III. Numerics: Energy-stable methods

Space and time discretization of phase-field models

1. Weak formulation
2. Galerkin approximation: System of ODEs
3. Time-stepping method: Algebraic system

Exercise

A. Discretization

1. Derive the system of ODEs for the space-discretized (Galerkin) Cahn–Hilliard equation, starting from:
   - the system of 2 second-order equations: $$\begin{cases} \dfrac{\partial \varphi}{\partial t} = \Delta \mu \\ \mu = \frac{1}{\varepsilon} f'(\varphi) - \epsilon \Delta \varphi \end{cases}$$
   - or, the fourth-order equation: $$\frac{\partial \varphi}{\partial t} = \Delta\Big(\tfrac{1}{\varepsilon} f'(\varphi) - \epsilon \Delta \varphi \Big)$$
2. How would you discretize in time?

B. Energy dissipation

Pick your problem of interest (NSCH, PFF, or AC),

and show that the total energy dissipates: $\boxed{\dfrac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} \leq 0}$

(NSCH: Add kinetic energy $\frac{1}{2}|\mathbf{u}|^2$.)
(PFF: Add elastic energy $W(c, \mathbf{e})$)
(Which boundary conditions did you choose?)

Exercise A

1. Derive the system of ODEs for the space-discretized (Galerkin) Cahn–Hilliard equation, starting from:
   - the system of 2 second-order equations: $$\begin{cases} \dfrac{\partial \varphi}{\partial t} = \Delta \mu \\ \mu = \frac{1}{\varepsilon} f'(\varphi) - \epsilon \Delta \varphi \end{cases}$$
   - or, the fourth-order equation: $$\frac{\partial \varphi}{\partial t} = \Delta\left(\tfrac{1}{\varepsilon} f'(\varphi) - \epsilon \Delta \varphi \right)$$
2. How would you discretize in time?

Exercise B

Pick your problem of interest (NSCH, PFF, or AC),

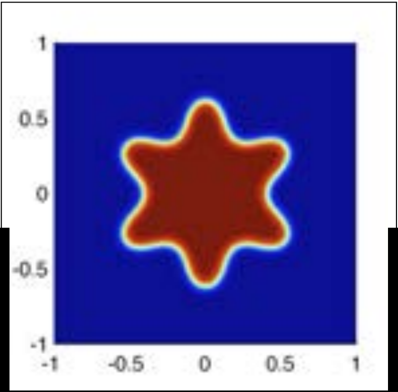
and show that the total energy dissipates: $\boxed{\dfrac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} \leq -\mathcal{D}}$

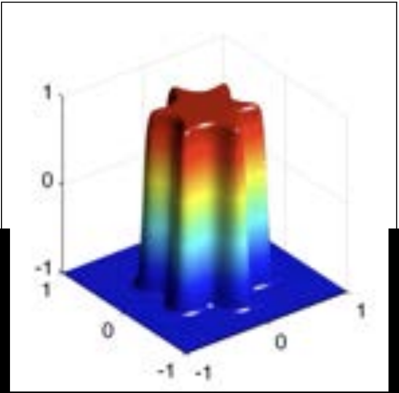
In other words, what is $\mathcal{D}$? (in general: $\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} \leq -\underbrace{\mathcal{D}}_{\geq 0} + \mathcal{W}$)

(Which boundary conditions did you choose?)

III. Numerics: Energy-stable methods

Time-discretization (Allen–Cahn equation)

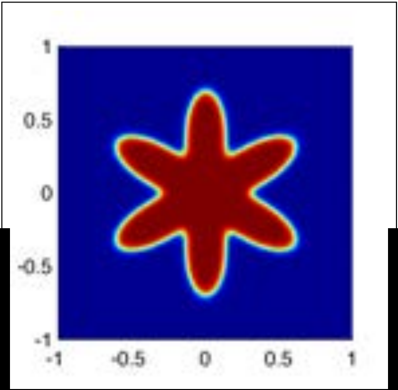


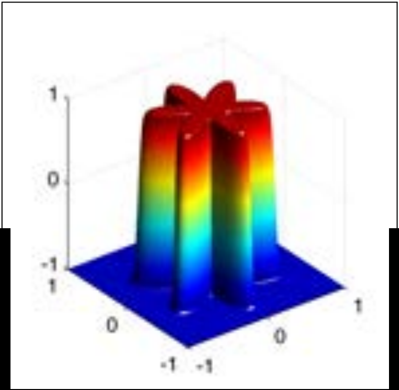


Using a stable scheme (convex-splitting)

III. Numerics: Energy-stable methods

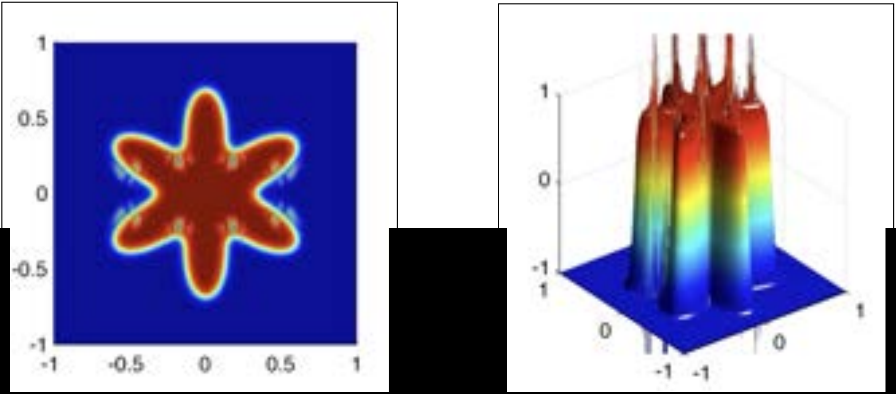
Time-discretization (Allen–Cahn equation)





Forward Euler scheme (explicit)

Time-discretization (Allen–Cahn equation)



Forward Euler scheme (explicit)

III. Numerics: Energy-stable methods

Time-discretization (Convex–splitting)

John Cahn (1968) :
"Uphill diffusion in a binary system is the dynamic hallmark of the [phase separation] mechanism."

Outline

IV Foundations: Thermomechanics and mixture theory

Questions: http://menti.com

1. How long ago did you study Continuum Mechanics?
2. Did you learn the "Second Law of Thermodynamics" in the context of Continuum Mechanics?

IV. Foundations: Thermomechanics . . .

Clifford Truesdell, 1984, p. 31:

"Textbooks by physicists hold up thermodynamics as perfect and closed. Thermodynamics today is a blend of statements from most of the founders: Gibbs, Planck, Boltzmann, even from information theory. Confusion is nearly universal. Constitutive properties are not delimited, just pulled out from under the table as needed."

IV. Foundations: Thermomechanics . . .

Marsden & Hughes, 1983, p. 176:

"The second law of thermodynamics is frequently shrouded in mysterious physical jargon and less than adequate mathematical treatment. The authors' education was no exception. Our own frustration is consistent with Truesdell's (1984, p. 62):

> *"The difference between mechanics and thermodynamics is that thermodynamics never grew up."*

IV. Foundations: Thermomechanics . . .

The unified, rational approach (> 1960)

1. (Mathematically precise) laws of physics
2. Constitutive class (dependence only)
3. Constitutive restrictions as logical consequences from the laws and other principles

1. The 5 Laws (for a continuous body)

$$\boxed{1} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{P}_t} \rho \,\mathrm{d}x = 0$$

$$\boxed{2} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{P}_t} \rho \boldsymbol{v} \,\mathrm{d}x = \int_{\mathcal{P}_t} \boldsymbol{b} \,\mathrm{d}x + \int_{\partial\mathcal{P}_t} \mathbf{T}\boldsymbol{n} \,\mathrm{d}s$$

$$\boxed{3} \qquad (\mathbf{T} = \mathbf{T}^{\mathsf{T}})$$

$\boxed{4}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\int_{\mathcal{P}_t} \epsilon \,\mathrm{d}x + \int_{\mathcal{P}_t} \tfrac{1}{2}\rho|\boldsymbol{v}|^2 \,\mathrm{d}x\Big) = \int_{\mathcal{P}_t} \boldsymbol{b}\cdot\boldsymbol{v}\,\mathrm{d}x + \int_{\partial\mathcal{P}_t} \mathbf{T}\boldsymbol{n}\cdot\boldsymbol{v}\,\mathrm{d}s - \int_{\partial\mathcal{P}_t} \boldsymbol{q}\cdot\boldsymbol{n}\,\mathrm{d}s + \int_{\mathcal{P}_t} r\,\mathrm{d}x$$

$\boxed{5}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{P}_t} \eta\,\mathrm{d}x \geq -\int_{\partial\mathcal{P}_t} \frac{\boldsymbol{q}}{\theta}\cdot\boldsymbol{n}\,\mathrm{d}s + \int_{\mathcal{P}_t} \frac{r}{\theta}\,\mathrm{d}x$$

2. Constitutive class. Example: $(\mathbf{T}, \epsilon, \boldsymbol{q}, \eta) = \hat{F}(\nabla\boldsymbol{v}, \theta, \nabla\theta, \ldots)$

3. Restrictions on the constitutive class

- Thermodynamic consistency
- Frame-indifference
- Equipresence, locality
- Well-posedness
- . . .

3. Restrictions on the constitutive class

Coleman–Noll procedure (1963)

The Thermodynamics of Elastic Materials with Heat Conduction and Viscosity

BERNARD D. COLEMAN & WALTER NOLL

Hilbert's 6th: Axiomatize all of physics

David Hilbert (1900):
"To treat in the same manner, by means of axioms, those physical sciences in which mathematics plays an important part; in the first rank are the theory of probabilities and mechanics."

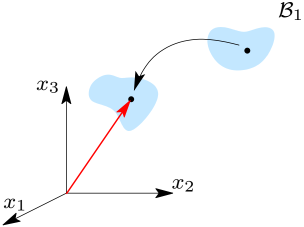
IV. Foundations: . . . and mixture theory

Definition: Mixture

A mixture is a material system made up by two or more different substances which are mixed together but not combined chemically.

Miscible mixtures $\leftrightarrow$ *Immiscible mixtures*

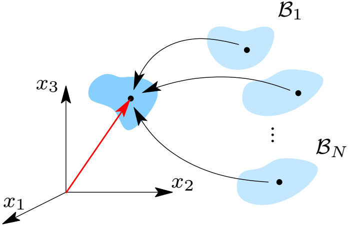
Mixture kinematics



Classical continuum

IV. Foundations: . . . and mixture theory

Mixture kinematics



Continuum mixture

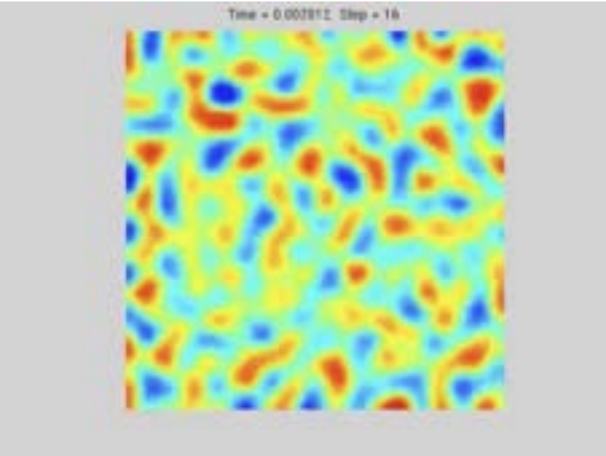
IV. Foundations: . . . and mixture theory

Derivation of Cahn–Hilliard eq. (binary mixture)

1958	1894	1996
John Cahn (1927–2016)	Diederik van der Waals (1837–1923)	Morton Gurtin
		

IV. Foundations: . . . and mixture theory

Derivation of Cahn–Hilliard eq. (binary mixture)



IV. Foundations: ... and mixture theory

Derivation of Cahn–Hilliard eq. (Coleman–Noll procedure)

i. Mixture assumptions / Balance laws

ii. Introduce free energy $\psi = \epsilon - \theta\eta$ / Dissipation ineq.

iii. Postulate constitutive class: $\psi = \hat{\psi}(\varphi, \nabla\varphi)$, $\boldsymbol{h} = \hat{\boldsymbol{h}}(\nabla\mu)$

iv. Infer restrictions (for phase-flux) using 2nd law

v. Take the canonical choice: $\psi = \frac{1}{\varepsilon} f(\varphi) + \frac{\varepsilon}{2}|\nabla\varphi|^2$, $\boldsymbol{h} = -\nabla\mu$

Derivation of the Cahn–Hilliard equation

i. Balance law: $$\frac{\partial \varphi}{\partial t} = -\operatorname{div} \boldsymbol{h}$$

ii. Free-energy dissipation: $$\frac{\mathrm{d}}{\mathrm{d}t} \int_V \psi \,\mathrm{d}V \le \mathcal{W}(\partial V)$$

iii. Constitutive dependence: $$\psi = \hat{\psi}\big(\varphi, \nabla\varphi\big), \; \boldsymbol{h} = \hat{\boldsymbol{h}}(\nabla\mu)$$

iv. Infer restrictions:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} \int_V \hat{\psi}\big(\varphi, \nabla\varphi\big) \,\mathrm{d}V &= \int_V \Big(\partial_\varphi \hat{\psi} \, \tfrac{\partial \varphi}{\partial t} + \partial_{\nabla\varphi} \hat{\psi} \, \tfrac{\partial \nabla\varphi}{\partial t}\Big) \,\mathrm{d}V \\
&= \int_V \underbrace{\Big(\partial_\varphi \hat{\psi} - \operatorname{div} \partial_{\nabla\varphi} \hat{\psi}\Big)}_{=:\mu} \underbrace{\tfrac{\partial \varphi}{\partial t}}_{=-\operatorname{div} \hat{\boldsymbol{h}}} \,\mathrm{d}V + \int_{\partial V} \tfrac{\partial \varphi}{\partial t} \, \partial_{\nabla\varphi} \hat{\psi} \cdot n \,\mathrm{d}A \\
&= \underbrace{\int_V \hat{\boldsymbol{h}} \cdot \nabla\mu \,\mathrm{d}V}_{\le 0 \text{ (dissipation)}} + \underbrace{\int_{\partial V} \Big(-\mu \hat{\boldsymbol{h}} \cdot n + \tfrac{\partial \varphi}{\partial t} \, \partial_{\nabla\varphi} \hat{\psi} \cdot n\Big) \,\mathrm{d}A}_{=:\mathcal{W}(\partial V) \text{ (work)}}
\end{aligned}$$

$$\Rightarrow \quad \boxed{\hat{\boldsymbol{h}} \cdot \nabla\mu \le 0}$$

v. Constitutive choice: $$\psi = \tfrac{1}{\varepsilon} f(\varphi) + \tfrac{\varepsilon}{2} |\nabla\varphi|^2, \quad \boldsymbol{h} = -\nabla\mu$$

$$\Rightarrow \quad \boxed{\frac{\partial \varphi}{\partial t} = \Delta\mu \,, \qquad \mu = \tfrac{1}{\varepsilon} f'(\varphi) - \varepsilon \Delta\varphi}$$

Summary and opportunities

- Main principle: Energy dissipation (Now: Coupled problems!)
- Numerics: Energy stable methods (Now: IGA & SAV !)
- Foundations: Thermomechanics (Now: Unifications!)

[Gomez, van der Zee, 2017]
Computational phase-field modeling, Encyclopedia of Computational Mechanics, 2nd Edition.

[Ten Eikelder, van der Zee, Akkerman, Schillinger, ARXIV 2021]
Unified Analysis of Navier–Stokes Cahn–Hilliard models with non-matching densities