



**Weierstrass Institute for
Applied Analysis and Stochastics**



Entropic solutions for systems of PDEs arising in complex fluids dynamics

Elisabetta Rocca

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- The dynamics we are interested in: **non-isothermal models** for
 - Liquid Crystals flows
 - Mixtures of two viscous incompressible Newtonian fluids
 - Damage phenomena in viscoelastic materials

- The common features of the PDEs

- The new notion of solution

- The analytical results

- Some open related problems

- Hydrodynamics of **liquid crystals flows**:
 - a liquid crystal may flow like a liquid, but its molecules may be oriented in a crystal-like way
 - **aim**: deal with the nematic liquid crystals in the [Landau-de Gennes theory](#), in which the order parameter describing the orientation of molecules is a matrix, the so-called [Q-tensor](#) and to include velocity and temperature dependence in the model

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- **Two-phase mixtures of fluids**:
 - avoid analytical problems of interface singularities: an alternative approach to the sharp interface models is the [diffuse interface models](#) (the H-model). The sharp interface is replaced by a thin interfacial region where a partial mixing of the fluids is allowed; a new variable φ represents the concentration difference of the fluids
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- **Damage** phenomena:
 - **aim**: deal with a non-isothermal diffuse interface models in [thermoviscoelasticity](#) accounting for the evolution of the displacement variables, the order (damage) parameter χ , indicating the local proportion of damage

■ Liquid crystals

$$\theta_t + \mathbf{v} \cdot \nabla_x \theta + \operatorname{div} \mathbf{q} = \theta (\partial_t f(\mathbb{Q}) + \mathbf{u} \cdot \nabla_x f(\mathbb{Q})) + \sigma : \nabla_x \mathbf{v} + \Gamma(\theta) |\mathbb{H}|^2$$

$$\operatorname{div} \mathbf{v} = 0, \quad \partial_t \mathbf{v} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) + \nabla_x p = \operatorname{div}(\sigma + \mathbb{T}(\theta, \mathbb{Q})), \quad \sigma = \nu(\theta) (\nabla_x \mathbf{v} + \nabla_x^t \mathbf{v})$$

$$\mathbb{Q}_t + \mathbf{v} \cdot \nabla_x \mathbb{Q} - \mathbb{S}(\nabla_x \mathbf{v}, \mathbb{Q}) = \Gamma(\theta) \mathbb{H}, \quad \mathbb{H} = \Delta \mathbb{Q} - \theta \frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} - \frac{\partial G(\mathbb{Q})}{\partial \mathbb{Q}}$$

■ Two-phase mixtures of fluids

$$\theta_t + \mathbf{v} \cdot \nabla_x \theta + \operatorname{div} \mathbf{q} = -\theta (\varphi_t + \mathbf{v} \cdot \nabla_x \varphi) + \sigma : \nabla_x \mathbf{v} + |\nabla_x \mu|^2$$

$$\operatorname{div} \mathbf{v} = 0, \quad \mathbf{v}_t + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) + \nabla_x p = \operatorname{div} \sigma - \mu \nabla_x \varphi, \quad \sigma = \nu(\theta) (\nabla_x \mathbf{v} + \nabla_x^t \mathbf{v})$$

$$\varphi_t + \mathbf{v} \cdot \nabla_x \varphi = \Delta \mu, \quad \mu = -\Delta \varphi + W'(\varphi) - \theta$$

■ Damage

$$\theta_t + \operatorname{div} \mathbf{q} = -\theta (\chi_t + \rho \operatorname{div} \mathbf{u}_t) + a(\chi) |\varepsilon(\mathbf{u}_t)|^2 + |\chi_t|^2$$

$$\mathbf{u}_{tt} - \operatorname{div}(a(\chi) \varepsilon(\mathbf{u}_t) + b(\chi) \varepsilon(\mathbf{u}) - \rho \theta \mathbf{1}) = \mathbf{f}, \quad \varepsilon(\mathbf{u}) = (\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u})/2$$

$$\chi_t + \partial I_{(-\infty, 0]}(\chi_t) - \operatorname{div}(|\nabla \chi|^{p-2} \nabla \chi) + W'(\chi) \ni -b'(\chi) |\varepsilon(\mathbf{u})|^2/2 + \theta$$

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1. a suitable *energy conservation* and *entropy inequality* inspired by:

- 1.1. the works of E. Feireisl and co-authors ([Feireisl, Comput. Math. Appl. (2007)] and [Bulíček, Feireisl, & Málek, Nonlinear Anal. Real World Appl. (2009)]) for heat conduction in fluids

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2. a *generalization of the principle of virtual powers* inspired by:

2.1. a notion of *weak solution* introduced by [Heinemann, Kraus, Adv. Math. Sci. Appl. (2011)] for non-degenerating isothermal diffuse interface models for phase separation and damage

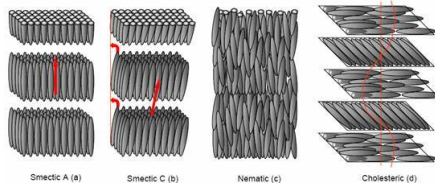
Liquid crystals

► The motivations:

- Theoretical studies of these types of materials are motivated by **real-world applications**: proper functioning of many practical devices relies on optical properties of certain liquid crystalline substances in the presence or absence of an electric field: **a multi-billion dollar industry**
- At the molecular level, what marks the difference between a liquid crystal and an ordinary, isotropic fluid is that, while the centers of mass of LC molecules do not exhibit any long-range correlation, **molecular orientations do exhibit orientational correlations**

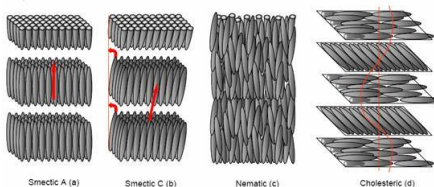
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- ▶ The objective: include the **temperature dependence** in models describing the **evolution of nematic liquid crystal flows** within the **Landau-De Gennes** theories (cf. [De Gennes, Prost (1995)])

To the present state of knowledge, three main types of liquid crystals are distinguished, termed *smectic*, *nematic* and *cholesteric*



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The *smectic* phase forms well-defined layers that can slide one over another in a manner very similar to that of a soap

The *nematic* phase: the molecules have long-range orientational order, but no tendency to the formation of layers. Their center of mass positions all point in the **same direction** (within each specific domain)

Crystals in the *cholesteric* phase exhibit a twisting of the molecules perpendicular to the director, with the molecular axis parallel to the director

- We consider the range of temperatures typical for the **nematic phase**



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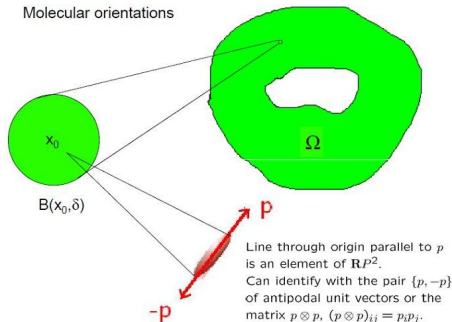


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- ▶ The flow **velocity v** evidently disturbs the alignment of the molecules and also the converse is true: a change in the alignment will produce a perturbation of the velocity field v . Moreover, we want to include in our model also the **changes of the temperature θ**

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- The distribution of molecular orientations in a ball $B(x_0, \delta)$, $x_0 \in \Omega$ can be represented as a probability measure μ on the unit sphere \mathbb{S}^2 satisfying $\mu(E) = \mu(-E)$ for $E \subset \mathbb{S}^2$
- For a continuously distributed measure we have $d\mu(p) = \rho(p)dp$ where dp is an element of the surface area on \mathbb{S}^2 and $\rho \geq 0$, $\int_{\mathbb{S}^2} \rho(p)dp = 1$, $\rho(p) = \rho(-p)$



- The first moment $\int_{\mathbb{S}^2} p d\mu(p) = 0$, the second moment $M = \int_{\mathbb{S}^2} p \otimes p d\mu(p)$ is a symmetric non-negative 3×3 matrix (for every $\mathbf{v} \in \mathbb{S}^2$,
 $\mathbf{v} \cdot M \cdot \mathbf{v} = \int_{\mathbb{S}^2} (\mathbf{v} \cdot p)^2 d\mu(p) = \langle \cos^2 \theta \rangle$, where θ is the angle between p and \mathbf{v})
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- If the orientation of molecules is equally distributed in all directions (the distribution is *isotropic*) and then $\mu = \mu_0$, where $d\mu_0(p) = \frac{1}{4\pi} dS$. In this case the second moment tensor is $M_0 = \frac{1}{4\pi} \int_{\mathbb{S}^2} p \otimes p dS = \frac{1}{3} \mathbf{1}$, because $\int_{\mathbb{S}^2} p_1 p_2 dS = 0$, $\int_{\mathbb{S}^2} p_1^2 dS = \int_{\mathbb{S}^2} p_2^2 dS$, etc., and $\text{tr}(M_0) = 1$

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- ▶ **The de Gennes \mathbb{Q} -tensor** measures the deviation of M from its isotropic value

$$\mathbb{Q} = M - M_0 = \int_{\mathbb{S}^2} \left(p \otimes p - \frac{1}{3} \mathbf{1} \right) d\mu(p)$$

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Note that (cf. [Ball, Majumdar, Molecular Crystals and Liquid Crystals (2010)])

1. $\mathbb{Q} = \mathbb{Q}^T$
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- 1.+2. implies $\mathbb{Q} = \lambda_1 \mathbf{n}_1 \otimes \mathbf{n}_1 + \lambda_2 \mathbf{n}_2 \otimes \mathbf{n}_2 + \lambda_3 \mathbf{n}_3 \otimes \mathbf{n}_3$, where $\{\mathbf{n}_i\}$ is an orthonormal basis of eigenvectors of \mathbb{Q} with corresponding eigenvalues λ_i such that $\lambda_1 + \lambda_2 + \lambda_3 = 0$
- 2.+3. implies $-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3}$
- $\mathbb{Q} = 0$ does not imply $\mu = \mu_0$ (e.g. $\mu = \frac{1}{6} \sum_{i=1}^3 (\delta_{e_i} + \delta_{-e_i})$)

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- In order to **naturally enforce the physical constraints in the eigenvalues of the symmetric, traceless tensors** \mathbb{Q} , Ball and Majumdar have recently introduced in [Ball, Majumdar, Molecular Crystals and Liquid Crystals (2010)] a **singular component**

$$f(\mathbb{Q}) = \begin{cases} \inf_{\rho \in \mathcal{A}_{\mathbb{Q}}} \int_{S^2} \rho(\mathbf{p}) \log(\rho(\mathbf{p})) \, d\mathbf{p} & \text{if } \lambda_i[\mathbb{Q}] \in (-1/3, 2/3), \, i = 1, 2, 3, \\ \infty & \text{otherwise,} \end{cases}$$

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to the bulk free-energy f_B enforcing the eigenvalues to stay in the interval $(-\frac{1}{3}, \frac{2}{3})$

[\Rightarrow] For the **Landau-de Gennes** free energy with “regular” potential, the hydrodynamic theory has been developed in [Paicu, Zarnescu, SIAM (2011) and ARMA (2012)] in the isothermal case

We study the **non-isothermal** evolutionary system for nematic liquid crystals within the recent Ball-Majumdar \mathbb{Q} -tensorial model preserving the physical eigenvalue constraint on the **traceless and symmetric matrices \mathbb{Q}** :

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We work in the three-dimensional torus $\Omega \subset \mathbb{R}^3$ in order to avoid complications connected with boundary conditions. We consider the evolution of the following variables:

- the mean velocity field \mathbf{v}
- the tensor field \mathbb{Q} , representing preferred (local) orientation of the crystals
- the absolute temperature θ

- The free energy density takes the form

$$\mathcal{F} = \frac{1}{2} |\nabla \mathbb{Q}|^2 + f_B(\theta, \mathbb{Q}) - \theta \log \theta - a\theta^m$$

where

- $f_B(\theta, \mathbb{Q}) = \theta f(\mathbb{Q}) + G(\mathbb{Q})$ is bulk the configuration potential
- f is the convex l.s.c. and singular Ball-Majumdar potential, G is a smooth function of \mathbb{Q}
- $a\theta^m$ prescribes a power-like specific heat

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 - $a\theta^m$ prescribes a power-like specific heat
- The dissipation pseudo-potential is given by

$$\mathcal{P} = \frac{\nu(\theta)}{4} |\nabla \mathbf{v} + \nabla^t \mathbf{v}|^2 + I_{\{0\}}(\operatorname{div} \mathbf{v}) + \frac{\kappa(\theta)}{2\theta} |\nabla \theta|^2 + \frac{1}{2\Gamma(\theta)} |D_t \mathbb{Q}|^2$$

- ν , κ and Γ are the smooth viscosity, the heat conductivity, and the collective rotational coefficients, $D_t \mathbb{Q}$ is a “generalized material derivative”
- **Incompressibility**: I_0 the indicator function of $\{0\}$: $I_0 = 0$ if $\operatorname{div} \mathbf{v} = 0$, $+\infty$ otherwise)

We assume that the driving force governing the dynamics of the director \mathbf{Q} is of “**gradient type**” $\partial_{\mathbf{Q}}\mathcal{F}$:

$$\partial_t \mathbf{Q} + \mathbf{v} \cdot \nabla \mathbf{Q} - \mathbb{S}(\nabla \mathbf{v}, \mathbf{Q}) = \Gamma(\theta) \mathbb{H}, \quad (\text{eq-Q})$$

- The left hand side is the “generalized material derivative”

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- $\Gamma(\theta)$ represents a collective rotational viscosity coefficient
- The function f represents the convex part of a singular potential of **[Ball-Majumdar]** type

The Ball-Majumdar potential (cf. [Ball, Majumdar (2010)]) exhibit a logarithmic divergence as the eigenvalues of \mathbb{Q} approaches $-\frac{1}{3}$ and $\frac{2}{3}$

$$f(\mathbb{Q}) = \begin{cases} \inf_{\rho \in \mathcal{A}_{\mathbb{Q}}} \int_{S^2} \rho(\mathbf{p}) \log(\rho(\mathbf{p})) \, d\mathbf{p} & \text{if } \lambda_i[\mathbb{Q}] \in (-1/3, 2/3), \, i = 1, 2, 3, \\ \infty & \text{otherwise,} \end{cases}$$

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\implies It explodes “logarithmically” as one of the eigenvalues of \mathbb{Q} approaches the limiting values $-1/3$ or $2/3$.

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- The **coupling term (or “extra-stress”)** \mathbb{T} depends both on θ and \mathbb{Q}

$$\mathbb{T} = 2\xi (\mathbb{H} : \mathbb{Q}) \left(\mathbb{Q} + \frac{1}{3} \mathbb{I} \right) - \xi \left[\mathbb{H} \left(\mathbb{Q} + \frac{1}{3} \mathbb{I} \right) + \left(\mathbb{Q} + \frac{1}{3} \mathbb{I} \right) \mathbb{H} \right] + (\mathbb{Q} \mathbb{H} - \mathbb{H} \mathbb{Q}) - \nabla \mathbb{Q} \odot \nabla \mathbb{Q}$$

where ξ is a fixed scalar parameter

The evolution of temperature is prescribed by stating the **entropy inequality**

$$s_t + \mathbf{v} \cdot \nabla s - \operatorname{div} \left(\frac{\kappa(\theta)}{\theta} \nabla \theta \right) \quad (\text{eq-}\theta)$$

$$\geq \frac{1}{\theta} \left(\frac{\nu(\theta)}{2} |\nabla \mathbf{v} + \nabla^t \mathbf{v}|^2 + \Gamma(\theta) |\mathbb{H}|^2 + \frac{\kappa(\theta)}{\theta} |\nabla \theta|^2 \right)$$

where $s'' = -\partial_\theta \mathcal{F}'' = -f(\mathbb{Q}) + 1 + \log \theta + m a \theta^{m-1}$

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- The viscosity ν is smooth and bounded - without any growth condition
- $\kappa(r) = A_0 + A_k r^k$, $A_0, A_k > 0$, $\frac{3k+2m}{3} > 9$, $\frac{3}{2} < m \leq \frac{6k}{5}$
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- $\Gamma(r) = \Gamma_0 + \Gamma_1 r$, $\Gamma_0, \Gamma_1 > 0$
- The “heat” balance can be recovered by (formally) multiplying by θ
- Due to the **quadratic** terms, we can only interpret (eq- θ) as an **inequality**

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$$\begin{aligned} & \partial_t \left(\frac{1}{2} |\mathbf{v}|^2 + e \right) + \operatorname{div} \left(\left(\frac{1}{2} |\mathbf{v}|^2 + e \right) \mathbf{v} \right) + \operatorname{div} \mathbf{q} && \text{(eq-bal)} \\ & = \operatorname{div}(\boldsymbol{\sigma} \mathbf{v}) + \operatorname{div} \left(\Gamma(\theta) \nabla \mathbb{Q} : \left(\Delta \mathbb{Q} - \theta \frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} + \lambda \theta \right) \right) + \mathbf{g} \cdot \mathbf{v} \end{aligned}$$

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- To control it, assuming periodic b.c.'s is essential

Theorem: existence of global in time “Entropic solutions”

We can prove existence of at least one “Entropic solution” to system (eq-v)+(eq-Q)+(eq- θ)+(eq-bal) for finite-energy initial data , namely

$$\theta_0 \in L^\infty(\Omega), \quad \text{ess\,inf}_{x \in \Omega} \theta_0(x) = \underline{\theta} > 0,$$

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- Notice that, if the solution is more regular, the **entropy inequality** becomes an **equality** and, multiplying it by θ we just get the standard **internal energy balance**

$$\theta_t + \mathbf{v} \cdot \nabla_x \theta + \text{div } \mathbf{q} = \theta (\partial_t f(\mathbb{Q}) + \mathbf{u} \cdot \nabla_x f(\mathbb{Q})) + \nu(\theta) |\nabla_x \mathbf{v} + \nabla_x^t \mathbf{v}|^2 + \Gamma(\theta) |\mathbb{H}|^2$$

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- However, this regularity is out of reach for this model: that is why this solution notion is significant

Two-phase mixtures of fluids

- A **non-isothermal** model for the flow of a **mixture of two**
 - viscous
 - incompressible
 - Newtonian fluids
 - of equal density

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- A partial mixing of the macroscopically immiscible fluids is allowed
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- The original idea of diffuse interface model for fluids: HOHENBERG and HALPERIN, '77
 - ⇒ **H-model**
 - Later, GURTIN ET AL., '96: continuum mechanical derivation based on microforces
- Models of two-phase or two-component fluids are receiving growing attention (e.g., ABELS, BOYER, GARCKE, GRÜN, GRASSELLI, LOWENGRUB, TRUSKINOVSKI, ...)

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- Our idea: a weak formulation of the system as a combination of *total energy balance* plus *entropy production inequality* \implies “**Entropic formulation**”

- This method has been recently proposed by [BULÍČEK-MÁLEK-FEIREISL, '09] for the Navier-Stokes-Fourier system and has been proved to be effective to study e.g.

- nonisothermal models for **phase transitions** ([FEIREISL-PETZELTOVÁ-R., '09]) and
- the evolution of **nematic liquid crystals** ([FRÉMOND, FEIREISL, R., SCHIMPERNA, ZARNESCU, '12,'13])

- We want to describe the behavior of a mixture of two incompressible fluids of the same density in terms of the following state variables
 - \mathbf{v} : macroscopic **velocity** (Navier-Stokes),
 - p : **pressure** (Navier-Stokes),
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 - θ : **absolute temperature** (Entropic formulation).
- We do not neglect convection and capillarity effects. We assume constant mobility and smooth configuration potential in Cahn-Hilliard. We take temperature dependent coefficients wherever possible. We assume the system being insulated from the exterior.

- We start by specifying two functionals:
 - the **free energy** Ψ , related to the equilibrium state of the material, and
 - the **dissipation pseudo-potential** Φ , describing the processes leading to dissipation of energy (i.e., transformation into heat)

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- The **thermodynamical consistency** of the model is then a direct consequence of the solution notion

The **total free energy** is given as a function of the state variables $E = (\theta, \varphi, \nabla_x \varphi)$

$$\Psi(E) = \int_{\Omega} \psi(E) \, dx, \quad \psi(E) = f(\theta) - \theta\varphi + \frac{\varepsilon}{2} |\nabla_x \varphi|^2 + \frac{1}{\varepsilon} F(\varphi)$$

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- $\varepsilon > 0$ is related to the interfacial thickness
- we need $F(\varphi)$ to be the classical smooth double well potential $F(\varphi) \sim \frac{1}{4}(\varphi^2 - 1)^2$

The **dissipation potential** is taken as function of $\delta E = (D\mathbf{u}, \frac{D\varphi}{Dt}, \nabla_x \theta)$ and E

$$\Phi(\delta E, E) = \int_{\Omega} \left(\frac{\nu(\theta)}{2} |D\mathbf{v}|^2 + I_{\{0\}}(\operatorname{div} \mathbf{v}) + \frac{\kappa(\theta)}{2\theta} |\nabla_x \theta|^2 + \frac{|\nabla_x \mu|^2}{2} \right) dx$$

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- the chemical potential μ is defined as $\frac{D\varphi}{Dt} = \Delta\mu$

- It is obtained (at least for no-flux b.c.'s) as the following **gradient-flow problem**

$$\partial_{L^2_{\#}(\Omega), \frac{D\varphi}{Dt}} \Phi + \partial_{L^2_{\#}(\Omega), \varphi_{\#}} \Psi = 0$$

where $L^2_{\#}(\Omega) = \{\xi \in L^2(\Omega) : \bar{\xi} := |\Omega|^{-1} \int_{\Omega} \xi \, dx = 0\}$, $\varphi_{\#} = \varphi - \bar{\varphi}_0$

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- Using the form of the Free energy

$$\Psi = \int_{\Omega} \left(f(\theta) - \theta\varphi + \frac{\varepsilon}{2} |\nabla_x \varphi|^2 + \frac{1}{\varepsilon} F(\varphi) \right) dx$$

and of the Pseudopotential of dissipation

$$\Phi = \int_{\Omega} \left(\frac{\nu(\theta)}{2} |D\mathbf{v}|^2 + I_{\{0\}}(\operatorname{div} \mathbf{v}) + \frac{\kappa(\theta)}{2\theta} |\nabla_x \theta|^2 + \frac{|\nabla_x \mu|^2}{2} \right) dx$$

we then arrive at **the Cahn-Hilliard system with Neumann hom. b.c. for μ and φ**

$$\frac{D\varphi}{Dt} = \Delta\mu, \quad \mu = -\varepsilon\Delta\varphi + \frac{1}{\varepsilon} F'(\varphi) - \theta, \quad \frac{\partial\varphi}{\partial\mathbf{n}} = \frac{\partial\mu}{\partial\mathbf{n}} = 0 \text{ on } \Gamma \quad (\text{CahnHill})$$

The **Navier-Stokes system** is obtained as a momentum balance by setting

$$\frac{D\mathbf{v}}{Dt} = \mathbf{v}_t + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) = \operatorname{div} \boldsymbol{\sigma}, \quad (\text{momentum})$$

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where the stress $\boldsymbol{\sigma}$ is split into its

- **dissipative part**

$$\boldsymbol{\sigma}^d := \frac{\partial \phi}{\partial D\mathbf{v}} = \nu(\theta) D\mathbf{v} - p\mathbb{I}, \quad \operatorname{div} \mathbf{v} = 0,$$

representing kinetic energy which **dissipates** (i.e. is transformed into heat) due to viscosity, and its

- **non-dissipative part** $\boldsymbol{\sigma}^{nd} = -\varepsilon \nabla_x \varphi \otimes \nabla_x \varphi$ which is determined in agreement with Thermodynamics

The balance of internal energy takes the form

$$(Q(\theta))_t + \mathbf{v} \cdot \nabla_x Q(\theta) + \theta \frac{D\varphi}{Dt} - \operatorname{div}(\kappa(\theta)\nabla_x \theta) = \nu(\theta)|D\mathbf{v}|^2 + |\nabla_x \mu|^2$$

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The **dissipation** terms on the right hand side are in perfect agreement with the Pseudopotential of dissipation

$$\Phi = \int_{\Omega} \left(\frac{\nu(\theta)}{2} |D\mathbf{v}|^2 + I_{\{0\}}(\operatorname{div} \mathbf{v}) + \frac{\kappa(\theta)}{2\theta} |\nabla_x \theta|^2 + \frac{|\nabla_x \mu|^2}{2} \right) dx$$

Following [BULÍČEK, FEIREISL, & MÁLEK], we replace the pointwise internal energy balance by the **total energy balance**

$$\begin{aligned} (\partial_t + \mathbf{v} \cdot \nabla_x) \left(\frac{|\mathbf{v}|^2}{2} + e \right) + \operatorname{div} (p\mathbf{v} - \kappa(\theta)\nabla_x\theta - (\nu(\theta)D\mathbf{v})\mathbf{v}) \\ = \operatorname{div} (\varphi_t\nabla_x\varphi + \mu\nabla_x\mu) \end{aligned} \quad \text{(energy)}$$

with the internal energy

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with the internal energy

$$e = F(\varphi) + \frac{1}{2}|\nabla_x\varphi|^2 + Q(\theta) \quad Q'(\theta) = c_v(\theta)$$

and the **entropy inequality**

$$\begin{aligned} (\Lambda(\theta) + \varphi)_t + \mathbf{v} \cdot \nabla_x(\Lambda(\theta) + \varphi) - \operatorname{div} \left(\frac{\kappa(\theta)\nabla_x\theta}{\theta} \right) \\ \geq \frac{\nu(\theta)}{\theta}|D\mathbf{v}|^2 + \frac{1}{\theta}|\nabla_x\mu|^2 + \frac{\kappa(\theta)}{\theta^2}|\nabla_x\theta|^2, \quad \text{where } \Lambda(\theta) = \int_1^\theta \frac{c_v(s)}{s} ds \sim \theta^\delta \end{aligned} \quad \text{(entropy)}$$

- a **weak form of the momentum balance** (in distributional sense)

$$\mathbf{v}_t + \mathbf{v} \cdot \nabla_x \mathbf{v} + \nabla_x p = \operatorname{div}(\nu(\theta) D\mathbf{v}) - \operatorname{div}(\nabla_x \varphi \otimes \nabla_x \varphi), \quad \operatorname{div} \mathbf{v} = 0;$$

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- the **Cahn-Hilliard system** in $H^1(\Omega)'$

$$\varphi_t + \mathbf{v} \cdot \nabla_x \varphi = \Delta \mu, \quad \mu = -\Delta \varphi + F'(\varphi) - \theta;$$

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$$\begin{aligned} \partial_t \left(\frac{1}{2} |\mathbf{v}|^2 + e \right) + \mathbf{v} \cdot \nabla_x \left(\frac{1}{2} |\mathbf{v}|^2 + e \right) + \operatorname{div} \left(p\mathbf{v} + \mathbf{q} - \mathbb{S}\mathbf{u} \right) \\ - \operatorname{div} \left(\varphi_t \nabla_x \varphi + \mu \nabla_x \mu \right) = 0 \quad \text{where} \quad e = F(\varphi) + \frac{1}{2} |\nabla_x \varphi|^2 + \int_1^\theta c_v(s) \, ds; \end{aligned}$$

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- the weak form of the **entropy production inequality**

$$\begin{aligned} (\Lambda(\theta) + \varphi)_t + \mathbf{v} \cdot \nabla_x (\Lambda(\theta)) + \mathbf{v} \cdot \nabla_x \varphi - \operatorname{div} \left(\frac{\kappa(\theta) \nabla_x \theta}{\theta} \right) \\ \geq \frac{\nu(\theta)}{\theta} |D\mathbf{v}|^2 + \frac{1}{\theta} |\nabla_x \mu|^2 + \frac{\kappa(\theta)}{\theta^2} |\nabla_x \theta|^2, \quad \text{where} \quad \Lambda(\theta) = \int_1^\theta \frac{c_v(s)}{s} ds. \end{aligned}$$

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 - The **viscosity** $\nu(\theta)$ is assumed **smooth and bounded**
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 - The potential $F(\varphi) = \frac{1}{4}(\varphi^2 - 1)^2$
- Concerning B.C.'s, our results are proved for **no-flux** conditions for θ , φ , and μ and **complete slip** conditions for \mathbf{v}

$\mathbf{v} \cdot \mathbf{n}|_\Gamma = 0$ (the fluid cannot exit Ω , it can move tangentially to Γ)

$[\mathbb{S}\mathbf{n}] \times \mathbf{n}|_\Gamma = 0$, where $\mathbb{S} = \nu(\theta)D\mathbf{v}$ (exclude friction effects with the boundary)

They can be easily extended to the case of periodic B.C.'s for all unknowns

Theorem

We can prove existence of **at least one global in time “Entropic solution”** $(\mathbf{v}, \varphi, \mu, \theta)$

$$\mathbf{v} \in L^\infty(0, T; L^2(\Omega; \mathbb{R}^3)) \cap L^2(0, T; \mathbf{V}_n)$$

$$\varphi \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^3(\Omega)) \cap H^1(0, T; H^1(\Omega)')$$

$$\mu \in L^2(0, T; H^1(\Omega)) \cap L^{\frac{14}{5}}((0, T) \times \Omega)$$

$$\theta \in L^\infty(0, T; L^{\delta+1}(\Omega)) \cap L^\beta(0, T; L^{3\beta}(\Omega)) \cap L^2(0, T; H^1(\Omega))$$

$$\theta > 0 \text{ a.e. in } (0, T) \times \Omega, \quad \log \theta \in L^2(0, T; H^1(\Omega))$$

to system given by (momentum), (CahnHill), (entropy) and (energy), in distributional sense and for finite-energy initial data

$$\mathbf{v}_0 \in L^2(\Omega), \quad \operatorname{div} \mathbf{v}_0 = 0, \quad \varphi_0 \in H^1(\Omega), \quad \theta_0 \in L^{\delta+1}(\Omega), \quad \theta_0 > 0 \text{ a.e.}$$

Damage phenomena

State variables:

- the absolute temperature θ
- the (small) displacement variables \mathbf{u} ($\varepsilon_{ij}(\mathbf{u}) := (u_{i,j} + u_{j,i})/2, i, j = 1, 2, 3$)
- the **damage** parameter $\chi \in [0, 1]$: $\chi = 0$ (completely damaged), $\chi = 1$ (completely undamaged)

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$$\theta_t + \chi_t \theta + \rho \theta \operatorname{div} \mathbf{u}_t - \operatorname{div}(\mathbf{K}(\theta) \nabla \theta) = g + a(\chi) |\varepsilon(\mathbf{u}_t)|^2 + |\chi_t|^2$$

$$\mathbf{u}_{tt} - \operatorname{div}(a(\chi) \varepsilon(\mathbf{u}_t) + b(\chi) \varepsilon(\mathbf{u}) - \rho \theta \mathbf{1}) = \mathbf{f}$$

$$\chi_t + \partial I_{(-\infty, 0]}(\chi_t) - \operatorname{div}(|\nabla \chi|^{p-2} \nabla \chi) + W'(\chi) \ni -b'(\chi) \frac{|\varepsilon(\mathbf{u})|^2}{2} + \theta$$

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- **Unidirectional:** $I_{(-\infty, 0]}(\chi_t) = 0$ if $\chi_t \in (-\infty, 0]$, $I_{(-\infty, 0]}(\chi_t) = +\infty$ otherwise;
- p -Laplacian: $-\Delta_p : W^{1,p}(\Omega) \rightarrow W^{1,p}(\Omega)^*$ ($p > d$ for this presentation);
- **The double-obstacle:** $W = \widehat{\beta} + \widehat{\gamma}$, $\widehat{\gamma} \in C^2(\mathbb{R})$, $\widehat{\beta}$ proper, convex, l.s.c. (e.g. $\widehat{\beta} = I_{[0,1]}$)

- **GLOBAL - in time - existence result for the FULL PDE system** displaying the high order dissipative terms on the right hand in side in the temperature equation:

$$\theta_t + \chi_t \theta + \rho \theta \operatorname{div} \mathbf{u}_t - \operatorname{div}(\mathbf{K}(\theta) \nabla \theta) = g + a(\chi) |\varepsilon(\mathbf{u}_t)|^2 + |\chi_t|^2$$

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- ⇒ These terms were neglected in most of the past contribution in the literature or considered only in the 1D case or in the framework of local - in time - existence (cf., e.g., [E. Bonetti, G. Bonfanti (2007)], [P. Krečí, J. Sprekels, U. Stefanelli (2003)], [F. Luterotti and U. Stefanelli (2002)], [E.R., R. Rossi (2013)])

The free-energy cf. [M. Frémond, Phase Change in Mechanics, Lecture Notes of UMI, Springer-Verlag, 2012]

$$\mathcal{F} = \int_{\Omega} \left(\theta(1 - \log \theta) + b(\chi) \frac{|\varepsilon(\mathbf{u})|^2}{2} + \frac{|\nabla \chi|^p}{p} + W(\chi) - \theta \chi - \rho \theta \operatorname{tr}(\varepsilon(\mathbf{u})) \right) dx$$

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The pseudo-potential of dissipation

$$\mathcal{P} = \frac{K(\theta)}{2} |\nabla \theta|^2 + \frac{1}{2} |\chi_t|^2 + a(\chi) \frac{|\varepsilon(\mathbf{u}_t)|^2}{2} + I_{(-\infty, 0]}(\chi_t)$$

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- e.g. $a(\chi) = \chi$: no viscosity when the material is completely damaged
- K is the heat conductivity, $K(\theta) \geq c_1(1 + \nu \theta^k)$ for some $c_1, \nu > 0, k > 1$
- $I_{(-\infty, 0]}(\chi_t) = 0$ if $\chi_t \in (-\infty, 0]$, $I_{(-\infty, 0]}(\chi_t) = +\infty$ otherwise (**irreversibility** of the damage)

The momentum equation

$$\mathbf{u}_{tt} - \operatorname{div} \sigma = \mathbf{f} \quad \left(\sigma = \sigma^d + \sigma^{nd} = \frac{\partial \mathcal{P}}{\partial \varepsilon(\mathbf{u}_t)} + \frac{\partial \mathcal{F}}{\partial \varepsilon(\mathbf{u})} \right) \quad \text{becomes}$$

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The “standard” principle of virtual powers

$$B - \operatorname{div} \mathbf{H} = 0 \quad \left(B = \frac{\partial \mathcal{P}}{\partial \chi_t} + \frac{\partial \mathcal{F}}{\partial \chi}, \mathbf{H} = \frac{\partial \mathcal{F}}{\partial \nabla \chi} \right) \quad \text{becomes}$$

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The internal energy balance

$$e_t + \operatorname{div} \mathbf{q} = g + \boldsymbol{\sigma} : \boldsymbol{\varepsilon}(\mathbf{u}_t) + B\chi_t + \mathbf{H} \cdot \nabla \chi_t \quad \left(e = \mathcal{F} - \theta \frac{\partial \mathcal{F}}{\partial \theta}, \quad \mathbf{q} = \frac{\partial \mathcal{P}}{\partial \nabla \theta} \right)$$

becomes

$$\theta_t + \chi_t \theta + \rho \theta \operatorname{div} \mathbf{u}_t - \operatorname{div}(\mathbf{K}(\theta) \nabla \theta) = g + a(\chi) |\boldsymbol{\varepsilon}(\mathbf{u}_t)|^2 + |\chi_t|^2$$

[The last result] [E.R., R. Rossi, preprint arXiv:1205.3578v2 (2012), to appear on M3AS]: **global existence result in 3D** using a suitable notion of solution and without enforcing the separation property, i.e. **allowing for degeneracy**: $a(\chi) = b(\chi) = \chi$, but always within the **small perturbations assumption, i.e. neglecting the quadratic terms** on the r.h.s. in the internal energy balance

[Our goals] We restrict to the non-degenerate case \implies replace a and b by $a + \delta$, $b + \delta$ in the momentum balance:

$$\mathbf{u}_{tt} - \operatorname{div}((a(\chi) + \delta)\varepsilon(\mathbf{u}_t) + (b(\chi) + \delta)\varepsilon(\mathbf{u}) - \rho\theta\mathbf{1}) = \mathbf{f} \quad \text{for } \delta > 0$$

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In order to handle

- the high order dissipative terms in the θ -equation
- the quadratic nonlinearity in the χ -equation

we need a suitable **weak formulation**

Hypothesis (I).

The function $K : [0, +\infty) \rightarrow (0, +\infty)$ is continuous and

$$\exists c_0, c_1, \nu > 0, k > 1 : \forall \theta \in [0, +\infty) \quad c_0(1 + \theta^k) \leq K(\theta) \leq c_1(1 + \nu\theta^k)$$

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Hypothesis (II). $a \in C^1(\mathbb{R})$, $b \in C^2(\mathbb{R})$ are such that $a(x)$, $b(x) \geq 0$, for all $x \in \mathbb{R}$

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Hypothesis (III). $W = \widehat{\beta} + \widehat{\gamma}$, where

$\widehat{\beta} : \text{dom}(\widehat{\beta}) \rightarrow \mathbb{R}$ is proper, l.s.c., convex;, $\text{dom}(\widehat{\beta}) \subseteq [0, +\infty)$ is bounded,

$$\widehat{\gamma} \in C^2(\mathbb{R}), \quad \exists c_w, c'_w > 0 : \quad W(r) \geq c_w r^2 - c'_w \quad \forall r \in \text{dom}(\widehat{\beta})$$

Hereafter, we shall denote by $\beta = \partial\widehat{\beta}$ the subdifferential of $\widehat{\beta}$, and set $\gamma := \widehat{\gamma}'$

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Hypothesis (IV).

$$\mathbf{f} \in L^2(0, T; L^2(\Omega)),$$

$$g \in L^1(0, T; L^1(\Omega)) \cap L^2(0, T; H^1(\Omega)'), \quad g \geq 0 \quad \text{a.e. in } \Omega \times (0, T),$$

and that the initial data comply with

$$\theta_0 \in L^1(\Omega), \quad \exists \theta_* > 0 : \min_{\Omega} \theta_0 \geq \theta_* > 0, \quad \log \theta_0 \in L^1(\Omega),$$

$$\mathbf{u}_0 \in H_0^2(\Omega), \quad \mathbf{v}_0 \in L^2(\Omega; \mathbb{R}^d), \quad \chi_0 \in W^{1,p}(\Omega), \quad \widehat{\beta}(\chi_0) \in L^1(\Omega).$$

Given $\delta > 0$ there exists (measurable) functions

$$\theta \in L^\infty(0, T; L^1(\Omega)) \cap L^2(0, T; H^1(\Omega)),$$

$$\mathbf{u} \in H^1(0, T; H_0^2(\Omega)) \cap W^{1,\infty}(0, T; H_0^1(\Omega; \mathbb{R}^d)) \cap H^2(0, T; L^2(\Omega; \mathbb{R}^d)),$$

$$\chi \in L^\infty(0, T; H^1(\Omega)) \cap H^1(0, T; L^2(\Omega)),$$

fulfilling the initial conditions

$$\mathbf{u}(0, x) = \mathbf{u}_0(x), \quad \mathbf{u}_t(0, x) = \mathbf{v}_0(x) \quad \text{for a.e. } x \in \Omega$$

$$\chi(0, x) = \chi_0(x) \quad \text{for a.e. } x \in \Omega$$

together with

the *entropy inequality*

the *total energy inequality*

the weak momentum equation (a.e. in $\Omega \times (0, T)$)

the *generalized principle of virtual powers*

The *entropy inequality*

$$\begin{aligned} & \int_0^T \int_{\Omega} (\log(\theta) + \chi) \varphi_t \, dx \, dt + \rho \int_0^T \int_{\Omega} \operatorname{div}(\mathbf{u}_t) \varphi \, dx \, dt - \int_0^T \int_{\Omega} \mathbf{K}(\theta) \nabla \log(\theta) \cdot \nabla \varphi \, dx \, dt \\ & \leq - \int_0^T \int_{\Omega} \mathbf{K}(\theta) \frac{\varphi}{\theta} \nabla \log(\theta) \cdot \nabla \theta \, dx \, dt - \int_0^T \int_{\Omega} ((a(\chi) + \delta) |\varepsilon(\mathbf{u}_t)|^2 + g + |\chi_t|^2) \frac{\varphi}{\theta} \, dx \, dt \end{aligned}$$

for all $\varphi \in \mathcal{D}(\bar{\Omega} \times [0, T])$ with $\varphi \geq 0$;

The *entropy inequality*

$$\int_0^T \int_{\Omega} (\log(\theta) + \chi) \varphi_t \, dx \, dt + \rho \int_0^T \int_{\Omega} \operatorname{div}(\mathbf{u}_t) \varphi \, dx \, dt - \int_0^T \int_{\Omega} \mathbf{K}(\theta) \nabla \log(\theta) \cdot \nabla \varphi \, dx \, dt$$

$$\leq - \int_0^T \int_{\Omega} \mathbf{K}(\theta) \frac{\varphi}{\theta} \nabla \log(\theta) \cdot \nabla \theta \, dx \, dt - \int_0^T \int_{\Omega} ((a(\chi) + \delta) |\varepsilon(\mathbf{u}_t)|^2 + g + |\chi_t|^2) \frac{\varphi}{\theta} \, dx \, dt$$

for all $\varphi \in \mathcal{D}(\bar{\Omega} \times [0, T])$ with $\varphi \geq 0$;

The *total energy inequality* for almost all $t \in (0, T)$ and almost all $s \in (0, t)$, and for $s = 0$

$$E(\theta(t), \mathbf{u}(t), \mathbf{u}_t(t), \chi(t)) \leq E(\theta(s), \mathbf{u}(s), \mathbf{u}_t(s), \chi(s)) + \int_s^t \int_{\Omega} g \, dx \, dr \int_s^t \int_{\Omega} \mathbf{f} \cdot \mathbf{u}_t \, dx \, dr$$

where

$$E(\theta, \mathbf{u}, \mathbf{u}_t, \chi) := \int_{\Omega} \theta + \frac{1}{2} \int_{\Omega} |\mathbf{u}_t|^2 + \frac{1}{2} (b(\chi(t)) + \delta) |\varepsilon(\mathbf{u})|^2(t) + \frac{1}{p} \int_{\Omega} |\nabla \chi|^p + \int_{\Omega} W(\chi)$$

The relations: $\chi_t(x, t) \leq 0$ for almost all $(x, t) \in \Omega \times (0, T)$, as well as

$$\int_{\Omega} \left(\chi_t(t)\varphi + |\nabla\chi(t)|^{p-2} \nabla\chi(t) \cdot \nabla\varphi + \xi(t)\varphi + \gamma(\chi(t))\varphi + b'(\chi(t)) \frac{|\varepsilon(\mathbf{u}(t))|^2}{2} \varphi - \theta(t)\varphi \right) \geq 0$$

for all $\varphi \in W_-^{1,p}(\Omega)$, for a.a. $t \in (0, T)$

with $\xi \in \partial I_{[0,+\infty)}(\chi)$ in the following sense:

$$\xi \in L^1(0, T; L^1(\Omega)) \quad \text{and} \quad \langle \xi(t), \varphi - \chi(t) \rangle_{W^{1,p}(\Omega)} \leq 0 \quad \forall \varphi \in W_+^{1,p}(\Omega), \text{ for a.a. } t \in (0, T)$$

and the energy inequality for all $t \in (0, T]$, for $s = 0$ and for almost all $0 < s \leq t$:

$$\begin{aligned} \int_s^t \int_{\Omega} |\chi_t|^2 \, dx \, dr + \int_{\Omega} \left(\frac{1}{p} |\nabla\chi(t)|^p + W(\chi(t)) \right) \, dx \\ \leq \int_{\Omega} \left(\frac{1}{p} |\nabla\chi(s)|^p + W(\chi(s)) \right) \, dx + \int_s^t \int_{\Omega} \chi_t \left(-b'(\chi) \frac{|\varepsilon(\mathbf{u})|^2}{2} + \theta \right) \, dx \, dr \end{aligned}$$

where

$$W_+^{1,p}(\Omega) := \left\{ \zeta \in W^{1,p}(\Omega) : \zeta(x) \geq 0 \text{ for a.a. } x \in \Omega \right\} \quad \text{and analogously for } W_-^{1,p}(\Omega)$$

- If $(\theta, \mathbf{u}, \chi)$ are "more regular" and satisfy the notion of *weak solution*:
the one-sided inequality ($\forall \varphi \in L^2(0, T; W_-^{1,p}(\Omega)) \cap L^\infty(Q)$):

$$\int_0^T \int_\Omega \chi_t \varphi + |\nabla \chi|^{p-2} \nabla \chi \nabla \varphi + \xi \varphi + \gamma(\chi) \varphi + b'(\chi) \frac{|\varepsilon(\mathbf{u})|^2}{2} \varphi - \theta \varphi \geq 0$$

(one-sided)

with $\xi \in \partial I_{[0,+\infty)}(\chi)$ and the energy inequality:

$$\begin{aligned} & \int_s^t \int_\Omega |\chi_t|^2 dx dr + \frac{1}{p} |\nabla \chi(t)|^p + \int_\Omega W(\chi(t)) dx \\ & \leq \frac{1}{p} |\nabla \chi(s)|^p + \int_\Omega W(\chi(s)) dx + \int_s^t \int_\Omega \chi_t \left(-b'(\chi) \frac{|\varepsilon(\mathbf{u})|^2}{2} + \theta \right) dx dr \end{aligned}$$

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(energy)

- “Differentiating in time” the *energy inequality* (energy) and using the chain rule, we conclude that $(\theta, \mathbf{u}, \chi, \xi)$ comply with

$$\langle \chi_t(t) - \Delta_p \chi(t) + \xi(t) + \gamma(\chi(t)) + b'(\chi) \frac{|\varepsilon(\mathbf{u})|^2}{2} - \theta(t), \chi_t(t) \rangle_{W^{1,p}(\Omega)} \leq 0 \text{ for a.e. } t$$

(ineq)

(one-sided) – (ineq) + “ $\chi_t \leq 0$ a.e.” are equivalent to the usual phase inclusion

$$\chi_t - \Delta_p \chi + \xi + \gamma(\chi) + b'(\chi) \frac{|\varepsilon(\mathbf{u})|^2}{2} - \theta \in -\partial I_{(-\infty, 0]}(\chi_t) \text{ in } W^{1,p}(\Omega)^*$$

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