

# Weak formulations of PDEs in thermomechanics

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- The most recent applications:
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- The main advantages and the potential future perspectives:
  - ◇ Non-isothermal mixtures of binary immiscible fluids [with S. Frigeri, G. Schimperna, ...]
  - ◇ The induction hardening of steel [with D. Hömberg], the SMA with possibility of voids [with M. Frémond], ...



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  - ▶ **aim**: deal with the nematic liquid crystals both in the [Oseen-Frank theory](#), in which the mean orientation of the rod-like molecules is described by a **vector field  $\mathbf{d}$**  and also in the [Landau-de Gennes theory](#), in which the order parameter describing the orientation of molecules is a matrix, the so-called **Q-tensor**
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- **Damage** phenomena:

- ▶ **aim**: deal with diffuse interface models in thermoviscoelasticity accounting for
  - the evolution of the displacement variables
  - the temperature
  - the order (damage) parameter  $\chi$

where the momentum equation for contains  $\chi$ -dependent elliptic operators, which may **degenerate** at the *pure phases*

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- Liquid crystals

$$\operatorname{div} \mathbf{v} = 0, \quad \mathbf{v}_t + \mathbf{v} \cdot \nabla_x \mathbf{v} + \nabla_x p = \operatorname{div} \mathbb{S} + \operatorname{div} \sigma^{nd} + \mathbf{g}$$

$$\mathbb{S} = \nu(\theta) (\nabla_x \mathbf{v} + \nabla_x^t \mathbf{v}), \quad \sigma^{nd} = -\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} + (\partial_d W(\mathbf{d}) - \Delta \mathbf{d}) \otimes \mathbf{d}$$

$$\theta_t + \mathbf{v} \cdot \theta + \operatorname{div} \mathbf{q} = \mathbb{S} : \nabla_x \mathbf{v} + |\Delta \mathbf{d} - \partial_d W(\mathbf{d})|^2$$

$$\mathbf{d}_t + \mathbf{v} \cdot \nabla_x \mathbf{d} - \mathbf{d} \cdot \nabla_x \mathbf{v} = \Delta \mathbf{d} - \partial_d W(\mathbf{d})$$

- Damage

$$c(\theta)\theta_t + \chi_t \theta - \rho \theta \operatorname{div} \mathbf{u}_t - \operatorname{div}(k(\theta) \nabla \theta) = g$$

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

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

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2. a *generalization of the principle of virtual powers* inspired by:
  - 2.1. the notion of *energetic solution* - A. Mielke and co-authors ([Bouchitté, Mielke, Roubíček, ZAMP. Angew. Math. Phys. (2009)] and [Mielke, Roubíček, Zeman, Comput. Methods Appl. Mech. Engrg. (2010)]) for rate-independent processes for damage phenomena and
  - 2.2. a notion of *weak solution* introduced by [Heinemann, Kraus, WIAS preprint 1569 and WIAS preprint 1520, to appear on Adv. Math. Sci. Appl. (2010)] for non-degenerating isothermal diffuse interface models for phase separation and damage

## Entropic formulation: a phase transitions model

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We consider there a model for solid-liquid phase transitions associated to a **nonlinear** PDE system

$$\begin{aligned}\theta_t + \chi_t \theta - \Delta \theta &= |\chi_t|^2 \\ \chi_t - \Delta \chi + W'(\chi) &= \theta - \theta_c\end{aligned}$$

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⇒ a new notion of solution is needed

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Finally, couple these relations to a suitable phase dynamics.



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$r$  represents the **entropy production rate**. Then, in order to comply with the Clausius-Duhem inequality, we assume:

- (i)  $r$  is a nonnegative measure on  $[0, T] \times \overline{\Omega} =: \overline{Q}_T$ ;
- (ii)  $r \geq \frac{1}{\theta} \left( |\chi_t|^2 - \frac{\mathbf{q} \cdot \nabla \theta}{\theta} \right) \geq 0$ .

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Taking  $\mathbf{q} = -\nabla \theta$ ,  $s = \log \theta + \chi$ , we get

$$\begin{aligned} \int_0^T \int_{\Omega} \left( (\log \theta + \chi) \partial_t \varphi - \nabla \log \theta \cdot \nabla \varphi \right) dx dt \\ \leq \int_0^T \int_{\Omega} \frac{1}{\theta} \left( -|\chi_t|^2 - \nabla \log \theta \cdot \nabla \theta \right) \varphi dx dt \end{aligned}$$

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$\Rightarrow$  the total entropy is controlled by dissipation.

## The energy conservation and phase relation

The total energy has to be preserved. Hence

$$E(t) = E(0) \text{ for a.e. } t \in [0, T],$$

where

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Finally, the phase dynamics results as

$$\chi_t - \Delta \chi + W'(\chi) = \theta - \theta_c \quad \text{a.e. in } \Omega \times (0, T),$$

where  $W$  is a double well or double obstacle potential:  $W = \widehat{\beta} + \widehat{\gamma}$  where

$\widehat{\beta} : \mathbb{R} \rightarrow [0, +\infty]$  is proper, lower semi-continuous, convex function

$\widehat{\gamma} \in C^2(\mathbb{R})$ ,  $\widehat{\gamma}' \in C^{0,1}(\mathbb{R}) : \widehat{\gamma}''(r) \geq -K$  for all  $r \in \mathbb{R}$ ,  $W(r) \geq c_w r^2$  for all  $r \in \text{dom}(\widehat{\beta})$

Examples:  $\widehat{\beta}(r) = r \ln(r) + (1 - r) \ln(1 - r)$  or  $\widehat{\beta}(r) = I_{[0,1]}(r)$ .

## The existence theorem [E. Feireisl, H. Petzeltová, E.R., M2AS (2009)]

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$$\theta \in L^\infty(0, T; L^1(\Omega)) \cap L^s(Q_T), \quad \theta(x, t) > 0 \quad \text{a. e. in } Q_T$$

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- However, in this case and similarly in many other situations, to prove that the solution has this extra regularity is **out of reach**
- **It can be suitable also in different applications** such as the ones related to phase transitions in viscoelastic materials, SMA, liquid crystal flows, etc.

## Entropic formulation: the hydrodynamics of liquid crystal flows

## A recent application: non-isothermal 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**

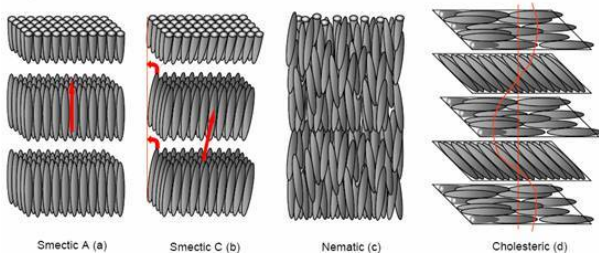
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## A recent application: non-isothermal liquid crystals

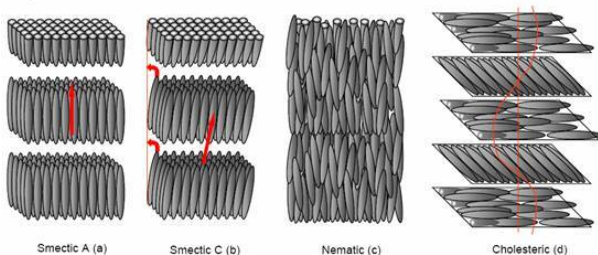
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  1. E. Feireisl, M. Frémond, E. R., G. Schimperna, A new approach to non-isothermal models for nematic liquid crystals, ARMA to appear, preprint arXiv:1104.1339v1 (2011)
  2. E. Feireisl, E.R., G. Schimperna, A. Zarnescu, Evolution of non-isothermal Landau-de Gennes nematic liquid crystals flows, paper in preparation

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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

# Our main aim



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



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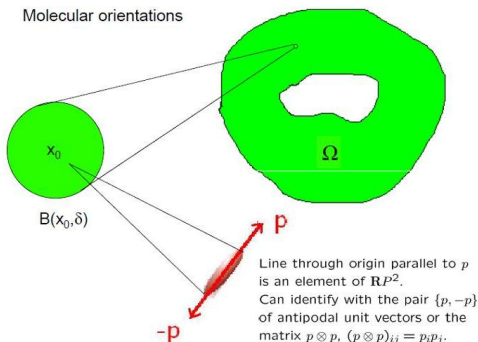
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- ▶ The flow **velocity  $\mathbf{u}$**  evidently disturbs the alignment of the molecules and also the converse is true: a change in the alignment will produce a perturbation of the velocity field  $\mathbf{u}$ . Moreover, we want to include in our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

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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  $\mu$  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 Landau-de Gennes theory: the $Q$ -tensor

- 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  $3 \times 3$  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  $\theta$  is the angle between  $p$  and  $\mathbf{v}$ ) satisfying  $\text{tr}(M) = 1$

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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

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

- ▶ 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  $\lambda_i$  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.  $\mu = \frac{1}{6} \sum_{i=1}^3 (\delta_{e_i} + \delta_{-e_i})$ )

# The reduction to the Oseen-Frank model

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- If the eigenvalues of  $\mathbb{Q}$  are all distinct then  $\mathbb{Q}$  is said to be *biaxial* (biaxiality implies the existence of more than one preferred direction of molecular alignment)
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**Reduction to the Oseen-Frank (1925, 1952) model (Ericksen model, 1991): the uniaxial case:**  $\lambda_1 = \lambda_2 = -\frac{s}{3}$ ,  $\lambda_3 = \frac{2s}{3}$ , setting  $\mathbf{n}_3 = \mathbf{d}$  where  $\mathbf{n}_i$  is an orthonormal basis of eigenvectors of  $\mathbb{Q}$  corresponding to  $\lambda_i$ , we have

$$\mathbb{Q} = -\frac{s}{3}(\mathbf{1} - \mathbf{d} \otimes \mathbf{d}) + \frac{2s}{3}\mathbf{d} \otimes \mathbf{d} = s \left( \mathbf{d} \otimes \mathbf{d} - \frac{1}{3}\mathbf{1} \right),$$

where  $-\frac{1}{2} \leq s \leq 1$ .

Here  $s \in \mathbb{R}$  is a real scalar order parameter that measures the degree of orientational ordering and  $\mathbf{d}$  is a **vector** representing the direction of preferred molecular alignment: the **director field**.

# The Landau-de Gennes free energy

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Suppose (for the moment) that the material is incompressible, homogeneous and at a constant temperature  $T$  in  $\Omega$ . At each  $x \in \Omega$  we have an order parameter tensor  $\mathbb{Q}(x)$  and **the Landau-de Gennes free energy** (defined in the space of traceless symmetric  $3 \times 3$  matrixes) is

$$\mathcal{F}_{LG}(\mathbb{Q}) = \int_{\Omega} \left( \frac{L}{2} |\nabla \mathbb{Q}(x)|^2 + f_B(\mathbb{Q}(x)) \right) dx,$$

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where

- $|\nabla \mathbb{Q}|^2 = \sum_{i,j,k=1}^3 \mathbb{Q}_{ij,k} \mathbb{Q}_{ij,k}$  is the elastic energy density that penalizes spatial inhomogeneities and  $L > 0$  is a material-dependent elastic constant
- $f_B(\mathbb{Q})$  is the **bulk free energy density**, e.g., (following [de Gennes, Prost (1995)])

$$f_B(\mathbb{Q}) = \frac{\alpha(T - T^*)}{2} \text{tr}(\mathbb{Q}^2) - \frac{b}{3} \text{tr}(\mathbb{Q}^3) + \frac{c}{4} (\text{tr}(\mathbb{Q}^2))^2$$

where  $\alpha$ ,  $b$ ,  $c$  are material-dependent positive constants,  $T$  is the absolute temperature and  $T^*$  is a characteristic liquid crystal temperature. Call  $a = \alpha(T - T^*)$

# The Oseen-Frank free energy



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it is reasonable to consider a theory where  $\mathbb{Q}$  is required to be uniaxial with constant scalar order parameter  $s > 0$ , i.e.

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- In this case  $f_B$  is constant and we can consider only the elastic energy and calculating it in terms of  $\mathbf{d}$  we obtain the simplest form of the **Oseen-Frank free energy** (1925, 1958)

$$\mathcal{F}_{OF} = Ls^2 \int_{\Omega} |\nabla \mathbf{d}(x)|^2 dx$$

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- In the Landau-de Gennes free energy there is no a-priori bound on the eigenvalues
- 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**

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

$$\mathcal{A}_{\mathbb{Q}} = \left\{ \rho : S^2 \rightarrow [0, \infty) \mid \int_{S^2} \rho(\mathbf{p}) \, d\mathbf{p} = 1; \mathbb{Q} = \int_{S^2} \left( \mathbf{p} \otimes \mathbf{p} - \frac{1}{3} \mathbb{I} \right) \rho(\mathbf{p}) \, d\mathbf{p} \right\}.$$

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

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

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⇒ The proposed model is shown compatible with *First and Second laws* of thermodynamics, and the existence of **global-in-time weak solutions** for the resulting PDE system is established, without any essential restriction on the size of the data, or on the space dimension, or on the viscosity coefficient

# The director field dynamics

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- We assume that the driving force governing the dynamics of the director  $\mathbf{d}$  is of “gradient type”  $\partial_{\mathbf{d}}\mathcal{F}$ , where the free-energy functional  $\mathcal{F}$  is given by

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where the last term accounts for **stretching** of the director field induced by the straining of the fluid

- The presence of **the stretching term  $\mathbf{d} \cdot \nabla_x \mathbf{u}$**  in the  $\mathbf{d}$ -equation prevents us from applying any maximum principle. Hence, we cannot find any  $L^\infty$  bound on  $\mathbf{d}$  (useful in order to handle the nonlinearities)

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- ◇ By virtue of Newton's second law, **the balance of momentum** reads

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla_x \mathbf{u} + \nabla_x p = \operatorname{div} \mathbb{S} + \operatorname{div} \boldsymbol{\sigma}^{nd} + \mathbf{g}$$

where  $p$  is the pressure, and

- the stress tensors are

$$\mathbb{S} = \frac{\mu(\theta)}{2} (\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u}), \quad \boldsymbol{\sigma}^{nd} = -\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} + (\partial_d W(\mathbf{d}) - \Delta \mathbf{d}) \otimes \mathbf{d}$$

where  $\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} := \sum_k \partial_i d_k \partial_j d_k$ ,  $\mu$  is a temperature-dependent viscosity coefficient

## The momentum balance

- ◇ In the context of nematic liquid crystals, we have the **incompressibility** constraint

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- The presence of **the stretching term**  $\mathbf{d} \cdot \nabla_x \mathbf{u}$  in the  $\mathbf{d}$ -equation prevents us from applying any maximum principle. Hence, we cannot find any  $L^\infty$  bound on  $\mathbf{d}$ . We will need a **weak formulation of the momentum balance**

## The total energy balance

$$\begin{aligned} \partial_t \left( \frac{1}{2} |\mathbf{u}|^2 + e \right) + \mathbf{u} \cdot \nabla_x \left( \frac{1}{2} |\mathbf{u}|^2 + e \right) + \operatorname{div} \left( \rho \mathbf{u} + \mathbf{q}^d + \mathbf{q}^{nd} - \mathbb{S} \mathbf{u} - \boldsymbol{\sigma}^{nd} \mathbf{u} \right) \\ = \mathbf{g} \cdot \mathbf{u} + \operatorname{div} \left( \nabla_x \mathbf{d} \cdot (\Delta \mathbf{d} - \partial_d W(\mathbf{d})) \right) \end{aligned}$$

with the internal energy

$$e = \frac{|\nabla_x \mathbf{d}|^2}{2} + W(\mathbf{d}) + \theta$$

and the flux

$$\mathbf{q} = \mathbf{q}^d + \mathbf{q}^{nd} = -k(\theta) \nabla_x \theta - h(\theta) (\mathbf{d} \cdot \nabla_x \theta) \mathbf{d} - \nabla_x \mathbf{d} \cdot \nabla_x \mathbf{u} \cdot \mathbf{d}$$

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## The entropy inequality

$$\begin{aligned} H(\theta)_t + \mathbf{u} \cdot \nabla_x H(\theta) + \operatorname{div}(H'(\theta) \mathbf{q}^d) \\ \geq H'(\theta) \left( \mathbb{S} : \nabla_x \mathbf{u} + |\Delta \mathbf{d} - \partial_d W(\mathbf{d})|^2 \right) + H''(\theta) \mathbf{q}^d \cdot \nabla_x \theta \end{aligned}$$

holding for any smooth, non-decreasing and concave function  $H$ .

## The initial and boundary conditions

In order to avoid the occurrence of boundary layers, we suppose that the boundary is impermeable and perfectly smooth imposing the **complete slip** boundary conditions:

$$\mathbf{u} \cdot \mathbf{n}|_{\partial\Omega} = 0, \quad [(\mathbb{S} + \sigma^{nd})\mathbf{n}] \times \mathbf{n}|_{\partial\Omega} = 0$$

together with the **no-flux** boundary condition for the temperature

$$\mathbf{q}^d \cdot \mathbf{n}|_{\partial\Omega} = 0$$

and the **Neumann** boundary condition for the director field

$$\nabla_x d_i \cdot \mathbf{n}|_{\partial\Omega} = 0 \text{ for } i = 1, 2, 3$$

The last relation accounts for the fact that there is no contribution to the surface force from the director  $\mathbf{d}$ . It is also suitable for implementation of a numerical scheme.

A **weak solution** is a triple  $(\mathbf{u}, \mathbf{d}, \theta)$  satisfying:

- the **momentum equations** ( $\varphi \in C_0^\infty([0, T) \times \bar{\Omega}; \mathbb{R}^3)$ ,  $\varphi \cdot \mathbf{n}|_{\partial\Omega} = 0$ ):

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- the **director equation**:  $\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d} - \mathbf{d} \cdot \nabla_x \mathbf{u} = \Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d})$  a.e.,  $\nabla_x \mathbf{d}_i \cdot \mathbf{n}|_{\partial\Omega} = 0$ ;

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- the **total energy balance** ( $\varphi \in C_0^\infty([0, T] \times \bar{\Omega})$ ,  $e_0 = \frac{\lambda}{2} |\nabla_x \mathbf{d}_0|^2 + \lambda W(\mathbf{d}_0) + \theta_0$ ):

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Assume that  $\Omega \subset \mathbb{R}^3$  is a bounded domain of class  $C^{2+\nu}$ ,  $\mathbf{g} \in L^2((0, T) \times \Omega; \mathbb{R}^3)$ ,

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- The transport coefficients  $\mu$ ,  $k$ , and  $h$  are continuously differentiable functions satisfying

$$0 < \underline{\mu} \leq \mu(\theta) \leq \bar{\mu}, \quad 0 < \underline{k} \leq k(\theta), \quad h(\theta) \leq \bar{k} \quad \text{for all } \theta \geq 0$$

and the initial data satisfy

$$\mathbf{u}_0 \in L^2(\Omega; \mathbb{R}^3), \quad \operatorname{div} \mathbf{u}_0 = 0, \quad \mathbf{d}_0 \in W^{1,2}(\Omega; \mathbb{R}^3), \quad W(\mathbf{d}_0) \in L^1(\Omega),$$

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Then **our problem possesses a weak solution  $(\mathbf{u}, \mathbf{d}, \theta)$**  belonging to the class

$$\mathbf{u} \in L^\infty(0, T; L^2(\Omega; \mathbb{R}^3)) \cap L^2(0, T; W^{1,2}(\Omega; \mathbb{R}^3)),$$

$$\mathbf{d} \in L^\infty(0, T; W^{1,2}(\Omega; \mathbb{R}^3)) \cap L^2(0, T; W^{2,2}(\Omega; \mathbb{R}^3)),$$

$$W(\mathbf{d}) \in L^\infty(0, T; L^1(\Omega)) \cap L^{5/3}((0, T) \times \Omega),$$

$$\theta \in L^\infty(0, T; L^1(\Omega)) \cap L^p(0, T; W^{1,p}(\Omega)), \quad 1 \leq p < 5/4, \quad \theta > 0 \text{ a.e. in } (0, T) \times \Omega,$$

with the pressure  $p$

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- It can be shown that **the solution set of our problem is weakly stable (compact) with respect to these bounds**, namely, any sequence of (weak) solutions that complies with the uniform bounds established above has a subsequence that converges to some limit
- Hence, we construct a suitable family of **approximate problems (via Faedo-Galerkin scheme + regularizing terms in the momentum equation)** whose solutions weakly converge (up to subsequences) to limit functions which solve the problem in the weak sense

## Model 2: the $\mathbb{Q}$ -tensorial Ball-Majumdar model

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

where  $f_B$  is bulk the configuration potential:

- $f_B(\theta, \mathbb{Q}) = f(\mathbb{Q}) - U(\theta)G(\mathbb{Q})$
- $f$  is the convex l.s.c. and singular Ball-Majumdar potential
- $U$  changes in sign at a critical temperature:  $U(\theta) = \alpha(\theta - \theta^*)$  for  $\theta \sim \theta^*$  with a controlled growth for large  $\theta$
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**Theorem [E. Feireisl, E.R., G. Schimperna, A. Zarnescu, paper in preparation]** There exists at least one weak solution to a system coupling

- a *weak momentum equation* for  $\mathbf{u}$
- a *gradient-type equation* for  $\mathbb{Q}$
- an *entropy inequality + total energy balance* for  $\theta$

for finite-energy initial data.



## The generalized principle of virtual powers: damage phenomena

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**The scope:** The analysis of the initial boundary-value problem for the following PDE system:

$$c(\theta)\theta_t + \chi_t\theta - \operatorname{div}(k(\theta)\nabla\theta) = g$$

$$\mathbf{u}_{tt} - \operatorname{div}(\chi\varepsilon(\mathbf{u}_t) + \chi\varepsilon(\mathbf{u})) = \mathbf{f}$$

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

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- $\theta$  is the absolute temperature of the system
- $\mathbf{u}$  the vector of *small displacements*
- $\chi$  is the **damage parameter**, assessing the soundness of the material in *damage* (for the **completely damaged**  $\chi = 0$  and the *undamaged* state  $\chi = 1$ , respectively, while  $0 < \chi < 1$ : *partial damage*)

[joint works with R. Rossi, *J. Differential Equations and Appl. Math* (2008) and preprint arXiv:1205.3578v1 (2012)]

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## The aim: deal with the possible degeneracy in the momentum equation

Main aim: We shall let  $\chi$  vanishes at the threshold value 0, not enforce separation of  $\chi$  from the threshold value 0, and accordingly we will allow for general initial configurations of  $\chi$

⇒ We shall approximate the system with a non-degenerating one, where we replace the momentum equation with

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

It seems to us that *both* the coefficients need to be truncated when taking the degenerate limit in the momentum equation. Indeed, on the one hand the truncation in front of  $\varepsilon(\mathbf{u}_t)$  allows us to deal with the *main part* of the elliptic operator. On the other hand, in order to pass to the limit in the quadratic term on the right-hand side of  $\chi$ -eq., we will also need to truncate the coefficient of  $\varepsilon(\mathbf{u})$ .

**Free energy and Dissipation, cf. [M. Frémond, Phase Change in Mechanics, Lecture Notes of the Unione Matematica Italiana 13, Springer-Verlag, Berlin, 2012]**

The free-energy  $\mathcal{F}$ :

$$\mathcal{F} = \int_{\Omega} \left( f(\theta) + \chi \frac{|\varepsilon(\mathbf{u})|^2}{2} + \frac{a_s(\chi, \chi)}{2} + W(\chi) - \theta \chi \right) dx$$

- $f$  is a concave function
- $a_s(\mathbf{z}_1, \mathbf{z}_2) := \int_{\Omega} \int_{\Omega} \frac{(\nabla \mathbf{z}_1(x) - \nabla \mathbf{z}_1(y)) \cdot (\nabla \mathbf{z}_2(x) - \nabla \mathbf{z}_2(y))}{|x - y|^{d+2(s-1)}} dx dy$  is the bilinear form associated to the **fractional  $s$ -Laplacian  $A_s$**
- $s > d/2$ : we need the embedding of  $H^s(\Omega)$  into  $C^0(\overline{\Omega})$
- $W = \widehat{\beta} + \widehat{\gamma}$ ,  $\widehat{\gamma} \in C^2(\mathbb{R})$ ,  $\widehat{\beta}$  proper, convex, l.s.c.,  $\overline{\text{dom}(\widehat{\beta})} = [0, 1]$



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### The pseudo-potential $\mathcal{P}$ :

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

- $k$  the **heat conductivity**: coupled conditions with the specific heat  $c(\theta) = f(\theta) - \theta f'(\theta)$
- $I_{(-\infty, 0]}(\chi_t) = 0$  if  $\chi_t \in (-\infty, 0]$ ,  $I_{(-\infty, 0]}(\chi_t) = +\infty$  otherwise

## The modelling

The momentum equation

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

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The principle of virtual powers

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

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The internal energy balance

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

becomes

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

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$$c(\theta)\theta_t + \chi_t\theta - \operatorname{div}(k(\theta)\nabla\theta) = g$$

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- For the analysis of the degenerate limit  $\delta \searrow 0$  we have carefully adapted techniques from [Bouchitté, Mielke, Roubíček, ZAMP (2009)] and [Mielke, Roubíček, Zeman, Comput. Methods Appl. Mech. Engrg. (2011)] to the case of a *rate-dependent* equation for  $\chi$ , also coupled with the temperature equation.

## Energy vs Enthalpy

In order to deal with the low regularity of  $\theta$ , rewrite the internal energy equation

$$c(\theta)\theta_t + \chi_t\theta - \operatorname{div}(k(\theta)\nabla\theta) = g$$

as the **enthalpy** equation

$$w_t + \chi_t\Theta(w) - \operatorname{div}(K(w)\nabla w) = g \quad \text{where}$$

$$w = h(\theta) := \int_0^\theta c(s) ds, \quad \Theta(w) := \begin{cases} h^{-1}(w) & \text{if } w \geq 0, \\ 0 & \text{if } w < 0, \end{cases} \quad K(w) := \frac{k(\Theta(w))}{c(\Theta(w))}$$

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We assume that

- $c \in C^0([0, +\infty); [0, +\infty))$
- $\exists \sigma_1 \geq \sigma > \frac{2d}{d+2} : c_0(1+\theta)^{\sigma-1} \leq c(\theta) \leq c_1(1+\theta)^{\sigma_1-1} \implies h$  is strictly increasing
- the function  $k : [0, +\infty) \rightarrow [0, +\infty)$  is continuous, and

$$\exists c_2, c_3 > 0 \quad \forall \theta \in [0, +\infty) : c_2c(\theta) \leq k(\theta) \leq c_3(c(\theta) + 1)$$

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$$\implies \exists \bar{c} > 0 \quad \forall w \in \mathbb{R} : \quad c_2 \leq K(w) \leq \bar{c}$$

$$\implies \text{for every } s \in (1, \infty) \exists C_s > 0 \quad \forall w \in L^1(\Omega) : \quad \|\Theta(w)\|_{L^s(\Omega)} \leq C_s(\|w\|_{L^{s/\sigma}(\Omega)}^{1/\sigma} + 1)$$

## The approximating non-degenerate Problem $[P_\delta]$

Given  $\delta > 0$ , take  $W' = \partial I_{[0,+\infty)} + \gamma$ ,  $\gamma \in C^1(\mathbb{R})$ , find (measurable) functions

$$\begin{aligned}w &\in L^r(0, T; W^{1,r}(\Omega)) \cap L^\infty(0, T; L^1(\Omega)) \cap \text{BV}([0, T]; W^{1,r'}(\Omega)^*) \\ \mathbf{u} &\in H^1(0, T; H^2(\Omega; \mathbb{R}^d)) \cap W^{1,\infty}(0, T; H_0^1(\Omega)) \cap H^2(0, T; L^2(\Omega; \mathbb{R}^d)) \\ \chi &\in L^\infty(0, T; H^s(\Omega)) \cap H^1(0, T; L^2(\Omega))\end{aligned}$$

for every  $1 \leq r < \frac{d+2}{d+1}$ , fulfilling the initial conditions

$$\begin{aligned}\mathbf{u}(0, x) &= \mathbf{u}_0(x), & \mathbf{u}_t(0, x) &= \mathbf{v}_0(x) & \text{for a.e. } x \in \Omega \\ \chi(0, x) &= \chi_0(x) & & & \text{for a.e. } x \in \Omega\end{aligned}$$

the equations (for every  $\varphi \in C^0([0, T]; W^{1,r'}(\Omega)) \cap W^{1,r'}(0, T; L^{r'}(\Omega))$  and  $t \in (0, T]$ )

$$\begin{aligned}&\int_{\Omega} \varphi(t) w(t) dx - \int_0^t \int_{\Omega} w \varphi_t dx + \int_0^t \int_{\Omega} \chi_t \Theta(w) \varphi dx + \int_0^t \int_{\Omega} K(w) \nabla w \nabla \varphi dx \\ &= \int_0^t \int_{\Omega} g \varphi + \int_{\Omega} w_0 \varphi(0) dx\end{aligned}$$

$$\mathbf{u}_{tt} - \text{div}((\chi + \delta)\varepsilon(\mathbf{u}_t) + (\chi + \delta)\varepsilon(\mathbf{u})) = \mathbf{f} \text{ in } H^{-1}(\Omega; \mathbb{R}^d) \text{ a.e. in } (0, T)$$

and the subdifferential inclusion “in a suitable sense”

$$\chi_t + \partial I_{(-\infty, 0]}(\chi_t) + A_s \chi + \partial I_{[0, +\infty)}(\chi) + \gamma(\chi) \ni -\frac{|\varepsilon(\mathbf{u})|^2}{2} + \Theta(w) \text{ in } H^{-s}(\Omega) \text{ and a.e. in } (0, T)$$

## Generalized principle of virtual powers for $\delta > 0$ [E.R., R. Rossi, preprint arXiv:1205.3578v1 (2012)]

**[Theorem 1]** ( $\delta > 0$ ) Under the previous assumptions on the data, then,

[1.] Problem  $[P_\delta]$  admits a *weak solution*  $(w, \mathbf{u}, \chi)$ , which, beside fulfilling the **enthalpy and momentum equations**, satisfies  $\chi_t(x, t) \leq 0$  for almost all  $t \in (0, T)$ , and  $(\forall \varphi \in L^2(0, T; H_+^s(\Omega)) \cap L^\infty(Q))$  the *one-sided inequality*

$$\int_0^T \int_\Omega \chi_t \varphi + a_s(\chi, \varphi) + \xi \varphi + \gamma(\chi) \varphi + \frac{|\varepsilon(\mathbf{u})|^2}{2} \varphi - \Theta(w) \varphi \leq 0$$

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

$$\xi \in L^1(0, T; L^1(\Omega)), \quad \langle \xi(t), \varphi - \chi(t) \rangle_{H^s(\Omega)} \leq 0 \quad \forall \varphi \in H_+^s(\Omega), \text{ a.e. } t \in (0, T)$$

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**Uniqueness of solutions for the irreversible system**, even in the isothermal case, **is still an open problem**. This is mainly due to the doubly nonlinear character of the  $\chi$  equation.

## Generalized principle of virtual powers vs classical phase inclusion

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- Any *weak solution*  $(w, \mathbf{u}, \chi)$  fulfills the **total energy inequality** for all  $t \in (0, T]$ , for  $s = 0$ , and for almost all  $0 < s \leq t$

$$\begin{aligned} & \int_{\Omega} w(t)(dx) + \frac{1}{2} \int_{\Omega} |\mathbf{u}_t(t)|^2 dx + \int_s^t \int_{\Omega} |\chi_t|^2 dx + \int_s^t (\chi + \delta) |\varepsilon(\mathbf{u}_t)|^2 \\ & \quad + \frac{1}{2} (\chi(t) + \delta) |\varepsilon(\mathbf{u}(t))|^2 + \frac{1}{2} a_s(\chi(t), \chi(t)) + \int_{\Omega} W(\chi(t)) dx \\ & \leq \int_{\Omega} w(s)(dx) + \frac{1}{2} \int_{\Omega} |\mathbf{u}_t(s)|^2 dx + \frac{1}{2} (\chi(s) + \delta) |\varepsilon(\mathbf{u}(s))|^2 + \frac{1}{2} a_s(\chi(s), \chi(s)) \\ & \quad + \int_{\Omega} W(\chi(s)) dx + \int_s^t \int_{\Omega} \mathbf{f} \cdot \mathbf{u}_t dx + \int_s^t \int_{\Omega} g dx \end{aligned}$$

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- If  $(w, \mathbf{u}, \chi)$  are “**more regular**” and satisfy the notion of *weak solution*, then, differentiating the **energy inequality** and using the chain rule, we conclude that  $(w, \mathbf{u}, \chi, \xi)$  comply with

$$\langle \chi_t(t) + A_s(\chi(t)) + \xi(t) + \gamma(\chi(t)) + \frac{|\varepsilon(\mathbf{u})|^2}{2} - \Theta(w(t)), \chi_t(t) \rangle_{H^s(\Omega)} \leq 0 \text{ for a.e. } t$$

Using the **one-sided inequality** we obtain the **classical phase inclusion**:

$$\exists \zeta \in L^2(0, T; L^2(\Omega)) \text{ with } \zeta(x, t) \in \partial I_{(-\infty, 0]}(\chi_t(x, t)) \text{ a.e. s.t.}$$

$$\chi_t + \zeta + A_s \chi + \xi + \gamma(\chi) = -\frac{|\varepsilon(\mathbf{u})|^2}{2} + \Theta(w) \text{ a.e.}$$

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- A BOCCARDO-GALLOUËT-type estimates combined with the Gagliardo-Nirenberg inequality applied to the enthalpy equation in order to obtain an  $L^r(0, T; W^{1,r}(\Omega))$ -estimate on the enthalpy  $w$  (and hence on  $\Theta(w)$ )

$$w_t + \chi_t \Theta(w) - \operatorname{div}(K(w) \nabla w) = g$$



## The total energy inequality in the degenerating case $\delta \searrow 0$

Rewrite the momentum equation

$$\partial_t^2 \mathbf{u}_\delta - \operatorname{div}((\chi + \delta)\varepsilon(\partial_t \mathbf{u}_\delta)) - \operatorname{div}((\chi + \delta)\varepsilon(\mathbf{u}_\delta)) = \mathbf{f}$$

using the new variables (*quasi-stresses*)  $\boldsymbol{\mu}_\delta := \sqrt{\chi_\delta + \delta} \varepsilon(\partial_t \mathbf{u}_\delta)$ , and  $\boldsymbol{\eta}_\delta := \sqrt{\chi_\delta + \delta} \varepsilon(\mathbf{u}_\delta)$ :

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$$\partial_t^2 \mathbf{u}_\delta - \operatorname{div}(\sqrt{\chi + \delta} \boldsymbol{\mu}_\delta) - \operatorname{div}(\sqrt{\chi + \delta} \boldsymbol{\eta}_\delta) = \mathbf{f}$$

The **total energy inequality** for  $(w_\delta, \mathbf{u}_\delta, \chi_\delta)$  is

$$\begin{aligned} & \int_{\Omega} w_\delta(t) \, dx + \frac{1}{2} \int_{\Omega} |\partial_t \mathbf{u}_\delta(t)|^2 \, dx + \int_s^t \int_{\Omega} |\partial_t \chi_\delta|^2 \, dx + \frac{1}{2} \int_s^t |\boldsymbol{\mu}_\delta(r)|^2 \\ & \quad + \frac{|\boldsymbol{\eta}_\delta(t)|^2}{2} + \frac{1}{2} a_s(\chi_\delta(t), \chi_\delta(t)) + \int_{\Omega} W(\chi_\delta(t)) \, dx \\ & \leq \int_{\Omega} w_\delta(s) \, dx + \frac{1}{2} \int_{\Omega} |\partial_t \mathbf{u}_\delta(s)|^2 \, dx + \frac{|\boldsymbol{\eta}_\delta(s)|^2}{2} + \frac{1}{2} a_s(\chi_\delta(s), \chi_\delta(s)) \\ & \quad + \int_{\Omega} W(\chi_\delta(s)) \, dx + \int_s^t \int_{\Omega} \mathbf{f} \cdot \partial_t \mathbf{u}_\delta \, dx + \int_s^t \int_{\Omega} \mathbf{g} \, dx \end{aligned}$$

# The degenerate problem ( $\delta = 0$ ): the existence theorem [E.R., R. Rossi, preprint arXiv:1205.3578v1 (2012)]

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together with the **total energy inequality** (for almost all  $t \in (0, T]$ )

$$\begin{aligned} & \int_\Omega w(t) \, dx + \int_0^t \int_\Omega |\chi_t|^2 \, dx + \frac{1}{2} \int_0^t |\boldsymbol{\mu}(r)|^2 + \int_\Omega W(\chi(t)) \, dx + \mathcal{J}(t) = \int_\Omega w_0 \, dx \\ & + \frac{1}{2} \int_\Omega |\mathbf{v}_0|^2 \, dx + \frac{1}{2} \chi_0 |\boldsymbol{\varepsilon}(\mathbf{u}_0)|^2 + \frac{1}{2} a_s(\chi_0, \chi_0) + \int_\Omega W(\chi_0) \, dx + \int_0^t \int_\Omega \mathbf{f} \cdot \mathbf{u}_t \, dx \, dr + \int_0^t \int_\Omega g \, dx \end{aligned}$$

$$\text{with } \int_0^t \mathcal{J}(r) \, dr \geq \frac{1}{2} \int_0^t \left( \int_\Omega |\mathbf{u}_t(r)|^2 \, dx + |\boldsymbol{\eta}(r)|^2 + a_s(\chi(r), \chi(r)) \right)$$

## A comparison between the solution notions

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$\forall \varphi \in L^2(0, T; H_+^s(\Omega)) \cap L^\infty(Q)$  and with  $\xi \in \partial I_{[0, +\infty)}(\chi)$ . Subtracting from the **degenerate total energy inequality** the weak enthalpy equation tested by 1, we recover (a.e. in  $(0, T]$ ) **the energy inequality**:

$$\begin{aligned} & \int_0^t \int_{\Omega} |\chi_t|^2 \, dx \, dr + \frac{1}{2} a_s(\chi(t), \chi(t)) + \int_{\Omega} W(\chi(t)) \, dx \\ & \leq \frac{1}{2} a_s(\chi_0, \chi_0) + \int_{\Omega} W(\chi_0) \, dx + \int_0^t \int_{\Omega} \chi_t \left( -\frac{|\varepsilon(\mathbf{u})|^2}{2} + \Theta(w) \right) \, dx \, dr \end{aligned}$$

## Work in progress: an entropic formulation for the damage phenomena

We worked here with the **small perturbation assumption**, i.e. neglecting the **quadratic** contribution on the r.h.s in the internal energy balance:

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✓ the **entropy production**

$$\begin{aligned} & \int_0^T \int_{\Omega} \left( (\log \theta + \chi) \partial_t \varphi - \nabla \log \theta \cdot \nabla \varphi \right) dx dt \\ & \leq \int_0^T \int_{\Omega} \frac{1}{\theta} \left( -|\chi_t|^2 - \chi |\varepsilon(\mathbf{u}_t)|^2 - \nabla \log \theta \cdot \nabla \theta \right) \varphi dx dt \end{aligned}$$

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- ✓ the **energy conservation**

$$E(t) = E(0) \text{ for a.e. } t \in [0, T],$$

where

$$E \equiv \int_{\Omega} \left( \theta + W(\chi) + \frac{1}{2} a_s(\chi, \chi) + \frac{|\mathbf{u}_t|^2}{2} + \chi \frac{|\varepsilon(\mathbf{u})|^2}{2} \right) dx.$$

This is still a **work in progress (with R. Rossi)**...

## Possible further application

- A fluid-mechanical theory for **two-phase mixtures of fluids** faces a well known mathematical difficulty:
  - ▶ the movement of the **interfaces**  $\implies$  **Lagrangian** description
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$$\operatorname{div} \mathbf{v} = 0, \quad \partial_t \mathbf{v} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) + \nabla p = \operatorname{div} \mathbb{S} - \mu \nabla_x \varphi, \quad \mathbb{S} = \nu(\theta, \varphi) (\nabla_x \mathbf{v} + \nabla_x^t \mathbf{v}) \quad (1)$$

$$\partial_t \theta + \operatorname{div}(\theta \mathbf{v}) + \operatorname{div} \mathbf{q} = \mathbb{S} : \nabla_x \mathbf{v} + |\nabla_x \mu|^2 \quad (2)$$

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**Entropic notion** of solution is needed in order to interpret the internal energy balance (2) ...

**Thanks for your attention!**

cf. <http://www.mat.unimi.it/users/rocca/>