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Role of thermodynamics in modeling the behavior of complex solids

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outline

- introduction & preliminaries
- Eulerian fluids? Lagrangian solids? Continuum mechanics!
- "standard" non-equilibrium thermodynamics for solids
- GENERIC for solids

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a bit more detail

comparison of Eulerian- & Lagrangian-based continuum mechanics

- configuration & fields
- derivatives (e.g., material time derivative)
- transport & balance relations
- elements of material theory for solids

comparison of non-equilibrium thermodynamic approaches

- generalized Gibbs / entropy-based
  e.g. Meixner and Reik (1959), de Groot and Mazur (1962), Liu (1972), Müller (1985)
- General Equation for Non-Equilibrium Reversible-Irreversible Coupling
  GENERIC: e.g. Öttinger and Grmela (1997), Öttinger (2005), Grmela (2010)

applications

- homogeneous thermoelastic solids (e.g., Hütter and Svendsen, 2011)
- homogeneous viscoplastic solids (e.g., Hütter and Svendsen, 2012)
- inhomogeneous thermoelastic solids (today)

a little notation

things Euclidean

- three-dimensional Euclidean space (E^3, V^3)
- first-order tensors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \ldots \in V^3$
- second-order tensors $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}, \ldots \in \mathrm{Lin}(V^3, V^3)$
- fourth-order tensors $\mathsf{\mathbf{A}}, \mathsf{\mathbf{B}}, \mathsf{\mathbf{C}}, \ldots \in \mathrm{Lin}(\mathrm{Lin}(V^3, V^3), \mathrm{Lin}(V^3, V^3))$

component form

- Cartesian basis vectors $(\boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3) = (\boldsymbol{i}_x, \boldsymbol{i}_y, \boldsymbol{i}_z)$
- arbitrary order $\mathcal{A} = \sum_{i,j,k,\ldots=1}^{3} A_{ijk\ldots} \boldsymbol{i}_i \otimes \boldsymbol{i}_j \otimes \boldsymbol{i}_k \cdots$

scalar product

- arbitrary order $\mathcal{A} \cdot \mathcal{B} = \sum_{i,j,k,\ldots=1}^{3} A_{ijk\ldots} B_{ijk\ldots}$

a little notation

partial derivative

$$\partial_a f(a,b,\ldots) \equiv \frac{\partial f}{\partial a}(a,b,\ldots)\bigg|_{b,\ldots} := \lim_{\epsilon\to 0} \frac{f(a+\epsilon,b,\ldots)-f(a,b,\ldots)}{\epsilon}$$

(total) time derivative

$$\dot{f}(t) := \lim_{\epsilon\to 0} \frac{f(t+\epsilon)-f(t)}{\epsilon}$$

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continuum mechanics & material behavior

some basic aspects

- kinematics (body, placement, configuration, motion, velocity, ...)
- balance relations (mass, momentum, energy, ...)
- constitutive relations / material theory
  - entropy / dissipation principle (second law)
  - frame-indifference (Euclidean & material)
  - material symmetry & constraints (solid, fluid, ..., incompressible, ...)
  - material heterogeneity (chemical, structural, ...)
  - ...
- environment / boundary conditions
- (variational) formulation of initial-boundary value problems & solution

basics: body, placement, configuration, deformation

kinematic space (classic spacetime): $E^3 \times \mathbb{R}$

material body: differentiable manifold M modeled on E^3

placement (chart)

$$\boldsymbol{\kappa}\colon M \longrightarrow E^3 \quad | \quad b \longmapsto \boldsymbol{x}_{\boldsymbol{\kappa}} = \boldsymbol{\kappa}(b)$$

configuration (chart image)

$$B_{\boldsymbol{\kappa}} = \boldsymbol{\kappa}[M] \subset E^3\,, \quad \boldsymbol{x}_{\boldsymbol{\kappa}} \in B_{\boldsymbol{\kappa}}$$

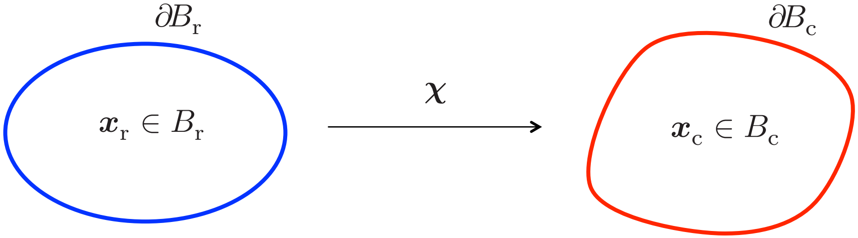
deformation (of $B_{\boldsymbol{\kappa}}$ into $B_{\boldsymbol{\gamma}}$)

$$\boldsymbol{\chi}_{\boldsymbol{\gamma}\boldsymbol{\kappa}}\colon B_{\boldsymbol{\kappa}} \longrightarrow B_{\boldsymbol{\gamma}} \quad | \quad \boldsymbol{x}_{\boldsymbol{\kappa}} \longmapsto \boldsymbol{x}_{\boldsymbol{\gamma}} = \boldsymbol{\gamma}(\boldsymbol{\kappa}^{-1}(\boldsymbol{x}_{\boldsymbol{\kappa}})) =: \boldsymbol{\chi}_{\boldsymbol{\gamma}\boldsymbol{\kappa}}(\boldsymbol{x}_{\boldsymbol{\kappa}})$$

motion

motion: time-dependent ($t \in \mathbb{R}$) sequence of deformations

$$\boldsymbol{\chi} \colon \mathbb{R} \times B_{\mathrm{r}} \longrightarrow E^3 \quad | \quad (t, \boldsymbol{x}_{\mathrm{r}}) \longmapsto \boldsymbol{x}_{\mathrm{c}} = \boldsymbol{\chi}_t(\boldsymbol{x}_{\mathrm{r}}) = \boldsymbol{\chi}(t, \boldsymbol{x}_{\mathrm{r}})$$



special configurations

- reference (e.g., undeformed, initial) $B_{\mathrm{r}} \subset E^3$
- current (deformed, time t) $B_{\mathrm{c}} = \boldsymbol{\chi}_t[B_{\mathrm{r}}] \subset E^3$

configurations & fields

two configurations B_r and B_c

$\Longrightarrow$ two representations of (time-dependent) physical fields $f(t, \boldsymbol{x})$

referential / material / Lagrangian: field on B_r

$$f_\mathrm{r}(t, \boldsymbol{x}_\mathrm{r})$$

current / spatial / Eulerian: field on B_c

$$f_\mathrm{c}(t, \boldsymbol{x}_\mathrm{c})$$

same physical quantity (e.g., temperature)

$$f_\mathrm{r}(t, \boldsymbol{x}_\mathrm{r}) = f_\mathrm{c}(t, \boldsymbol{x}_\mathrm{c}) = f_\mathrm{c}(t, \boldsymbol{\chi}(t, \boldsymbol{x}_\mathrm{r}))$$

abstract form (partial composition notation)

$$f_\mathrm{r} = f_\mathrm{c} \circ \boldsymbol{\chi}$$

derivatives of fields

partial derivatives (notation)

$$\partial_t f_{\mathrm{r}} \equiv \left.\frac{\partial f_{\mathrm{r}}}{\partial t}\right|_{\boldsymbol{x}_{\mathrm{r}}}, \quad \partial_t f_{\mathrm{c}} \equiv \left.\frac{\partial f_{\mathrm{c}}}{\partial t}\right|_{\boldsymbol{x}_{\mathrm{c}}}, \quad \nabla f_{\mathrm{r}} \equiv \left.\frac{\partial f_{\mathrm{r}}}{\partial \boldsymbol{x}_{\mathrm{r}}}\right|_t, \quad \nabla f_{\mathrm{c}} \equiv \left.\frac{\partial f_{\mathrm{c}}}{\partial \boldsymbol{x}_{\mathrm{c}}}\right|_t$$

material time derivative: with respect to / at fixed B_{r}

- Lagrangian / referential field

$$\dot{f}_{\mathrm{r}} \equiv \partial_t f_{\mathrm{r}}$$

- Eulerian / spatial field

$$\begin{aligned} \dot{f}_{\mathrm{c}} &:= \dot{\overline{f_{\mathrm{c}} \circ \boldsymbol{\chi}}} \circ \boldsymbol{\chi}^{-1} = \partial_t f_{\mathrm{c}} + \nabla f_{\mathrm{c}} \cdot \dot{\boldsymbol{\chi}} \circ \boldsymbol{\chi}^{-1} \\ &= \partial_t f_{\mathrm{c}} + \nabla f_{\mathrm{c}} \cdot \boldsymbol{v} \end{aligned}$$

- spatial velocity field

$$\boldsymbol{v} := \dot{\boldsymbol{\chi}} \circ \boldsymbol{\chi}^{-1} = \partial_t \boldsymbol{\chi} \circ \boldsymbol{\chi}^{-1}$$

deformation & velocity gradients

deformation gradient ("mixed" or "two-point" tensor field on B_{r})

$$\boldsymbol{F} := \nabla \boldsymbol{\chi}$$

velocity gradient ("Eulerian" tensor field on B_{c})

$$\boldsymbol{L} := \nabla \boldsymbol{v} \quad \text{or} \quad \boldsymbol{L} := \nabla \boldsymbol{v} \circ \boldsymbol{\chi}$$

connection (chain rule)

$$\dot{\boldsymbol{F}} = \dot{\overline{\nabla \boldsymbol{\chi}}} = \nabla \dot{\boldsymbol{\chi}} = \nabla(\boldsymbol{v} \circ \boldsymbol{\chi}) = (\nabla \boldsymbol{v} \circ \boldsymbol{\chi})\, \nabla \boldsymbol{\chi} = \boldsymbol{L}\boldsymbol{F}$$

Eulerian & Lagrangian densities, fluxes

area $d\boldsymbol{a} = d\boldsymbol{x} \times d\boldsymbol{y}$ & volume $dv = d\boldsymbol{x} \times d\boldsymbol{y} \cdot d\boldsymbol{z}$ elements

$$\begin{aligned} \boldsymbol{\chi}^* \, d\boldsymbol{a} &= \boldsymbol{F} d\boldsymbol{x} \times \boldsymbol{F} d\boldsymbol{y} &&= (\operatorname{cof} \boldsymbol{F}) \, d\boldsymbol{a} = (\det \boldsymbol{F}) \, \boldsymbol{F}^{-\mathrm{T}} \, d\boldsymbol{a} \\ \boldsymbol{\chi}^* dv &= \boldsymbol{F} d\boldsymbol{x} \times \boldsymbol{F} d\boldsymbol{y} \cdot \boldsymbol{F} d\boldsymbol{z} &&= (\det \boldsymbol{F}) \, dv \end{aligned}$$

relation between volume densities

$$\int_{B_\mathrm{r}} f_\mathrm{r} \, dv = \int_{B_\mathrm{c}} f_\mathrm{c} \, dv = \int_{B_\mathrm{r}} \boldsymbol{\chi}^*(f_\mathrm{c} \, dv)$$

$$\Longrightarrow \quad f_\mathrm{r} \, dv = \boldsymbol{\chi}^*(f_\mathrm{c} \, dv) \quad \Longrightarrow \quad f_\mathrm{r} = (\det \boldsymbol{F}) \, f_\mathrm{c} \circ \boldsymbol{\chi}$$

relation between surface densities (fluxes)

$$\int_{\partial B_\mathrm{r}} \boldsymbol{f}_\mathrm{r} \cdot d\boldsymbol{a} = \int_{\partial B_\mathrm{c}} \boldsymbol{f}_\mathrm{c} \cdot d\boldsymbol{a} = \int_{\partial B_\mathrm{r}} \boldsymbol{\chi}^*(\boldsymbol{f}_\mathrm{c} \cdot d\boldsymbol{a})$$

$$\Longrightarrow \quad \boldsymbol{f}_\mathrm{r} \cdot d\boldsymbol{a} = \boldsymbol{\chi}^*(\boldsymbol{f}_\mathrm{c} \cdot d\boldsymbol{a}) \quad \Longrightarrow \quad \boldsymbol{f}_\mathrm{r} = (\operatorname{cof} \boldsymbol{F})^\mathrm{T} \boldsymbol{f}_\mathrm{c} \circ \boldsymbol{\chi}$$

transport relations

extensive quantity with density f

$$\int_{B_\mathrm{r}} f_\mathrm{r}\, dv = \int_{B_\mathrm{c}} f_\mathrm{c}\, dv$$

Lagrangian rate of change (∂B_r fixed)

$$\overline{\int_{B_\mathrm{r}} f_\mathrm{r}\, dv}^{\cdot} = \int_{B_\mathrm{r}} \partial_t f_\mathrm{r}\, dv = \int_{B_\mathrm{r}} \dot{f}_\mathrm{r}\, dv$$

Eulerian rate of change ($\partial B_\mathrm{c} = \boldsymbol{\chi}_t[\partial B_\mathrm{r}]$ moving)

$$\overline{\int_{B_\mathrm{c}} f_\mathrm{c}\, dv}^{\cdot} = \int_{B_\mathrm{c}} \partial_t f_\mathrm{c}\, dv + \int_{\partial B_\mathrm{c}} f_\mathrm{c} \boldsymbol{v} \cdot \boldsymbol{n}\, da$$

Eulerian transport

divergence theorem

$$\int_{\partial B_{\mathrm{c}}} f_{\mathrm{c}} \boldsymbol{v} \cdot \boldsymbol{n} \; da = \int_{B_{\mathrm{c}}} \operatorname{div} f_{\mathrm{c}} \boldsymbol{v} \; dv$$

divergence form

$$\overline{\int_{B_{\mathrm{c}}} f_{\mathrm{c}} \; dv}^{\,\cdot} = \int_{B_{\mathrm{c}}} (\partial_t f_{\mathrm{c}} + \operatorname{div} f_{\mathrm{c}} \boldsymbol{v}) \; dv = \int_{B_{\mathrm{c}}} (\dot{f}_{\mathrm{c}} + f_{\mathrm{c}} \operatorname{div} \boldsymbol{v}) \; dv$$

pull-back form

$$\overline{\int_{B_{\mathrm{c}}} f_{\mathrm{c}} \; dv}^{\,\cdot} = \int_{B_{\mathrm{r}}} \overline{(f_{\mathrm{c}} \circ \boldsymbol{\chi}) \det \boldsymbol{F}}^{\,\cdot} \; dv = \int_{B_{\mathrm{c}}} (\dot{f}_{\mathrm{c}} + f_{\mathrm{c}} \operatorname{div} \boldsymbol{v}) \; dv$$

balance relation

for extensive quantity with density f

$$\overline{\int_B f \, dv}^{\,\cdot} = \underbrace{\int_B p \, dv}_{\text{production rate}} + \underbrace{\int_{\partial B} \boldsymbol{f} \cdot \boldsymbol{n} \, da}_{\text{flux rate}} + \underbrace{\int_B s \, dv}_{\text{supply rate}}$$

differential forms in terms of material time derivative

$$\begin{aligned} \dot{f}_{\mathrm{r}} &= p_{\mathrm{r}} + \operatorname{div} \boldsymbol{f}_{\mathrm{r}} + s_{\mathrm{r}} \\ \dot{f}_{\mathrm{c}} + f_{\mathrm{c}} \operatorname{div} \boldsymbol{v} &= p_{\mathrm{c}} + \operatorname{div} \boldsymbol{f}_{\mathrm{c}} + s_{\mathrm{c}} \end{aligned}$$

in terms of partial time derivatives

$$\begin{aligned} \partial_t f_{\mathrm{r}} &= p_{\mathrm{r}} + \operatorname{div} \boldsymbol{f}_{\mathrm{r}} + s_{\mathrm{r}} \\ \partial_t f_{\mathrm{c}} &= p_{\mathrm{c}} + \operatorname{div}(\boldsymbol{f}_{\mathrm{c}} - f_{\mathrm{c}} \boldsymbol{v}) + s_{\mathrm{c}} \end{aligned}$$

specfic balance relations

mass (no supply)

$$\dot{\varrho}_{\rm r} = m_{\rm r} - \operatorname{div} \boldsymbol{j}_{\rm r}\,, \quad \dot{\varrho}_{\rm c} + \varrho_{\rm c} \operatorname{div} \boldsymbol{v} = m_{\rm c} - \operatorname{div} \boldsymbol{j}_{\rm c}$$

linear momentum (no production)

$$\dot{\boldsymbol{m}}_{\rm r} = \operatorname{div} \boldsymbol{S}_{\rm r} + \boldsymbol{b}_{\rm r}\,, \quad \dot{\boldsymbol{m}}_{\rm c} + \boldsymbol{m}_{\rm c} \operatorname{div} \boldsymbol{v} = \operatorname{div} \boldsymbol{S}_{\rm c} + \boldsymbol{b}_{\rm c}$$

total energy (no production)

$$\dot{e}_{\rm r} = \operatorname{div} \boldsymbol{h}_{\rm r} + s_{\rm r}\,, \quad \dot{e}_{\rm c} + e_{\rm c} \operatorname{div} \boldsymbol{v} = \operatorname{div} \boldsymbol{h}_{\rm c} + s_{\rm c}$$

entropy

$$\dot{\eta}_{\rm r} = \pi_{\rm r} - \operatorname{div} \boldsymbol{\phi}_{\rm r} + \sigma_{\rm r}\,, \quad \dot{\eta}_{\rm c} + \eta_{\rm c} \operatorname{div} \boldsymbol{v} = \pi_{\rm c} - \operatorname{div} \boldsymbol{\phi}_{\rm c} + \sigma_{\rm c}$$

From now on: only "Lagrangian" ("r" subscript will be dropped)

a little material / constitutive theory

balance relations contain constitutive quantities: $\boldsymbol{j}, m, \boldsymbol{S}, \boldsymbol{h}, s, \boldsymbol{\phi}, \ldots$

momentum flux: first Piola-Kirchhoff stress, Cauchy stress

$$\boldsymbol{P} \equiv \boldsymbol{S}_{\mathrm{r}}\,, \quad \boldsymbol{T} \equiv \boldsymbol{S}_{\mathrm{c}}$$

example: constitutive model for stress, free energy density $\psi(\boldsymbol{F})$

$$\boldsymbol{P}(\boldsymbol{F}) = \partial_{\boldsymbol{F}}\psi(\boldsymbol{F})$$

material frame-indifference (observer independence)

$$\psi(\boldsymbol{F}) = \psi(\boldsymbol{Q}\boldsymbol{F}) \quad \forall \boldsymbol{Q} \in \mathrm{Orth}(V^3, V^3)$$

material symmetry (e.g., anisotropy)

$$\psi(\boldsymbol{F}) = \psi(\boldsymbol{F}\boldsymbol{Q}) \quad \forall \boldsymbol{Q} \in \mathcal{G} \subset \mathrm{Orth}(V^3, V^3)$$

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setting

kinematics & balance relations ✓

material class: materially inhomogeneous solids

selected applications of phase field modeling

- precipitate formation (phase separation) in multicomponent solids
- recrystallization in polycrystalline systems
- austenite $\rightarrow$ martensite transformation in metallic systems
- dislocation dissociation / core-solute interaction in metallic nanocrystals
- polarization domain microstructure formation in ferroelectrics
- magnetization domain microstrcture formation in ferromagnetics
- ...

today: simple ideal case

- two-component, two-phase solid mixture
- for simplicity: thermoelastic phases with heat and mass transfer
- for simplicity: no mass production, no supplies

mass balance for two-component mixture

component mass balance (no production)

$$\dot{\varrho}_1 = -\mathrm{div}\, \boldsymbol{j}_1 \,, \quad \dot{\varrho}_2 = -\mathrm{div}\, \boldsymbol{j}_2$$

mixture mass density

$$\rho = \varrho_1 + \varrho_2$$

for simplicity: assume mixture mass density constant

$$\dot{\rho} = 0 \quad \Longrightarrow \quad \dot{\varrho}_2 = -\dot{\varrho}_1$$

one independent component / mass balance relation

$$\varrho \equiv \varrho_1 \,, \quad \boldsymbol{j} \equiv \boldsymbol{j}_1 \quad \Longrightarrow \quad \dot{\varrho} = -\mathrm{div}\, \boldsymbol{j}$$

linear momentum & energy balance

linear momentum, total energy balance for mixture (no supplies)

$$\dot{\boldsymbol{m}} = \operatorname{div} \boldsymbol{P} \,, \quad \dot{e} = \operatorname{div} \boldsymbol{h}$$

densities (linear momentum, total energy, kinetic energy)

$$\boldsymbol{m} = \rho \, \dot{\boldsymbol{\chi}} \,, \quad e = k + \varepsilon \,, \quad k = \frac{\rho \, \dot{\boldsymbol{\chi}} \cdot \dot{\boldsymbol{\chi}}}{2} = \frac{\boldsymbol{m} \cdot \boldsymbol{m}}{2\rho}$$

total energy flux: mechanical + non-mechanical

$$\boldsymbol{h} = \boldsymbol{P}^{\mathrm{T}} \dot{\boldsymbol{\chi}} - \boldsymbol{e}$$

mixture internal energy balance

$$\dot{\varepsilon} = \boldsymbol{P} \cdot \nabla \dot{\boldsymbol{\chi}} - \operatorname{div} \boldsymbol{e}$$

entropy balance & generalized Gibbs

mixture entropy balance

$$\dot{\eta} = \pi - \operatorname{div} \boldsymbol{\phi}$$

(absolute) temperature, inverse temperature ("coldness")

$$\theta\,, \quad \vartheta = \theta^{-1}$$

generalized Gibbs relation

$$\begin{aligned} \dot{\eta} - \vartheta\,\dot{\varepsilon} &= \pi - \boldsymbol{e}\cdot\nabla\vartheta - \vartheta\boldsymbol{P}\cdot\nabla\dot{\boldsymbol{\chi}} - \operatorname{div}(\boldsymbol{\phi} - \vartheta\,\boldsymbol{e}) \\ &= -\dot{\check{\psi}} + \varepsilon\,\dot{\vartheta} \end{aligned}$$

(negative) free entropy density, free energy density

$$\check{\psi} := \vartheta\,\varepsilon - \eta = \vartheta\,\psi\,, \quad \psi := \varepsilon - \theta\,\eta$$

internal energy flux & entropy flux

notation (energetic $\rightarrow$ entropic)

$$\check{f} := \vartheta\, f = \theta^{-1} f$$

for heat & mass transport

- entropy flux: purely thermal (Clausius-Duhem)
  e.g. Eckart (1940), Truesdell and Noll (1965), Gurtin and Vargas (1971), Šilhavý (1997)

$$\boldsymbol{\phi} = \check{\boldsymbol{q}}\,, \quad \boldsymbol{e} = \boldsymbol{q} + \mu\, \boldsymbol{j}$$

- (energetic) chemical potential μ
- internal energy flux: purely thermal
  e.g. Meixner and Reik (1959), de Groot and Mazur (1962), Müller (1968)

$$\boldsymbol{e} = \boldsymbol{q}\,, \quad \boldsymbol{\phi} = \check{\boldsymbol{q}} - \check{\mu}\, \boldsymbol{j}$$

- (entropic) chemical potential $\check{\mu} = \vartheta\, \mu$

entropy production rate & dissipation rate

entropy production-rate density

$$\pi = \check{\boldsymbol{P}} \cdot \nabla \dot{\boldsymbol{\chi}} + \check{\mu}\, \dot{\varrho} + \varepsilon\, \dot{\vartheta} - \dot{\check{\psi}} + \boldsymbol{q} \cdot \nabla \vartheta - \boldsymbol{j} \cdot \nabla \check{\mu}$$

entropy principle: non-negative entropy production-rate (density)

$$\pi \geqslant 0$$

in terms of dissipation-rate density

$$\delta = \theta\, \pi = \boldsymbol{P} \cdot \nabla \dot{\boldsymbol{\chi}} + \mu\, \dot{\varrho} - \eta\, \dot{\theta} - \dot{\psi} - \boldsymbol{\phi} \cdot \nabla \theta - \boldsymbol{j} \cdot \nabla \mu$$

dissipation principle: non-negative dissipation-rate (density)

$$\theta \geqslant 0\,, \quad \pi \geqslant 0 \quad \Longrightarrow \quad \delta = \theta\, \pi \geqslant 0$$

a brief aside: Müller-Liu entropy principle

entropy principle with balance relations as constraints

e.g. Liu (1972), Müller (1985), Muschik et al. (2001)

$$\begin{aligned} \pi &= \dot{\eta} + \operatorname{div} \boldsymbol{\phi} \\ &- \lambda^{\varrho}(\dot{\varrho} + \operatorname{div} \boldsymbol{j}) \\ &- \boldsymbol{\lambda}^{\boldsymbol{m}} \cdot (\dot{\boldsymbol{m}} - \operatorname{div} \boldsymbol{P}) \\ &- \lambda^{e}(\dot{e} - \operatorname{div} \boldsymbol{P}^{\mathrm{T}} \dot{\boldsymbol{\chi}} + \operatorname{div} \boldsymbol{q}) \geqslant 0 \end{aligned}$$

Lagrange multipliers

$$\lambda^{\varrho}, \quad \boldsymbol{\lambda}^{\boldsymbol{m}}, \quad \lambda^{e}$$

not today!

model class: isothermal phase field

a (very) few landmarks

- van der Waals (1893): non-uniform density (see Rowlison, 1979)
- Landau (1937): order parameter PT (see Provatas and Elder, 2010)
- Cahn and Hilliard (1958): conservative (mass)
- Allen and Cahn (1979): non-conservative (structural)
- Khachaturyan (1983): defective solid mechanics (structural)
- Elder and Grant (2004): phase field crystal

models for materially inhomogeneous free energy (density)

weakly non-local (e.g., Cahn and Hilliard, 1958)

$$\psi(\ldots,\boldsymbol{x}) \equiv \psi(\ldots,\varrho(\boldsymbol{x}),\phi(\boldsymbol{x}),\nabla\varrho(\boldsymbol{x}),\nabla\phi(\boldsymbol{x}),\nabla\nabla\varrho(\boldsymbol{x}),\nabla\nabla\phi(\boldsymbol{x}),\ldots)$$

more general: strongly non-local

$$\psi(\ldots,\boldsymbol{x}) = \int w(\boldsymbol{x}-\boldsymbol{x}')\,\varphi(\ldots,\varrho(\boldsymbol{x}),\phi(\boldsymbol{x}),\varrho(\boldsymbol{x}'),\phi(\boldsymbol{x}'))\,dv(\boldsymbol{x}')$$

isothermal formulation of Cahn and Hilliard (1958)

isothermal, purely chemical case

$$\psi(\varrho, \nabla\varrho, \nabla\nabla\varrho, \ldots)$$

expand ψ about the "homogeneous" state

$$(\varrho, \nabla\varrho, \nabla\nabla\varrho, \ldots)|_{\mathrm{H}} = (\varrho, \mathbf{0}, \mathbf{0}, \ldots)$$

expansion up to second order

$$\begin{aligned} \psi &= \psi|_{\mathrm{H}} + \partial_{\nabla\varrho}\psi|_{\mathrm{H}} \cdot \nabla\varrho + \partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}} \cdot \nabla\nabla\varrho + \cdots \\ &+ \tfrac{1}{2}\,\nabla\varrho \cdot \partial_{\nabla\varrho}\partial_{\nabla\varrho}\psi|_{\mathrm{H}}\nabla\varrho + \cdots \end{aligned}$$

reduce order: partial integration, divergence theorem

$$\int_B \partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}} \cdot \nabla\nabla\varrho\, dv = \int_{\partial B} \partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}}\, \boldsymbol{n} \cdot \nabla\varrho\, da - \int_B \operatorname{div} \partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}} \cdot \nabla\varrho\, dv$$

isothermal formulation of Cahn and Hilliard (1958)

no-flux boundary conditions

$$\partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}}\,\boldsymbol{n}|_{\partial B} = \mathbf{0} \quad \Longrightarrow \quad \partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}} \cdot \nabla\nabla\varrho \equiv -\operatorname{div}\partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}} \cdot \nabla\varrho$$

dependence of $\partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}}$ on ϱ

$$\operatorname{div}\partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}} \cdot \nabla\varrho = \nabla\varrho \cdot (\partial_\varrho \partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}})\nabla\varrho$$

reduced free energy model

$$\psi(\varrho, \nabla\varrho) = \psi|_{\mathrm{H}}(\varrho) + \partial_{\nabla\varrho}\psi|_{\mathrm{H}}(\varrho) \cdot \nabla\varrho + \tfrac{1}{2}\,\nabla\varrho \cdot \boldsymbol{\Lambda}_{\mathrm{H}}(\varrho)\nabla\varrho$$

second-order coefficient

$$\boldsymbol{\Lambda}_{\mathrm{H}} = \partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}} - 2\,\partial_\varrho \partial_{\nabla\nabla\varrho}\psi|_{\mathrm{H}}$$

generalization: deformation & material inhomogeneity

free energy density

$$\psi(\nabla\boldsymbol{\chi}, \varrho, \nabla\varrho, \phi, \nabla\phi)$$

elastic phases

$$\boldsymbol{P} = \partial_{\nabla\boldsymbol{\chi}}\psi$$

inhomogeneous (local) dissipation rate density

$$\delta \;=\; (\mu - \partial_\varrho\psi)\,\dot{\varrho} - \partial_{\nabla\varrho}\psi\cdot\nabla\dot{\varrho} - \partial_\phi\psi\,\dot{\phi} - \partial_{\nabla\phi}\psi\cdot\nabla\dot{\phi} - \boldsymbol{j}\cdot\nabla\mu$$

dissipation rate form

$$\begin{aligned}\int_B \delta\,dv \;&=\; \int_B (\mu - \delta_\varrho\psi)\,\dot{\varrho}\,dv - \int_B (\boldsymbol{j}\cdot\nabla\mu + \delta_\phi\psi\,\dot{\phi})\,dv \\ &-\; \int_{\partial B} (\partial_{\nabla\varrho}\psi\cdot\boldsymbol{n}\,\dot{\varrho} + \partial_{\nabla\phi}\psi\cdot\boldsymbol{n}\,\dot{\phi})\,da\end{aligned}$$

chemical potential & boundary conditions

inhomogeneous chemical potential

$$\mu = \delta_\varrho \psi$$

variational derivative

$$\delta_x a := \partial_x a - \operatorname{div} \partial_{\nabla x} a$$

boundary conditions

$$\partial_{\nabla \varrho} \psi \cdot \boldsymbol{n} \; \dot{\varrho} \, |_{\partial B} = 0 \, , \quad \partial_{\nabla \phi} \psi \cdot \boldsymbol{n} \; \dot{\phi} \, |_{\partial B} = 0$$

"residual" dissipation-rate density

$$\delta = -\boldsymbol{j} \cdot \nabla \mu - \dot{\phi} \, \delta_\phi \psi$$

kinetics

thermodynamic fluxes & forces

$$\mathbf{j} := (-\boldsymbol{j}, -\dot{\phi})\,, \quad \mathbf{f} := (\nabla\mu, \delta_\phi \psi)$$

quasi-linear flux-force relation

$$\mathbf{j} = \mathbf{L}(\ldots, \mathbf{f})\mathbf{f}$$

dissipation principle

$$\delta = \mathbf{j} \cdot \mathbf{f} = \mathbf{f} \cdot \mathbf{L}\mathbf{f} \geqslant 0 \quad \Longleftarrow \quad \mathbf{D} = \operatorname{sym} \mathbf{L} \geqslant 0 \;\; \text{(non-negative definite)}$$

simplest case: "diagonal" flux-force relations (no coupling)

$$\boldsymbol{j} = -\boldsymbol{D}(\ldots)\,\nabla\mu\,, \quad \dot{\phi} = -m(\ldots)\,\delta_\phi\psi$$

dissipation-rate density

$$\delta = \nabla\mu \cdot \boldsymbol{D}\,\nabla\mu + \delta_\phi\psi\; m\,\delta_\phi\psi \geqslant 0 \quad \Longleftarrow \quad \boldsymbol{D}^{\mathrm{T}} = \boldsymbol{D}\,, \quad \boldsymbol{D} \geqslant 0\,, \quad m \geqslant 0$$

the case of a dissipation potential

potential-based flux-force relations

$$\boldsymbol{j} = -\partial_{\nabla\mu} d\,, \quad \dot{\phi} = -\partial_{\delta_\phi \psi}\, d$$

dissipation potential

$$d(\ldots, \nabla\mu, \delta_\phi \psi)$$

dissipation-rate density

$$\delta \;=\; \nabla\mu \cdot \partial_{\nabla\mu} d + \delta_\phi \psi \; \partial_{\delta_\phi \psi}\, d$$

d non-negative, convex in forces (sufficient for $\delta \geqslant 0$)

$$\nabla\mu \cdot \partial_{\nabla\mu} d + \delta_\phi \psi \; \partial_{\delta_\phi \psi}\, d \geqslant d \geqslant 0$$

treatment in the GENERIC framework: Hütter and Svendsen (2013)

summary of isothermal model relations

Cahn-Hilliard mass balance

$$\mu = \delta_\varrho \psi = \partial_\varrho \psi - \operatorname{div} \partial_{\nabla\varrho} \psi \,, \quad \partial_{\nabla\varrho} \psi \cdot \boldsymbol{n} \; \dot{\varrho} \,|_{\partial B} = 0$$

$$\dot{\varrho} = -\operatorname{div} \boldsymbol{j} = \operatorname{div} \boldsymbol{D} \nabla \mu \,, \quad \boldsymbol{j}|_{\partial B} \cdot \boldsymbol{n} = 0$$

reduced momentum balance

$$\varrho \, \ddot{\boldsymbol{\chi}} = \dot{\boldsymbol{m}} = \operatorname{div} \boldsymbol{P} = \operatorname{div} \partial_{\nabla \boldsymbol{\chi}} \psi$$

time-dependent Ginzburg-Landau, Allen-Cahn phase field

$$\dot{\phi} = -m \, \delta_\phi \psi = m \left(\operatorname{div} \partial_{\nabla \phi} \psi - \partial_\phi \psi \right) , \quad \partial_{\nabla \phi} \psi \cdot \boldsymbol{n} \; \dot{\phi} \,|_{\partial B} = 0$$

model class: non-isothermal phase field

free entropy density

$$\check{\psi}(\vartheta, \nabla\boldsymbol{\chi}, \varrho, \nabla\varrho, \phi, \nabla\phi)$$

thermoelastic internal energy & entropy

$$\varepsilon = \partial_\vartheta \check{\psi} \quad \Longrightarrow \quad \eta = \check{\psi} - \vartheta\, \partial_\vartheta \check{\psi}$$

thermoelastic stress, chemical potential

$$\boldsymbol{P} = \theta\, \partial_{\nabla\boldsymbol{\chi}} \check{\psi}\,, \quad \mu = \theta\, \delta_\varrho \check{\psi}$$

boundary conditions

$$\partial_{\nabla\varrho} \check{\psi} \cdot \boldsymbol{n}\ \dot{\varrho}\,|_{\partial B} = 0\,, \quad \partial_{\nabla\phi} \check{\psi} \cdot \boldsymbol{n}\ \dot{\phi}\,|_{\partial B} = 0$$

"residual" entropy production rate density

$$\pi = \boldsymbol{q} \cdot \nabla\vartheta - \boldsymbol{j} \cdot \nabla\check{\mu} - \dot{\phi}\, \delta_\phi \check{\psi}$$

non-isothermal kinetics

for simplicity: "diagonal" flux-force relations

$$\boldsymbol{q} = \theta^2 \boldsymbol{K}(\ldots)\, \nabla\vartheta\,, \quad \boldsymbol{j} = -\theta \boldsymbol{D}(\ldots)\, \nabla\check{\mu}\,, \quad \dot{\phi} = -\theta\, m(\ldots)\, \delta_\phi \check{\psi}$$

entropy production-rate density

$$\pi \;=\; \nabla\vartheta \cdot \theta^2 \boldsymbol{K}\, \nabla\vartheta + \nabla\check{\mu} \cdot \theta \boldsymbol{D}\, \nabla\check{\mu} + \delta_\phi \check{\psi}\, \theta\, m\, \delta_\phi \check{\psi}$$

dissipation-rate density

$$\delta \;=\; \nabla\vartheta \cdot \theta \boldsymbol{K}\, \nabla\vartheta + \nabla\check{\mu} \cdot \boldsymbol{D}\, \nabla\check{\mu} + \delta_\phi \check{\psi}\, m\, \delta_\phi \check{\psi}$$

summary of non-isothermal model relations

Cahn-Hilliard mass balance

$$\begin{aligned} \check{\mu} &= \delta_\varrho \check{\psi} &&= \partial_\varrho \check{\psi} - \operatorname{div} \partial_{\nabla\varrho} \check{\psi} \,, \quad && \partial_{\nabla\varrho} \check{\psi} \cdot \boldsymbol{n} \; \dot{\varrho} \,|_{\partial B} = 0 \\ \dot{\varrho} &= -\operatorname{div} \boldsymbol{j} &&= \operatorname{div} \theta \boldsymbol{D} \nabla \check{\mu} \,, && \boldsymbol{j}|_{\partial B} \cdot \boldsymbol{n} = 0 \end{aligned}$$

reduced momentum balance

$$\varrho \, \ddot{\boldsymbol{\chi}} = \dot{\boldsymbol{m}} = \operatorname{div} \boldsymbol{P} = \operatorname{div} \theta \, \partial_{\nabla \boldsymbol{\chi}} \check{\psi}$$

time-dependent Ginzburg-Landau (TDGL), Allen-Cahn phase field

$$\dot{\phi} = -\theta \, m \, \delta_\phi \check{\psi} = m \, (\operatorname{div} \partial_{\nabla\phi} \check{\psi} - \partial_\phi \check{\psi}) \,, \quad \vartheta \, \partial_{\nabla\phi} \check{\psi} \cdot \boldsymbol{n} \; \dot{\phi} \,|_{\partial B} = 0$$

temperature relation (sketch)

from energy balance & free entropy

$$\dot{\varepsilon} = \boldsymbol{P} \cdot \nabla \dot{\boldsymbol{\chi}} - \operatorname{div} \boldsymbol{q} \,, \quad \varepsilon = \partial_\vartheta \check{\psi}$$

time derivative

$$\dot{\varepsilon} \;=\; \partial_\vartheta \varepsilon \, \dot{\vartheta} + \partial_{\nabla \boldsymbol{\chi}} \varepsilon \cdot \nabla \dot{\boldsymbol{\chi}} + \partial_\varrho \varepsilon \, \dot{\varrho} + \partial_{\nabla \varrho} \varepsilon \cdot \nabla \dot{\varrho} + \partial_\phi \varepsilon \, \dot{\phi} + \partial_{\nabla \phi} \varepsilon \cdot \nabla \dot{\phi}$$

from entropy balance & free entropy

$$\dot{\eta} = \pi - \operatorname{div} \boldsymbol{\phi} \,, \quad \eta = \check{\psi} - \vartheta \, \partial_\vartheta \check{\psi}$$

time derivative

$$\dot{\eta} \;=\; \partial_\vartheta \eta \, \dot{\vartheta} + \partial_{\nabla \boldsymbol{\chi}} \eta \cdot \nabla \dot{\boldsymbol{\chi}} + \partial_\varrho \eta \, \dot{\varrho} + \partial_{\nabla \varrho} \eta \cdot \nabla \dot{\varrho} + \partial_\phi \eta \, \dot{\phi} + \partial_{\nabla \phi} \eta \cdot \nabla \dot{\phi}$$

outline

- introduction & preliminaries
- Eulerian fluids? Lagrangian solids? Continuum mechanics!
- "standard" non-equilibrium thermodynamics for solids
- GENERIC for solids

GENERIC: brief review

General Equation for Non-Equilibrium Reversible-Irreversible Coupling

$$\dot{x} = \mathcal{L}\,\mathcal{D}_x E + \mathcal{M}\,\mathcal{D}_x S$$

- energy E, entropy S: functionals $A[x]$ of x
- $\mathcal{D}_x A$ functional derivative ("gradient") of A
- skew-symmetric Poisson operator $\mathcal{L}$
- symmetric, non-negative definite friction operator $\mathcal{M}$

inner product, transpose of operator $\mathcal{O}$

$$\langle \mathcal{D}_x B, \mathcal{O}^{\mathrm{T}} \mathcal{D}_x A \rangle := \langle \mathcal{D}_x A, \mathcal{O}\,\mathcal{D}_x B \rangle$$

skew-symmetry of $\mathcal{L}$

$$\langle \mathcal{D}_x A, \mathcal{L}^{\mathrm{T}} \mathcal{D}_x B \rangle = -\langle \mathcal{D}_x A, \mathcal{L}\,\mathcal{D}_x B \rangle$$

symmetry, non-negative definiteness of $\mathcal{M}$

$$\langle \mathcal{D}_x A, \mathcal{M}^{\mathrm{T}} \mathcal{D}_x B \rangle = \langle \mathcal{D}_x A, \mathcal{M}\,\mathcal{D}_x B \rangle\,, \quad \langle \mathcal{D}_x A, \mathcal{M}\,\mathcal{D}_x A \rangle \geqslant 0$$

brackets & identities

Poisson & dissipation brackets

$$\{A, B\} := \langle \mathcal{D}_x A, \mathcal{L}\, \mathcal{D}_x B \rangle\,, \quad [A, B] := \langle \mathcal{D}_x A, \mathcal{M}\, \mathcal{D}_x B \rangle$$

bracket symmetry

$$\mathcal{L}^{\mathrm{T}} = -\mathcal{L} \implies \{B, A\} = -\{A, B\}$$
$$\mathcal{M}^{\mathrm{T}} = \mathcal{M} \implies [B, A] = [A, B]$$
$$\mathcal{M} \text{ NND} \implies [A, A] \geqslant 0$$

Jacobi identity

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$$

functional evolution & orthogonality

functional evolution

$$\dot{A} = \langle \mathcal{D}_x A, \dot{\boldsymbol{x}} \rangle = \langle \mathcal{D}_x A, \mathcal{L}\, \mathcal{D}_{\boldsymbol{x}} E \rangle + \langle \mathcal{D}_x A, \mathcal{M}\, \mathcal{D}_{\boldsymbol{x}} S \rangle = \{A, E\} + [A, S]$$

orthogonality

$$\mathcal{L}\, \mathcal{D}_{\boldsymbol{x}} S = 0\,, \quad \mathcal{M}\, \mathcal{D}_{\boldsymbol{x}} E = 0$$

energy conservation

$$\dot{E} = \{E, E\} = 0$$

non-negative entropy production

$$\dot{S} = [S, S] \geqslant 0$$

functionals & gradient for phase field models

volume density representation of functionals

$$A[\boldsymbol{x}] = \int_B a(\boldsymbol{x}, \nabla \boldsymbol{x})\, dv$$

variation

$$\begin{aligned} \delta A &= \int_B (\partial_{\boldsymbol{x}} a \cdot \delta \boldsymbol{x} + \partial_{\nabla \boldsymbol{x}} a \cdot \delta \nabla \boldsymbol{x})\, dv \\ &= \int_B \delta_{\boldsymbol{x}} a \cdot \delta \boldsymbol{x}\, dv + \int_{\partial B} (\partial_{\nabla \boldsymbol{x}} a) \boldsymbol{n} \cdot \delta \boldsymbol{x}\, da \end{aligned}$$

(bulk & boundary) functional derivative

$$\mathcal{D}_{\boldsymbol{x}} A|_B \equiv \delta_{\boldsymbol{x}} a = \partial_{\boldsymbol{x}} a - \operatorname{div} \partial_{\nabla \boldsymbol{x}} a\,, \quad \mathcal{D}_{\boldsymbol{x}} A|_{\partial B} \equiv (\partial_{\nabla \boldsymbol{x}} a)|_{\partial B} \boldsymbol{n}$$

no-flux boundary conditions (energy, entropy)

$$\mathcal{D}_{\boldsymbol{x}} A|_{\partial B} = (\partial_{\nabla \boldsymbol{x}} a)|_{\partial B} \boldsymbol{n} = 0$$

choice of GENERIC variables

GENERIC variables

$$\boldsymbol{x} = (\boldsymbol{\chi}, \boldsymbol{m}, \theta, \varrho, \phi)\,, \quad \boldsymbol{m} = \rho\,\dot{\boldsymbol{\chi}}$$

total energy and entropy

$$E[\boldsymbol{x}] \;=\; \int_B e(\nabla\boldsymbol{\chi}, \boldsymbol{m}, \theta, \varrho, \nabla\varrho, \phi, \nabla\phi)\; dv$$

$$S[\boldsymbol{x}] \;=\; \int_B \eta(\nabla\boldsymbol{\chi}, \theta, \varrho, \nabla\varrho, \phi, \nabla\phi)\; dv$$

total energy density

$$e(\nabla\boldsymbol{\chi}, \boldsymbol{m}, \theta, \varrho, \nabla\varrho, \phi, \nabla\phi) = \frac{1}{2\rho}\,\boldsymbol{m}\cdot\boldsymbol{m} + \varepsilon(\nabla\boldsymbol{\chi}, \theta, \varrho, \nabla\varrho, \phi, \nabla\phi)$$

gradients

driving "forces" / gradients

$$\mathcal{D}_{\boldsymbol{x}} E = \begin{bmatrix} \mathcal{D}_{\boldsymbol{\chi}} E \\ \mathcal{D}_{\boldsymbol{m}} E \\ \mathcal{D}_{\theta} E \\ \mathcal{D}_{\varrho} E \\ \mathcal{D}_{\phi} E \end{bmatrix} = \begin{bmatrix} \delta_{\boldsymbol{\chi}} e \\ \delta_{\boldsymbol{m}} e \\ \delta_{\theta} e \\ \delta_{\varrho} e \\ \delta_{\phi} e \end{bmatrix}, \quad \mathcal{D}_{\boldsymbol{x}} S = \begin{bmatrix} \mathcal{D}_{\boldsymbol{\chi}} S \\ \mathcal{D}_{\boldsymbol{m}} S \\ \mathcal{D}_{\theta} S \\ \mathcal{D}_{\varrho} S \\ \mathcal{D}_{\phi} S \end{bmatrix} = \begin{bmatrix} \delta_{\boldsymbol{\chi}} \eta \\ \delta_{\boldsymbol{m}} \eta \\ \delta_{\theta} \eta \\ \delta_{\varrho} \eta \\ \delta_{\phi} \eta \end{bmatrix}$$

particular energy gradient "components"

$$\delta_{\boldsymbol{\chi}} e = \delta_{\boldsymbol{\chi}} \varepsilon \,, \quad \delta_{\boldsymbol{m}} e = \frac{\boldsymbol{m}}{\rho} = \dot{\boldsymbol{\chi}} \,, \quad \delta_{\theta} e = \partial_{\theta} \varepsilon = c$$

particular entropy gradient "components", temperature

$$\delta_{\boldsymbol{m}} \eta = \boldsymbol{0} \,, \quad \delta_{\theta} \eta = \partial_{\theta} \eta \,, \quad \theta = \frac{\partial_{\theta} \varepsilon}{\partial_{\theta} \eta}$$

reversible part

GENERIC variable evolution

- momentum evolution reversible (stress thermoelastic)
- temperature evolution reversible & irreversible
- mass evolution irreversible (flux diffusive)
- order parameter evolution irreversible (relaxation)

reversible-irreversible split

$$\boldsymbol{x}_{\text{rev}} = (\boldsymbol{\chi}, \boldsymbol{m}, \theta_{\text{rev}}, 0, 0)\,, \quad \boldsymbol{x}_{\text{irr}} = (\mathbf{0}, \mathbf{0}, \theta_{\text{irr}}, \varrho, \phi)$$

reversible part $\dot{\boldsymbol{x}}_{\text{rev}} = \mathcal{L}\,\mathcal{D}_{\boldsymbol{x}} E$

$$\begin{bmatrix} \dot{\boldsymbol{\chi}} \\ \dot{\boldsymbol{m}} \\ \dot{\theta}_{\text{rev}} \end{bmatrix} = \begin{bmatrix} 0 & L_{\boldsymbol{\chi}\boldsymbol{m}} & L_{\boldsymbol{\chi}\theta} \\ L_{\boldsymbol{m}\boldsymbol{\chi}} & 0 & L_{\boldsymbol{m}\theta} \\ L_{\theta\boldsymbol{\chi}} & L_{\theta\boldsymbol{m}} & 0 \end{bmatrix} \begin{bmatrix} \delta_{\boldsymbol{\chi}} e \\ \delta_{\boldsymbol{m}} e \\ \delta_{\theta} e \end{bmatrix} = \begin{bmatrix} L_{\boldsymbol{\chi}\boldsymbol{m}}\,\delta_{\boldsymbol{m}} e + L_{\boldsymbol{\chi}\theta}\,\delta_{\theta} e \\ L_{\boldsymbol{m}\boldsymbol{\chi}}\,\delta_{\boldsymbol{\chi}} e + L_{\boldsymbol{m}\theta}\,\delta_{\theta} e \\ L_{\theta\boldsymbol{\chi}}\,\delta_{\boldsymbol{\chi}} e + L_{\theta\boldsymbol{m}}\,\delta_{\boldsymbol{m}} e \end{bmatrix}$$

consequences of orthogonality

orthogonality $\mathcal{L}\,\mathcal{D}_{\boldsymbol{x}}S = \mathbf{0}$

$$
\begin{aligned}
L_{\boldsymbol{\chi m}}\,\delta_{\boldsymbol{m}}\eta \;+\; L_{\boldsymbol{\chi}\theta}\,\delta_{\theta}\eta &= \mathbf{0} \;\overset{\delta_{\boldsymbol{m}}\eta=\mathbf{0},\;\delta_\theta\eta\neq 0}{\Longrightarrow}\; L_{\boldsymbol{\chi}\theta} = \mathbf{0}\\
L_{\boldsymbol{m}\theta}\,\delta_{\theta}\eta \;+\; L_{\boldsymbol{m\chi}}\,\delta_{\boldsymbol{\chi}}\eta &= \mathbf{0} \;\Longrightarrow\; L_{\boldsymbol{m}\theta} = -L_{\boldsymbol{m\chi}}\delta_{\boldsymbol{\chi}}\eta\,\frac{1}{\partial_\theta\eta}\\
L_{\theta\boldsymbol{\chi}}\,\delta_{\boldsymbol{\chi}}\eta \;+\; L_{\theta\boldsymbol{m}}\,\delta_{\boldsymbol{m}}\eta &= 0 \;\overset{\delta_{\boldsymbol{m}}\eta=\mathbf{0},\;\delta_{\boldsymbol{\chi}}\eta\neq\mathbf{0}}{\Longrightarrow}\; L_{\theta\boldsymbol{\chi}} = \mathbf{0}
\end{aligned}
$$

reduced evolution relations ($L_{\boldsymbol{\chi}\theta} = \mathbf{0}$, $L_{\theta\boldsymbol{\chi}} = \mathbf{0}$, $\delta_{\boldsymbol{m}}e = \dot{\boldsymbol{\chi}}$, $\partial_\theta\varepsilon = \theta\,\partial_\theta\eta$)

$$
\begin{aligned}
\dot{\boldsymbol{\chi}} &= L_{\boldsymbol{\chi m}}\,\delta_{\boldsymbol{m}}e + L_{\boldsymbol{\chi}\theta}\,\delta_\theta e = L_{\boldsymbol{\chi m}}\,\dot{\boldsymbol{\chi}}\\
\dot{\boldsymbol{m}} &= L_{\boldsymbol{m\chi}}\,\delta_{\boldsymbol{\chi}}\varepsilon + L_{\boldsymbol{m}\theta}\,\partial_\theta\varepsilon = L_{\boldsymbol{m\chi}}\,\delta_{\boldsymbol{\chi}}(\varepsilon - \theta\,\eta)\\
\dot{\theta}_{\mathrm{rev}} &= L_{\theta\boldsymbol{\chi}}\,\delta_{\boldsymbol{\chi}}e + L_{\theta\boldsymbol{m}}\,\delta_{\boldsymbol{m}}e = L_{\theta\boldsymbol{m}}\,\dot{\boldsymbol{\chi}}
\end{aligned}
$$

Poisson operator components

operator component

$$\dot{\boldsymbol{\chi}} = L_{\boldsymbol{\chi}\boldsymbol{m}}\,\dot{\boldsymbol{\chi}} \quad \Longrightarrow \quad L_{\boldsymbol{\chi}\boldsymbol{m}} = \boldsymbol{I}$$

skew-symmetry

$$\langle \mathcal{D}_{\boldsymbol{m}} A, L_{\boldsymbol{m}\boldsymbol{\chi}}\,\mathcal{D}_{\boldsymbol{\chi}} B\rangle = -\langle \mathcal{D}_{\boldsymbol{\chi}} B, L_{\boldsymbol{\chi}\boldsymbol{m}}\,\mathcal{D}_{\boldsymbol{m}} A\rangle \quad \Longrightarrow \quad L_{\boldsymbol{m}\boldsymbol{\chi}} = -\boldsymbol{I}$$

orthogonality, skew-symmetry

$$L_{\boldsymbol{m}\theta} = -L_{\boldsymbol{m}\boldsymbol{\chi}}\delta_{\boldsymbol{\chi}}\eta\,\frac{1}{\partial_\theta \eta} = -\operatorname{div}\partial_{\nabla\boldsymbol{\chi}}\eta\,\frac{1}{\partial_\theta\eta}$$

$$\Longrightarrow \quad \begin{aligned} \langle \mathcal{D}_\theta A, L_{\theta\boldsymbol{m}}\,\mathcal{D}_{\boldsymbol{m}} B\rangle &= -\langle \mathcal{D}_{\boldsymbol{m}} B, L_{\boldsymbol{m}\theta}\,\mathcal{D}_\theta A\rangle \\ &= \int_B dv\,\mathcal{D}_{\boldsymbol{m}} B\cdot\operatorname{div}\partial_{\nabla\boldsymbol{\chi}}\eta\,\frac{\mathcal{D}_\theta A}{\partial_\theta\eta} \end{aligned}$$

Poisson operator components

integration by parts

$$\int_B dv\, \mathcal{D}_{\boldsymbol{m}} B \cdot \operatorname{div} \partial_{\nabla \boldsymbol{\chi}} \eta \, \frac{1}{\partial_\theta \eta} \, \mathcal{D}_\theta A$$
$$= \int_{\partial B} da\, \mathcal{D}_\theta A \, \frac{1}{\partial_\theta \eta} \, (\partial_{\nabla \boldsymbol{\chi}} \eta) \boldsymbol{n} \cdot \mathcal{D}_{\boldsymbol{m}} B - \int_B dv\, \mathcal{D}_\theta A \, \frac{1}{\partial_\theta \eta} \, \partial_{\nabla \boldsymbol{\chi}} \eta \cdot \nabla \mathcal{D}_{\boldsymbol{m}} B$$

boundary condition $(\partial_{\nabla \boldsymbol{\chi}} \eta) \, \boldsymbol{n}|_{\partial B} = \mathbf{0}$

$$\langle \mathcal{D}_\theta A, L_{\theta \boldsymbol{m}} \, \mathcal{D}_{\boldsymbol{m}} B \rangle = - \int_B dv\, \mathcal{D}_\theta A \, \frac{1}{\partial_\theta \eta} \, \partial_{\nabla \boldsymbol{\chi}} \eta \cdot \nabla \mathcal{D}_{\boldsymbol{m}} B$$

Poisson operator component

$$L_{\theta \boldsymbol{m}} = - \frac{1}{\partial_\theta \eta} \, \partial_{\nabla \boldsymbol{\chi}} \eta \cdot \nabla$$

summary: reversible part

reversible part

$$\begin{bmatrix} \dot{\boldsymbol{\chi}} \\ \dot{\boldsymbol{m}} \\ \dot{\theta}_{\mathrm{rev}} \end{bmatrix} = \begin{bmatrix} 0 & \boldsymbol{I} & 0 \\ -\boldsymbol{I} & 0 & -\operatorname{div}\partial_{\nabla\boldsymbol{\chi}}\eta\,\dfrac{1}{\partial_\theta\eta} \\ 0 & -\dfrac{1}{\partial_\theta\eta}\,\partial_{\nabla\boldsymbol{\chi}}\eta\cdot\nabla & 0 \end{bmatrix} \begin{bmatrix} \delta_{\boldsymbol{\chi}} e \\ \delta_{\boldsymbol{m}} e \\ \delta_\theta e \end{bmatrix}$$

$$= \begin{bmatrix} \dfrac{\boldsymbol{m}}{\rho} \\ \operatorname{div}\partial_{\nabla\boldsymbol{\chi}}\psi \\ -\dfrac{1}{\partial_\theta\eta}\,\partial_{\nabla\boldsymbol{\chi}}\eta\cdot\nabla\dot{\boldsymbol{\chi}} \end{bmatrix}$$

momentum balance, temperature evolution

$$\dot{\boldsymbol{m}} = -\delta_{\boldsymbol{\chi}}\psi = \operatorname{div}\partial_{\nabla\boldsymbol{\chi}}\psi = \operatorname{div}\boldsymbol{P}\,, \quad \dot{\theta}_{\mathrm{rev}} = L_{\theta\boldsymbol{m}}\delta_{\boldsymbol{m}} e = -\frac{1}{\partial_\theta\eta}\,\partial_{\nabla\boldsymbol{\chi}}\eta\cdot\nabla\dot{\boldsymbol{\chi}}$$

irreversible part

GENERIC variable evolution

- temperature evolution reversible & irreversible
- mass evolution, order parameter irreversible (flux diffusive)
- heat conduction affects only θ_{irr}
- mass diffusion, structural evolution affect $\theta_{\text{irr}}, \varrho, \phi$

reversible-irreversible split

$$\boldsymbol{x}_{\text{rev}} = (\boldsymbol{\chi}, \boldsymbol{m}, \theta_{\text{rev}}, 0, 0)\,, \quad \boldsymbol{x}_{\text{irr}} = (\mathbf{0}, \mathbf{0}, \theta_{\text{irr}}, \varrho, \phi)$$

irreversible part $\dot{\boldsymbol{x}}_{\text{irr}} = \mathcal{M}\,\mathcal{D}_{\boldsymbol{x}} S$

$$\begin{bmatrix} \dot{\theta}_{\text{irr}} \\ \dot{\varrho} \\ \dot{\phi} \end{bmatrix} = \begin{bmatrix} M_{\theta\theta} & M_{\theta\varrho} & M_{\theta\phi} \\ M_{\varrho\theta} & M_{\varrho\varrho} & 0 \\ M_{\phi\theta} & 0 & M_{\phi\phi} \end{bmatrix} \begin{bmatrix} \delta_\theta \eta \\ \delta_\varrho \eta \\ \delta_\phi \eta \end{bmatrix} = \begin{bmatrix} M_{\theta\theta}\,\delta_\theta\eta + M_{\theta\varrho}\,\delta_\varrho\eta + M_{\theta\phi}\,\delta_\phi\eta \\ M_{\varrho\theta}\,\delta_\theta\eta + M_{\varrho\varrho}\,\delta_\varrho\eta \\ M_{\phi\theta}\,\delta_\theta\eta + M_{\phi\phi}\,\delta_\phi\eta \end{bmatrix}$$

consequences of orthogonality

orthogonality $\mathcal{M}\,\mathcal{D}_x E = 0$

$$M_{\varrho\theta}\,\delta_\theta\varepsilon + M_{\varrho\varrho}\,\delta_\varrho\varepsilon \;=\; 0 \implies M_{\varrho\theta} \;=\; -M_{\varrho\varrho}\,\delta_\varrho\varepsilon\,\frac{1}{\partial_\theta\varepsilon}$$

$$M_{\phi\theta}\,\delta_\theta\varepsilon + M_{\phi\phi}\,\delta_\phi\varepsilon \;=\; 0 \implies M_{\phi\theta} \;=\; -M_{\phi\phi}\,\delta_\phi\varepsilon\,\frac{1}{\partial_\theta\varepsilon}$$

reduced phase field relations

$$\dot\varrho \;=\; M_{\varrho\theta}\,\delta_\theta\eta + M_{\varrho\varrho}\,\delta_\varrho\eta \;=\; M_{\varrho\varrho}\,\delta_\varrho(\eta - \vartheta\,\varepsilon) \;=\; -M_{\varrho\varrho}\,\delta_\varrho\check\psi$$

$$\dot\phi \;=\; M_{\phi\theta}\,\delta_\theta\eta + M_{\phi\phi}\,\delta_\phi\eta \;=\; M_{\phi\phi}\,\delta_\phi(\eta - \vartheta\,\varepsilon) \;=\; -M_{\phi\phi}\,\delta_\phi\check\psi$$

$\implies$ same driving force as in "standard" formulation

comparison with Ginzburg-Landau driving force

$$\theta\,\delta_x\check\psi - \delta_x\psi = \theta^{-1}\partial_{\nabla x}\psi\cdot\nabla\theta$$

mass diffusion & structural transition

friction operator component for mass diffusion

$$M_{\varrho\varrho} = -\nabla \cdot \theta \boldsymbol{D} \, \nabla$$

friction operator component for mobility

$$M_{\phi\phi} = \theta \, m$$

reduced phase field relations

$$\begin{aligned} \dot{\varrho} &= M_{\varrho\theta}\delta_\theta\eta + M_{\varrho\varrho}\delta_\varrho\eta &= \operatorname{div} \theta \boldsymbol{D} \nabla \delta_\varrho \check{\psi} \\ \dot{\phi} &= M_{\phi\theta}\delta_\theta\eta + M_{\phi\phi}\delta_\phi\eta &= -\theta \, m \, \delta_\phi \check{\psi} \end{aligned}$$

consistent with relations from standard NE thermodynamics

thermal friction operator

split of $M_{\theta\theta}$ (heat conduction affects only θ)

$$M_{\theta\theta} = M_{\mathrm{C}\theta\theta} + M_{\mathrm{P}\theta\theta}\,, \quad M_{\mathrm{C}\theta\theta} = -\frac{1}{c}\,\nabla\cdot\theta^2\boldsymbol{K}\,\nabla\,\frac{1}{c}\,, \quad c = \partial_\theta\varepsilon$$

conduction ($\partial_\theta\varepsilon = \theta\,\partial_\theta\eta$)

$$M_{\mathrm{C}\theta\theta}\,\delta_\theta\eta \;=\; -\frac{1}{c}\,\mathrm{div}\,\theta^2\boldsymbol{K}\nabla\frac{\partial_\theta\eta}{c} \;=\; \frac{1}{c}\,\mathrm{div}\,\boldsymbol{K}\nabla\theta$$

$$M_{\mathrm{C}\theta\theta}\,\delta_\theta\varepsilon \;=\; -\frac{1}{c}\,\mathrm{div}\,\theta^2\boldsymbol{K}\nabla\frac{c}{c} \;=\; 0$$

orthogonality $\mathcal{M}\,\mathcal{D}_x E = 0$ and $M_{\mathrm{C}\theta\theta}\,\delta_\theta\varepsilon = 0$

$$M_{\theta\theta}\,\delta_\theta\varepsilon + M_{\theta\varrho}\,\delta_\varrho\varepsilon + M_{\theta\phi}\,\delta_\phi\varepsilon = 0$$

$$\Longrightarrow \quad M_{\mathrm{P}\theta\theta} \;=\; -M_{\theta\varrho}\,\delta_\varrho\varepsilon\,\frac{1}{c} - M_{\theta\phi}\,\delta_\phi\varepsilon\,\frac{1}{c}$$

consequences of symmetry

symmetry

$$\langle \mathcal{D}_\theta A, M_{\theta\varrho}\, \mathcal{D}_\varrho B\rangle = \langle \mathcal{D}_\varrho B, M_{\varrho\theta}\, \mathcal{D}_\theta A\rangle = \int_B \mathcal{D}_\varrho B \;\operatorname{div} \theta \boldsymbol{D}\, \nabla \delta_\varrho \varepsilon\, \frac{1}{c}\, \mathcal{D}_\theta A\, dv$$

integration by parts & boundary condition $\mathcal{D}_\varrho B|_{\partial B} = 0$

$$\int_B \mathcal{D}_\varrho B \;\operatorname{div} \theta \boldsymbol{D}\, \nabla \delta_\varrho \varepsilon\, \frac{1}{c}\, \mathcal{D}_\theta A\, dv = -\int_B \mathcal{D}_\theta A\, \frac{1}{c}\, \theta \boldsymbol{D}\, \nabla \delta_\varrho \varepsilon \cdot \nabla \mathcal{D}_\varrho B\, dv$$

temperature / mass density coupling

$$M_{\theta\varrho} = -\frac{1}{c}\, \theta \boldsymbol{D}\, \nabla \delta_\varrho \varepsilon \cdot \nabla$$

likewise $\langle \mathcal{D}_\theta A, M_{\theta\phi}\, \mathcal{D}_\phi B\rangle = \langle \mathcal{D}_\phi B, M_{\phi\theta}\, \mathcal{D}_\theta A\rangle$ yields θ-ϕ coupling

$$M_{\theta\phi} = -\frac{1}{c}\, \delta_\phi \varepsilon\; \theta\, m$$

phase field part $M_{\mathrm{P}\theta\theta}$

previous result from $\mathcal{M}\,\mathcal{D}_{\boldsymbol{x}}E = 0$ and $M_{\mathrm{C}\theta\theta}\,\delta_\theta\varepsilon = 0$

$$M_{\mathrm{P}\theta\theta} = -M_{\theta\varrho}\,\delta_\varrho\varepsilon\,\frac{1}{c} - M_{\theta\phi}\,\delta_\phi\varepsilon\,\frac{1}{c}$$

θ-ϱ component

$$M_{\theta\varrho} = -\frac{1}{c}\,\theta\boldsymbol{D}\,\nabla\delta_\varrho\varepsilon\cdot\nabla \quad\Longrightarrow\quad -M_{\theta\varrho}\,\delta_\varrho\varepsilon\,\frac{1}{c} = \frac{1}{c}\,\theta\boldsymbol{D}\,\nabla\delta_\varrho\varepsilon\cdot\nabla\delta_\varrho\varepsilon\,\frac{1}{c}$$

θ-ϕ component

$$M_{\theta\phi} = -\frac{1}{c}\,\delta_\phi\varepsilon\;\theta\,m \quad\Longrightarrow\quad -M_{\theta\phi}\,\delta_\phi\varepsilon\,\frac{1}{c} = \frac{1}{c}\,\delta_\phi\varepsilon\;\theta\,m\,\delta_\phi\varepsilon\,\frac{1}{c}$$

result

$$M_{\mathrm{P}\theta\theta} = \frac{1}{c}\,\theta\boldsymbol{D}\,\nabla\delta_\varrho\varepsilon\cdot\nabla\delta_\varrho\varepsilon\,\frac{1}{c} + \frac{1}{c}\,\delta_\phi\varepsilon\;\theta\,m\,\delta_\phi\varepsilon\,\frac{1}{c}$$

summary: irreversible part

friction operator

$$\mathcal{M} = \begin{bmatrix} -\frac{1}{c}\nabla\cdot\theta^2\boldsymbol{K}\,\nabla\,\frac{1}{c} + M_{\mathrm{P}\theta\theta} & -\frac{1}{c}\,\theta\boldsymbol{D}\,\nabla\delta_\varrho\varepsilon\cdot\nabla & -\frac{1}{c}\,\delta_\phi\varepsilon\,\theta\,m \\ \nabla\cdot\theta\boldsymbol{D}\,\nabla\,\delta_\varrho\varepsilon\,\frac{1}{c} & -\nabla\cdot\theta\boldsymbol{D}\,\nabla & 0 \\ -\theta\,m\,\delta_\phi\varepsilon\,\frac{1}{c} & 0 & \theta\,m \end{bmatrix}$$

phase field part of $M_{\theta\theta}$

$$M_{\mathrm{P}\theta\theta} = \frac{1}{c}\left\{\nabla\delta_\varrho\varepsilon\cdot\theta\boldsymbol{D}\,\nabla\delta_\varrho\varepsilon + \delta_\phi\varepsilon\;\theta\,m\,\delta_\phi\varepsilon\right\}\frac{1}{c}$$

irreversible temperature evolution

$$\dot{\theta}_{\mathrm{irr}} = \frac{1}{c}\,\mathrm{div}\,\boldsymbol{K}\nabla\theta + \frac{1}{c}\,\nabla\delta_\varrho\varepsilon\cdot\theta\boldsymbol{D}\,\nabla\delta_\varrho\check{\psi} + \frac{1}{c}\,\delta_\phi\varepsilon\;\theta\,m\,\delta_\phi\check{\psi}$$

summary & outlook

comparison of Eulerian- & Lagrangian-based continuum mechanics

comparison of non-equilibrium thermodynamic approaches

- "standard" non-equilibrium thermodynamics
- GENERIC

applications / outlook

- homogeneous & inhomogeneous thermoelastic-viscoplastic solids
- strongly non-local GENERIC-based phase field (Hütter & S., in prep.)
- multiscale dislocation ensemble modeling (Koimann et al. 2015; in prog.)

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