An Integral Framework for Modeling in Continuum Thermodynamics

Martin Heida[1]

[1]TU Dortmund

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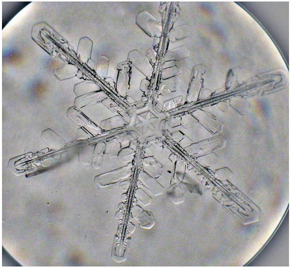
Outline

Outline

Multiphase and Multifluid Systems



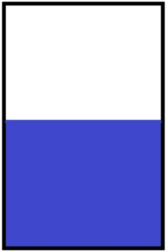
Phase Field Models

M. Van der Waals 1893/1894

"It is highly probable that the sharp interface observed at the interface between a liquid and its vapor is only ostensible. In fact it seems that there is a small transition zone in which the density continuously decreases."

Phase Field Models: Example

- Consider a system of a tank Ω filled with two fluids, say air and water.
- Introduce a function $c : \Omega \to [0,1]$ having values
  - $c(x) \equiv 1$ whenever x is occupied by water
  - $c(x) \equiv 0$ whenever x is occupied by air
  - $c(x) \in]0,1[$ whenever x is in the boundary region between water and air



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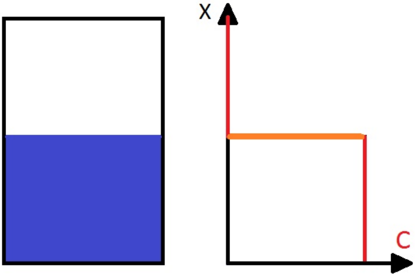

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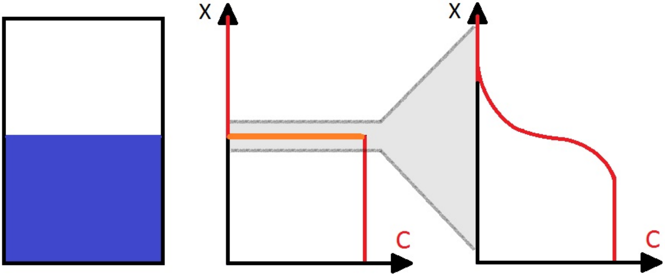


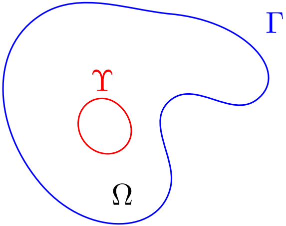
Phase Field Models

Examples for phase field models

- Korteweg model (1901)
- Cahn-Hilliard model (1958)
- Allen-Cahn model (1979)
- Cahn-Hilliard-Navier-Stokes model (Lowengrub & Truskinovsky 1998)

Outline

Thermodynamical Systems

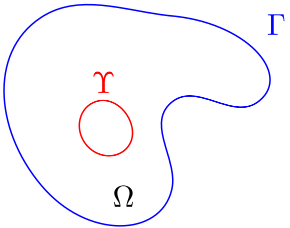


- The most essential parameters in classical equilibrium Thermodynamics: Internal Energy $\mathcal{E}$ and Entropy $\mathcal{S}$, depending on extensive variables

- Here:
  Internal Energy $\mathcal{E}$ and Entropy $\mathcal{S}$, depend on several parameters that are intersting to us, in order to provide a complete description of the system

- As the parameters usually are given as functions on Ω, Γ, Υ, the quantities $\mathcal{E}$ and $\mathcal{S}$ are functionals

Thermodynamical Systems



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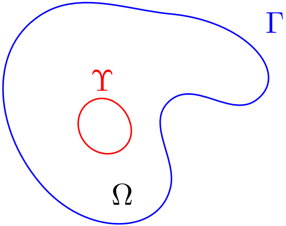

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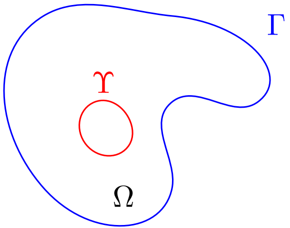
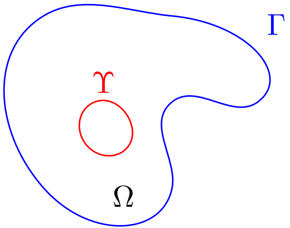


- As the parameters usually are given as functions on Ω, Γ, Υ, the quantities $\mathcal{E}$ and $\mathcal{S}$ are functionals
- Examples are
  - velocity, density, concentrations on Ω
  - normal velocity, tangential velocity, concentration on Γ or Υ
  - shape of Γ and Υ

Thermodynamical Systems

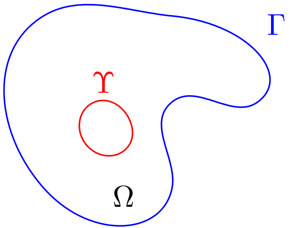


We consider isolated systems, i.e.

- $\dfrac{d}{dt}\mathcal{E} = 0$ and
- there is no exchange of entropy with the surrounding of Ω (to be specified later), in particular,

$$\frac{d}{dt}\mathcal{S} \geq 0.$$

Thermodynamical Systems



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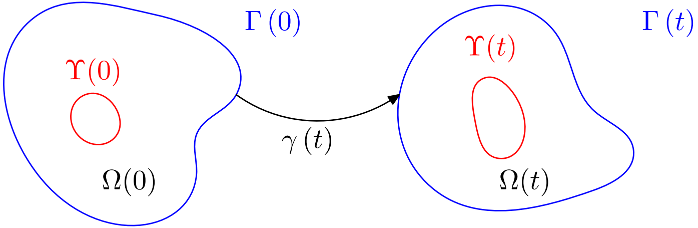
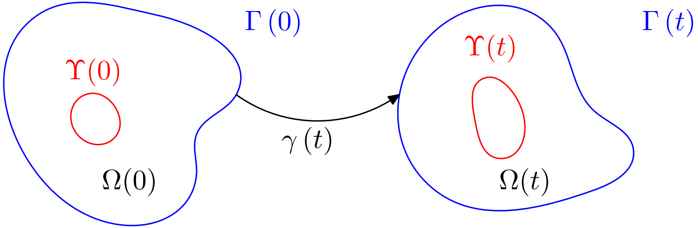
Assumptions



The evolution is given by an evolution trajectory $\gamma(t)$, containing information on

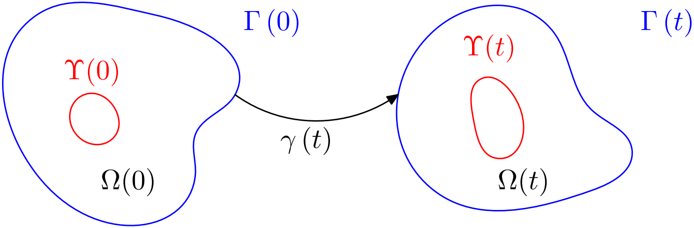
- parameters such as density ϱ, velocity $\boldsymbol{v}$ etc.
- shape of $\Omega(t), \Gamma(t)$ and subdomains $\Upsilon(t)$

Assumptions



- The dissipation of the system along any valid trajectory $\gamma(t)$ is given through $\Xi\left(\gamma(t), "\partial_t \gamma(t)"\right)$
- any physical trajectory is such that it maximizes Ξ with respect to the constraint $\Xi\left(\gamma(t), \partial_t \gamma(t)\right) = \frac{d}{dt}\mathcal{S}(\gamma(t))$.
- Physical interpretation (as we will see later):
  - Ξ adds a (Riemannian) geometry to the space of thermodynamical states.
  - Any admissible trajectory is such that it follows the steepest decent of $\mathcal{S}$ according to this geometry.

Assumptions



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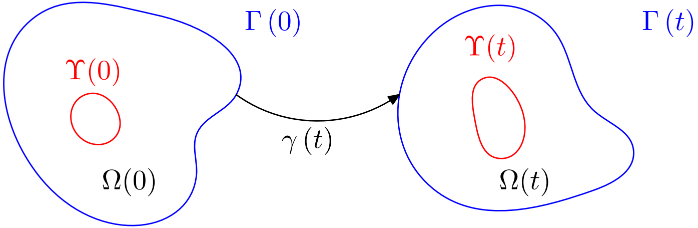

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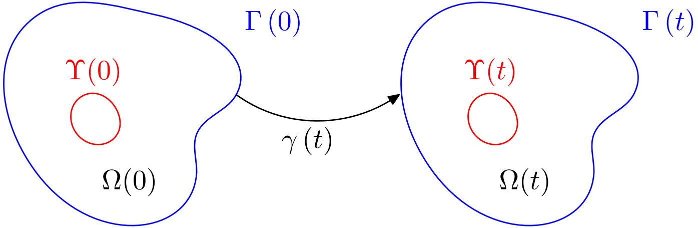

- We assume that the shape is preserved
- $\gamma(t)$ is then given by internal variables such as ϱ, $\boldsymbol{v}$, etc. ....
- we assume there are no further (fixed ore evolving) structures $\Upsilon \equiv \emptyset$.

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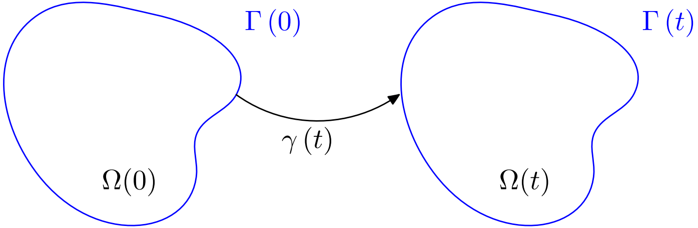

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Quantities and Parameters

$$\mathcal{E} = \int_\Omega \varrho E + \int_\Gamma E_\Gamma \qquad \mathcal{S} = \int_\Omega \varrho\eta(\varrho, c, E, \boldsymbol{v}) + \int_\Gamma \eta_\Gamma(E_\Gamma, c)$$

In Ω:
Energy $E = \tilde{e}(\varrho, c, \eta) + \frac{1}{2}|\boldsymbol{v}|^2$ where
$\varrho \hat{=}$ mass density
$\boldsymbol{v} \hat{=}$ velocity
$c \hat{=}$ mass concentration of one of the constituents
$e = \tilde{e}(\varrho, c, \eta) \hat{=}$ internal energy per mass
$\eta \hat{=}$ entropy per mass
Assume $\frac{\partial \tilde{e}}{\partial \eta} > 0$, $\Rightarrow$

$$\eta = \tilde{\eta}(\varrho, c, E, \boldsymbol{v})$$

On Γ
$E_\Gamma = \tilde{E}_\Gamma(c, \eta_\Gamma) \hat{=}$ surface energy
$\eta_\Gamma \hat{=}$ surface entropy
Assume $\frac{\partial \tilde{E}_\Gamma}{\partial \eta_\Gamma} > 0$, $\Rightarrow$

$$\eta_\Gamma = \tilde{\eta}_\Gamma(c, E_\Gamma)$$

Basic Assumptions

Using the notation $\dot{a} = \partial_t a + \boldsymbol{v} \cdot \nabla a\,, \quad \dot{\mathbf{a}} = \partial_t \mathbf{a} + (\nabla \mathbf{a})\, \boldsymbol{v}\,,$
we start from continuum mechanics

$$\dot{\varrho} + \varrho \operatorname{div} \boldsymbol{v} = 0 \qquad \varrho \dot{E} - \operatorname{div} \mathbf{h} = 0$$

$$\varrho \dot{\boldsymbol{v}} - \operatorname{div} \mathbb{T} = 0 \qquad \varrho \dot{c} + \operatorname{div} \mathbf{j} = \overset{+}{c}$$

where $\mathbb{T}$ is the stress tensor, $\mathbf{j}$ is diffusive flux of c, $\overset{+}{c}$ is production of c and $\mathbf{h}$ is the generalized heat flux.

Aim: Find constitutive equations for $\mathbb{T}$, $\mathbf{h}$, $\mathbf{j}$ and $\overset{+}{c}$

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We assume either

$$\overset{+}{c} = 0 \quad \Rightarrow \quad \text{Cahn-Hilliard models}$$

$$\mathbf{j} = \mathbf{0} \quad \Rightarrow \quad \text{Allen-Cahn models}$$

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We have the following balance equations on Γ:

$$\varrho \partial_t c + \varrho \boldsymbol{\upsilon}_\tau \cdot \nabla_\tau c = \overset{\oplus}{c}$$

$$\partial_t E_\Gamma - \operatorname{div}_\tau \mathbf{h}_\Gamma = \overset{\oplus}{E}$$

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$$E = \tilde{E}\,(\eta, \varrho, \boldsymbol{v}, c, \nabla c) = \frac{1}{2}\,|\boldsymbol{v}|^2 + E_0(\eta, \varrho, c) + \frac{\sigma}{2\varrho}\,|\nabla c|^2$$

$$E_\Gamma = \tilde{E}_\Gamma(\eta_\Gamma, c, \nabla_\tau c) = \hat{E}(\eta_\Gamma, c) + \frac{\sigma_\Gamma}{2}\,|\nabla_\tau c|^2 \,.$$

Energy conservation

Local energy conservation:

$$\overset{\oplus}{E} = -\mathbf{h} \cdot \mathbf{n}_\Gamma$$

yields

$$\frac{d}{dt}\mathcal{E} = 0$$

Time derivative of $\mathcal{S}$

$$\mathcal{S} = \int_\Omega \varrho\eta(\varrho, c, E, \boldsymbol{v}) + \int_\Gamma \eta_\Gamma(E_\Gamma, c)$$

leads to

$$\frac{d}{dt}\mathcal{S} = \int_\Omega \varrho\dot{\eta} + \int_\Gamma \frac{d}{dt}\eta_\Gamma$$

where we get the time derivatives from constitutive assumptions via

$$\varrho\dot{E} = \varrho\frac{\partial E}{\partial \eta}\dot{\eta} + \varrho\frac{\partial E}{\partial \varrho}\dot{\varrho} + \varrho\frac{\partial E}{\partial \boldsymbol{v}}\cdot\dot{\boldsymbol{v}} + \varrho\frac{\partial E}{\partial c}\dot{c} + \varrho\frac{\partial E}{\partial \nabla c}\cdot\dot{\overline{\nabla c}}\,,$$

$$\partial_t E_\Gamma = \frac{\partial E_\Gamma}{\partial \eta_\Gamma}\partial_t\eta_\Gamma + \frac{\partial E_\Gamma}{\partial c}\partial_t c + \frac{\partial E_\Gamma}{\partial(\nabla_\tau c)}\partial_t(\nabla_\tau c)\,.$$

Assume for simplicity $\quad \vartheta := \frac{\partial E}{\partial \eta} \quad = \quad \vartheta_\Gamma := \frac{\partial E_\Gamma}{\partial \eta_\Gamma} \quad$ on Γ.

Rate of Entropy Production

$$\frac{d}{dt}\mathcal{S} = \int_\Omega \frac{1}{\vartheta}\xi + \int_\Gamma \frac{1}{\vartheta}\xi_\Gamma$$

We find two local rates of entropy production:

$$\xi = \left(\tilde{\mathbb{S}} \cdot \mathbb{D}^d \boldsymbol{\upsilon} + \frac{\mathbf{q}}{\vartheta} \cdot \nabla\vartheta + (\tilde{m} + p)\operatorname{div}\boldsymbol{\upsilon}\right) - \mathbf{j} \cdot \nabla\left(\mu_c + \mu\right)$$

$$\xi_\Gamma = -\check{\mathbb{S}} \cdot \boldsymbol{\upsilon}_\tau + \mathbf{q}_\Gamma \cdot \frac{\nabla_\tau \vartheta}{\vartheta} - \mu_{\Gamma,c}\overset{\oplus}{c}$$

where

$$\check{\mathbb{S}} := \left((\mathbb{T}\mathbf{n}_\Gamma)_\tau + \mu_{\boldsymbol{\upsilon},\Gamma}\right) \qquad \tilde{\mathbb{S}} := (\mathbb{T} + \mathbb{T}_c) - \tilde{m}\mathbb{I}$$

$$\mathbf{q}_\Gamma := \mathbf{h}_\Gamma + \varrho c \mu_{\Gamma,2}\boldsymbol{\upsilon}_\tau - \frac{\partial E_\Gamma}{\partial(\nabla_\tau c)}\partial_t c \qquad \mathbb{D}\boldsymbol{\upsilon} := \frac{1}{2}(\nabla\boldsymbol{\upsilon} + \nabla\boldsymbol{\upsilon}^T)$$

$$\tilde{m} := \frac{1}{3}\operatorname{tr}(\mathbb{T} + \mathbb{T}_c) \qquad \mathbb{D}^d\boldsymbol{\upsilon} := \mathbb{D}\boldsymbol{\upsilon} - \frac{1}{3}\left(\operatorname{tr}\mathbb{D}\boldsymbol{\upsilon}\right)\mathbb{I}$$

$$\mathbf{q} = (\mu_c + \mu)\,\mathbf{j} + \partial_{\nabla c}E \operatorname{div}\mathbf{j} + \mathbf{h} - \mathbb{T}\boldsymbol{\upsilon}\,,$$

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$$\mathbb{D}^d\boldsymbol{v} := \mathbb{D}\boldsymbol{v} - \frac{1}{3}\left(\mathrm{tr}\mathbb{D}\boldsymbol{v}\right)\mathbb{I}$$

Maximum Rate of Entropy Production

We assume that global dissipation is given through

$$\Xi(\check{\mathbb{S}}, \mathbf{q}_\Gamma, \overset{\oplus}{c}, \tilde{\mathbb{S}}, \mathbf{q}, (\tilde{m}+p), \mathbf{j}) = \int_\Omega \tilde{\xi}(\tilde{\mathbb{S}}, \mathbf{q}, (\tilde{m}+p), \mathbf{j}) + \int_\Gamma \tilde{\xi}_\Gamma(\check{\mathbb{S}}_\tau, \mathbf{q}_\Gamma, \overset{\oplus}{c})$$

while we calculated

$$\frac{d}{dt}\mathcal{S} = \int_\Omega \frac{1}{\vartheta}\xi + \int_\Gamma \frac{1}{\vartheta}\xi_\Gamma$$

with

$$\xi = \left(\tilde{\mathbb{S}} \cdot \mathbb{D}^d \boldsymbol{v} + \frac{\mathbf{q}}{\vartheta} \cdot \nabla\vartheta + (\tilde{m}+p)\,\mathrm{div}\,\boldsymbol{v}\right) - \mathbf{j} \cdot \nabla\left(\mu_c + \mu\right)$$

$$\xi_\Gamma = -\check{\mathbb{S}} \cdot \boldsymbol{v}_\tau + \mathbf{q}_\Gamma \cdot \frac{\nabla_\tau \vartheta}{\vartheta} - \mu_{\Gamma,c}\overset{\oplus}{c}$$

and

$$\tilde{\xi}(\tilde{\mathbb{S}}, \mathbf{q}, (\tilde{m}+p), \mathbf{j}_1) = \frac{1}{\nu}\left|\tilde{\mathbb{S}}\right|^2 + \frac{3}{\nu+3\lambda}(\tilde{m}+p)^2 + \frac{1}{\kappa}|\mathbf{q}|^2 + \frac{1}{J}|\mathbf{j}|^2\ ,$$

$$\tilde{\xi}_\Gamma(\check{\mathbb{S}}_\tau, \mathbf{q}_\Gamma, \overset{\oplus}{c}) = \frac{1}{\beta}\left|\check{\mathbb{S}}_\tau\right|^2 + \frac{1}{\kappa_\Gamma}|\mathbf{q}_\Gamma|^2 + \frac{1}{\alpha_c}\left|\overset{\oplus}{c}\right|^2$$

Maximum Rate of Entropy Production

We whish to maximize $\Xi(\check{\mathbb{S}}, \mathbf{q}_\Gamma, \overset{\oplus}{c}, \tilde{\mathbb{S}}, \mathbf{q}, (\tilde{m}+p), \mathbf{j})$ w.r.t. $\check{\mathbb{S}}, \mathbf{q}_\Gamma, \overset{\oplus}{c}, \tilde{\mathbb{S}}, \mathbf{q}, (\tilde{m}+p), \mathbf{j}$ under the constraint

$$\Xi = \frac{d}{dt}\mathcal{S}\,.$$

This is equivalent with

- maximizing $\tilde{\xi}(\tilde{\mathbb{S}}, \mathbf{q}, (\tilde{m}+p), \mathbf{j})$ under the constraint

$$\tilde{\xi}(\tilde{\mathbb{S}}, \mathbf{q}, (\tilde{m}+p), \mathbf{j}) = \left(\tilde{\mathbb{S}} \cdot \mathbb{D}^d \boldsymbol{\upsilon} + \frac{\mathbf{q}}{\vartheta} \cdot \nabla\vartheta + (\tilde{m}+p)\,\mathrm{div}\,\boldsymbol{\upsilon}\right) - \mathbf{j} \cdot \nabla\left(\mu_c + \mu\right)$$

  and

- maximizing $\tilde{\xi}_\Gamma(\check{\mathbb{S}}_\tau, \mathbf{q}_\Gamma, \overset{\oplus}{c})$ under the constraint

$$\tilde{\xi}_\Gamma(\check{\mathbb{S}}_\tau, \mathbf{q}_\Gamma, \overset{\oplus}{c}) = -\check{\mathbb{S}} \cdot \boldsymbol{\upsilon}_\tau + \mathbf{q}_\Gamma \cdot \frac{\nabla_\tau \vartheta}{\vartheta} - \mu_{\Gamma,c}\overset{\oplus}{c}$$

Resulting equations

H., Málek & Rajagopal

$$
\begin{aligned}
\partial_t \varrho + \operatorname{div}(\varrho \boldsymbol{v}) &= 0 \\
\varrho \partial_t \boldsymbol{v} + \varrho (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} - \operatorname{div}(\nu(\varrho, c) \nabla \boldsymbol{v}) + \nabla p + \operatorname{div}(\sigma \nabla c \otimes \nabla c) &= 0 \\
\varrho \partial_t c + \varrho \boldsymbol{v} \nabla c - \operatorname{div}(f'(c) \nabla c) + \operatorname{div}\left(\nabla\left(\frac{\sigma}{\varrho} \Delta c\right)\right) &= 0
\end{aligned}
$$

with the boundary conditions

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(2011 / 2012)

$$
\varrho \partial_t c + \varrho \boldsymbol{v}_\tau \cdot \nabla_\tau c = \alpha_c \left(\frac{\sigma}{\varrho} \Delta_\tau c - \frac{\mu_\Gamma}{\varrho} - \nabla c \cdot \mathbf{n}_\Gamma \right)
$$

Resulting equations

H., Málek & Rajagopal

$$
\begin{aligned}
\partial_t \varrho + \operatorname{div}(\varrho \boldsymbol{v}) &= 0 \\
\varrho \partial_t \boldsymbol{v} + \varrho (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} - \operatorname{div}(\nu(\varrho, c) \nabla \boldsymbol{v}) + \nabla p + \operatorname{div}(\sigma \nabla c \otimes \nabla c) &= 0 \\
\varrho \partial_t c + \varrho \boldsymbol{v} \nabla c - \operatorname{div}(f'(c) \nabla c) + \operatorname{div}\left(\nabla \left(\frac{\sigma}{\varrho} \Delta c\right)\right) &= 0
\end{aligned}
$$

with the boundary conditions

H. (2011 / 2012)

$$
\mathbf{h}_\Gamma = \kappa_\Gamma \frac{\nabla_\tau \vartheta}{\vartheta} - (\varrho c \mu_{\Gamma,2} \boldsymbol{v}_\tau - \partial_z E_\Gamma \partial_t c) \qquad (\mathbb{T}\mathbf{n}_\Gamma)_\tau = -\beta \boldsymbol{v}_\tau - (\sigma \Delta_\tau c - \mu_\Gamma) \nabla_\tau c
$$

$$
\mathbf{h} = \mathbb{T}\boldsymbol{v} + \kappa \nabla \vartheta - (\mu_c + \mu)\,\mathbf{j} - \partial_{\nabla c} E \operatorname{div} \mathbf{j} \qquad \overset{\oplus}{c} = \alpha_c \left(\frac{\sigma}{\varrho} \Delta_\tau c - \frac{\mu_\Gamma}{\varrho} - \nabla c \cdot \mathbf{n}_\Gamma\right)
$$

Outline

Example

We consider the following system:

$$\begin{aligned} \partial_t u + \operatorname{div}\left(A(u,\nabla u)\,\nabla\left(\Delta u - s'(u)\right)\right) \ni 0 \qquad & \text{on } (0,T]\times\Omega\,, \\ \left(A(u,\nabla u)\,\nabla\left(\Delta u - s'(u)\right)\right)\cdot \mathbf{n}_\Gamma = \nabla u\cdot\mathbf{n}_\Gamma = 0 \qquad & \text{on } (0,T]\times\Gamma\,, \\ u(0) = u_0 \qquad & \text{for } t = 0\,. \end{aligned}$$

with the weak formulation

$$\int_0^T\int_\Omega \partial_t u\psi - \int_0^T\int_\Omega \left(A(u,\nabla u)\,\nabla\left(\Delta u - s'(u)\right)\right)\cdot\nabla\psi = 0 \qquad \forall\psi\in L^2(0,T;H^1_{(0)}(\Omega))$$

$$\nabla u\cdot\mathbf{n}_\Gamma = 0 \text{ on } (0,T]\times\Gamma\,, \qquad u(0) = u_0 \text{ for } t = 0\,.$$

Example

- Set $\quad H^1_{(0)}(\Omega) := \left\{ u \in H^1(\Omega) \,:\, \int_\Omega u = 0 \right\}, \qquad \|u\|_{H^1_{(0)}} = \int_\Omega |\nabla u|^2$
- For $u \in \tilde{\mathcal{H}} := H^1_{(0)}(\Omega)$, we define for $r_1, r_2 \in \mathcal{H} := H^{-1}_{(0)}(\Omega)$:

$$g_u(r_1, r_2) = \int_\Omega \nabla p_1^u A(u, \nabla u) \nabla p_2^u = \int_\Omega r_1 p_2^u = \langle r_1, p_2 \rangle_{H^{-1}_{(0)}, H^1_{(0)}} \ ,$$

where $A : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^{3\times 3}$, $A \in C^{1,1}(\mathbb{R} \times \mathbb{R}^n)$, $\xi \cdot A(c,d)\xi \geq a_0 |\xi|^2$ $\forall\, \xi \in \mathbb{R}^3$ a.e. $(c,d) \in \mathbb{R} \times \mathbb{R}^3$, A symmetric and

- $p_i^u \in H^1_{(0)}(\Omega)$ is the unique solution to

$$-\mathrm{div}\,\left(A(u, \nabla u)\nabla p_i^u\right) = r_i \quad \text{for } i = 1, 2\,.$$

Example

- $g_u(r_1, r_2) = \int_\Omega r_1 p_2 = \langle r_1, p_2 \rangle_{H^{-1}_{(0)}, H^1_{(0)}} = \langle r_2, p_1 \rangle_{H^{-1}_{(0)}, H^1_{(0)}}$
- We introduce

$$\mathcal{S} : \ \mathcal{H} = H^{-1}_{(0)}(\Omega) \to \mathbb{R}$$
$$\mathcal{S}(u) = \begin{cases} \int_\Omega \frac{1}{2} |\nabla u|^2 + \int_\Omega s(u) & \text{for } u \in H^1_{(0)}(\Omega) \\ +\infty & \text{for } u \in \mathcal{H} \backslash H^1_{(0)}(\Omega) \end{cases}$$

- with subdifferential (Abels & Wilke 2008) $\quad d\mathcal{S}(u) = -\Delta(\Delta u - s'(u))$
- and the notation:

$$\delta \in \nabla_u \mathcal{S}(u) \quad \Leftrightarrow \quad \exists \tilde{\delta} \in d\mathcal{S}(u) \quad s.t. \quad g_u(\delta, \varphi) = \left\langle \tilde{\delta}, \varphi \right\rangle_{\mathcal{H}} \ \forall \varphi \in \mathcal{H}$$

Example

$$\int_0^T \int_\Omega \partial_t u \psi - \int_0^T \int_\Omega \left(A(u, \nabla u)\, \nabla \left(\Delta u - s'(u)\right)\right) \cdot \nabla \psi = 0 \qquad \forall \psi \in L^2(0, T; H^1_{(0)}(\Omega))$$

$$\nabla u \cdot \mathbf{n}_\Gamma = 0 \text{ on } (0, T] \times \Gamma\,, \qquad u(0) = u_0 \text{ for } t = 0\,.$$

$$\Leftrightarrow$$

$$g_u(\partial_t u, \varphi) = g_u(-\nabla \mathcal{S}, \varphi) \quad \forall \varphi \in \mathcal{H}\,, \quad u(0) = u_0 \text{ for } t = 0\,.$$

$$\Leftrightarrow$$

$$\partial_t u = -\nabla_u \mathcal{S}(u), \qquad \nabla_u \mathcal{S}(u) = -\mathrm{div}\, \left(A(u, \nabla u)\, \nabla \left(\Delta u - s'(u)\right)\right)$$

General Setting

Definition

We call any tuple $(\mathcal{H}_0, \tilde{\mathcal{H}}, \mathcal{H}, g)$ of Hilbert spaces $\mathcal{H}_0$, $\tilde{\mathcal{H}}$, $\mathcal{H}$ and a mapping $g_\bullet : \tilde{\mathcal{H}} \to B(\mathcal{H})$ satisfying 1 and 2 an entropy space:

1. $\mathcal{H}_0 \hookrightarrow \tilde{\mathcal{H}} \hookrightarrow \mathcal{H}$, densely, $\mathcal{H}_0 \hookrightarrow \tilde{\mathcal{H}}$ is compactly.

2. $\exists\, 1 \leq G^* < +\infty$ such that

$$\sqrt{G^*}^{-1} |\langle x, y\rangle_{\mathcal{H}}| \leq |g_u(x,y)| \leq \sqrt{G^*}\, |\langle x, y\rangle_{\mathcal{H}}| \quad \forall u \in \tilde{\mathcal{H}}, \quad \forall x, y \in \mathcal{H}\,,$$

and : if $u_n \to u$ strongly in $\tilde{\mathcal{H}}$ and $\varphi_n \rightharpoonup \varphi$ weakly in $\mathcal{H}$ as $n \to \infty$, then

$$g_{u_n}(\varphi_n, \psi) \to g_u(\varphi, \psi) \quad \text{as } n \to \infty \qquad \forall \psi \in \mathcal{H}\,.$$

General Setting

Definition

$\mathcal{S} : \mathcal{H} \to (-\infty, +\infty]$ is an entropy functional on $(\mathcal{H}_0, \tilde{\mathcal{H}}, \mathcal{H}, g)$ if it satisfies :

1. $D(\mathcal{S}) \subset \tilde{\mathcal{H}}$ and $\mathcal{S} : \mathcal{H} \to \mathbb{R}$ being proper, lower semicontinuous.
2. $\exists\ \tau_* > 0$ such that sets
$$\left\{ v \in \mathcal{H} \,:\, \mathcal{S}(v) + \frac{1}{2\tau} \min\left\{1, \sqrt{G^*}^{-1}\right\} \|v\|^2_{\mathcal{H}} < C \right\}$$
are compact for any $\tau < \tau_*$ and any $C > 0$ and $\exists\ S_0 > 0$ s. t.
$$\mathcal{S}(v) + \frac{1}{2\tau_*} \min\left\{1, \sqrt{G^*}^{-1}\right\} \|v\|^2_{\mathcal{H}} \geq -S_0 \qquad (1)$$
3. $$\|u\|_{\mathcal{H}_0} \leq C\left(\mathcal{S}(u) + |\nabla S|^2(u) + 1\right)$$

Theorem (H. 2012)

Let $d_l\mathcal{S}(u)$ the strong-weak closure of $d\mathcal{S}(u)$ be convex and closed for all $u \in \mathcal{H}$. Then, for each $u_0 \in \mathcal{H}_0$ and every $0 < T \in \mathbb{R}$, there exists a solution $u \in H^1(0,T;\mathcal{H}) \cap L^2(0,T;\mathcal{H}_0)$ to

$$\partial_t u = -\nabla_{l,u}\mathcal{S}(u)$$

satisfying the Lyapunov inequality

$$\frac{1}{2}\int_0^t g_u(\partial_t u, \partial_t u) + \frac{1}{2}\int_0^t |\nabla_l \mathcal{S}(u)|^2 + \mathcal{S}(u(t)) \le \mathcal{S}(u(0)) \qquad \text{for a.e. } t \in (0,T).$$

If $\mathcal{S}$ additionally fulfills the continuity assumption

$$v_n \to v, \ \sup_n \left(|\nabla \mathcal{S}(v_n)|, \mathcal{S}(v_n)\right) < +\infty \ \Rightarrow \ \mathcal{S}(v_n) \to \mathcal{S}(v) \quad \text{as } n \nearrow \infty$$

then, there is a negligible set $\mathcal{N} \subset (0,T)$ such that

$$\frac{1}{2}\int_s^t |u'|^2 + \frac{1}{2}\int_s^t |\nabla_l \mathcal{S}(u)|^2 + \mathcal{S}(u(t)) \le \mathcal{S}(u(s)) \qquad \forall t \in (s,T), \forall s \in (0,T)\backslash\mathcal{N}.$$

Application

We get solutions to a variety of problems:

H. 2012

$$
\begin{aligned}
\partial_t u + \operatorname{div}\left(A(u,\nabla u)\,\nabla\left(\Delta u - s'(u)\right)\right) &\ni 0 && \text{on } (0,T]\times\Omega\,,\\
\left(A(u,\nabla u)\,\nabla\left(\Delta u - s'(u)\right)\right)\cdot \mathbf{n}_\Gamma = \nabla u\cdot\mathbf{n}_\Gamma &= 0 && \text{on } (0,T]\times\Gamma\,,\\
u(0) &= u_0 && \text{for } t=0\,.
\end{aligned}
$$

$s(\cdot) = s_0(\cdot) + s_1(\cdot)$

$s_0 \in C^2((a,b))$ convex , $\qquad s_1 \in C^2(\mathbb{R})$

$\lim_{x\to a} s_0'(x) = -\infty, \qquad \lim_{x\to b} s_0'(x) = +\infty$

Application

We get solutions to a variety of problems:

H. 2012

$$
\begin{aligned}
\partial_t u &\in -\mathrm{div}\,\left(A(u,\nabla u)\nabla\left(s'(u)-\Delta u\right)\right) && \text{on } \Omega\,,\\
0 &= A(u,\nabla u)\nabla\left(s'(u)-\Delta u\right)\cdot \mathbf{n}_\Gamma && \text{on } \Gamma\,,\\
\partial_t u &\in A_\Gamma(u)\left(\Delta_\Gamma u - s_\Gamma'(u) - \nabla u\cdot\mathbf{n}_\Gamma\right) && \text{on } \Gamma\,,
\end{aligned}
$$

$s(\cdot) = s_0(\cdot) + s_1(\cdot)$ $\qquad$ $s_\Gamma(\cdot) = s_0(\cdot) + s_2(\cdot)$

$s_0 \in C^2((a,b))$ convex , $\qquad$ $s_1, s_2 \in C^2(\mathbb{R})$

$\lim_{x\to a} s_0'(x) = -\infty,$ $\qquad$ $\lim_{x\to b} s_0'(x) = +\infty$

Application

We get solutions to a variety of problems:

H. 2012

$$
\begin{aligned}
\partial_t u - \operatorname{div}\left(A(u, \nabla u, w)\, \nabla w\right) &\ni 0 && \text{on } (0, T] \times \Omega\,, \\
w + \Delta u - s'(u) &= 0 && \text{on } (0, T] \times \Omega\,, \\
\left(A(u, \nabla u, w)\, \nabla w\right) \cdot \mathbf{n}_\Gamma = \nabla u \cdot \mathbf{n}_\Gamma &= 0 && \text{on } (0, T] \times \Gamma\,, \\
u(0) &= u_0 && \text{for } t = 0\,.
\end{aligned}
$$

$s(u) = s_0(u) + s_1(u)$

$s_0(u) = |u|^p$ for some $p > 0$

$s_1 \in C_b^{3,1}(\mathbb{R})$

Connection to Maximum Rate of Entropy Production

(2012)

In case there is no convection, we can show that Maximum Rate of Entropy Production is equivalent with a gradient flow, provided we can identify a suitable Hilbert spaces with suitable generalized Riemannian metric tensor.

Conjecture

Can we discribe evolution of thermodynamical systems equivalently as a "generalized version" of "gradient flows" or via the maximum rate of entropy production???
Here, we mean by generalized gradient flows equations of the form

$$\frac{\Delta u}{\Delta t} = -\nabla_u \mathcal{S}(u)$$

where $\frac{\Delta u}{\Delta t}$ *is a generalized time derivative, such as*

$$\frac{\Delta u}{\Delta t} \equiv \varrho \dot{u}\,, \qquad \frac{\Delta u}{\Delta t} \equiv \partial_t u\,, \qquad \ldots\ldots$$

Interpretation

The evolution is given in such a way as to locally follow the steepest decent of the entropy in the space of states of a system with respect to a given geometry. With regard to Maupertuis' principle, this geometry can be interpreted as the "inertia" or "inertial mass" of the system.

Outline

Outlook

Open Questions

- Moving interfaces, membranes, interactions fluid / elastic body
- Better understanding of physical implications
- Is the conjecture true, i.e. are MREP and gradient flows at least informally equivalent?
- In particular: What about Navier-Stokes or Cahn-Hilliard-Navier-Stokes?
- More mathematics is needed