Entropic solutions arising in complex fluids dynamics and damage phenomena

E. Rocca

Università degli Studi di Pavia

Implicitly constituted materials: Modeling, Analysis and Computing
Roztoky, July 31 - August 4, 2017

joint with E. Feireisl, C. Heinemann, C. Kraus, R. Rossi, G. Schimperna, A. Zarnescu

Fondazione Cariplo and Regione Lombardia Grant MEGAsTaR 2016-2019

Outline

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Mathematical problems arising from Thermomechanics

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- 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 $\mathbb{Q}$-tensor and to include velocity and temperature dependence in the model

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- Damage phenomena:
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- Another problem: Two-phase mixtures of fluids (see Giulio's talk on Thursday):
  - 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
  - aim: to consider the non-isothermal version of the model

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- Liquid crystals

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

$$\operatorname{div}\boldsymbol{v} = 0,\ \ \boldsymbol{v}_t + \operatorname{div}(\boldsymbol{v}\otimes\boldsymbol{v}) = \operatorname{div}\sigma + \boldsymbol{g}, \quad \sigma = \nu(\theta)(\nabla_x\boldsymbol{v} + \nabla_x^t\boldsymbol{v}) - p\mathbb{I} + \mathbb{T}(\theta,\mathbb{Q})$$

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

- Two-phase mixtures of fluids

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

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

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

- Damage

$$\theta_t + c_t\theta + z_t\theta + \rho\theta\operatorname{div}(\boldsymbol{u}_t) + \operatorname{div}\boldsymbol{q} = g + |c_t|^2 + |z_t|^2 + a(c,z)\epsilon(\boldsymbol{u}_t) : \mathbb{V}\epsilon(\boldsymbol{u}_t) + m(c,z)|\nabla\mu|^2$$

$$\boldsymbol{u}_{tt} - \operatorname{div}\left(a(c,z)\mathbb{V}\epsilon(\boldsymbol{u}_t) + b(c,z)\mathbb{C}(\epsilon(\boldsymbol{u}) - \epsilon^*(c)) - \rho\theta 1\right) = \boldsymbol{f}$$

$$z_t + \partial I_{(-\infty,0]}(z_t) - \Delta_p(z) + \partial I_{[0,\infty)}(z) + \sigma'(z) \ni -\frac{1}{2}b_{,z}\mathbb{C}(\epsilon(\boldsymbol{u}) - \epsilon^*(c)) : (\epsilon(\boldsymbol{u}) - \epsilon^*(c)) + \theta$$

$$c_t = \operatorname{div}(m(c,z)\nabla\mu)$$

$$\mu = -\Delta_p(c) + \phi'(c) + \frac{1}{2}\big(b(c,z)\mathbb{C}(\epsilon(\boldsymbol{u}) - \epsilon^*(c)) : (\epsilon(\boldsymbol{u}) - \epsilon^*(c))\big)_{,c} - \theta + c_t$$

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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

Outline

Liquid Crystals flows

- 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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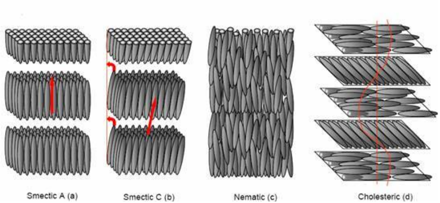
  - At the molecular level, what marks the difference between a liquid crystal and an ordinary, isotropic fluid is that, while the centers of mass of LC molecules do not exhibit any long-range correlation, molecular orientations do exhibit orientational correlations
- The objective: include the temperature dependence in models describing the evolution of nematic liquid crystal flows within the Landau-De Gennes theories (cf. [De Gennes, Prost (1995)])

Main LC types

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



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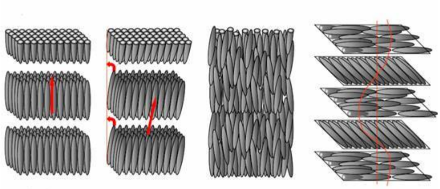

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The *smectic* phase forms well-defined layers that can slide one over another in a manner very similar to that of a soap

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

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- Most mathematical work has been done on the Oseen-Frank theory, in which the mean orientation of the rod-like molecules is described by a vector field $\boldsymbol{d}$. However, more popular among physicists is the Landau-de Gennes theory, in which the order parameter describing the orientation of molecules is a matrix, the so-called $\mathbb{Q}$-tensor

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▶ The flow velocity $\boldsymbol{v}$ 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 $\boldsymbol{v}$. Moreover, we want to include in our model also the changes of the temperature θ

The Landau-de Gennes theory: the molecular orientation

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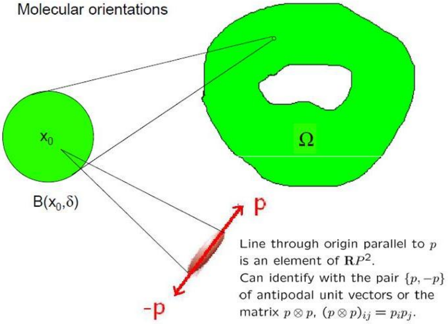
- Consider a nematic liquid crystal filling a bounded connected container Ω in $\mathbb{R}^3$ with "regular" boundary
- The distribution of molecular orientations in a ball $B(x_0, \delta)$, $x_0 \in \Omega$ can be represented as a probability measure μ on the unit sphere $\mathbb{S}^2$ satisfying $\mu(E) = \mu(-E)$ 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 Landau-de Gennes theory: the $\mathbb{Q}$-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 3×3 matrix (for every $\mathrm{v} \in \mathbb{S}^2$, $\mathrm{v} \cdot M \cdot \mathrm{v} = \int_{\mathbb{S}^2} (\mathrm{v} \cdot p)^2 \, d\mu(p) =< \cos^2 \theta >$, where θ is the angle between p and v) satisfying $\mathrm{tr}(M) = 1$

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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 $M_0 = \frac{1}{4\pi} \int_{\mathbb{S}^2} p \otimes p\, dS = \frac{1}{3} \mathbb{1}$, 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 $\mathrm{tr}(M_0) = 1$

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

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

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1.+2. implies $\mathbb{Q} = \lambda_1 \mathrm{n}_1 \otimes \mathrm{n}_1 + \lambda_2 \mathrm{n}_2 \otimes \mathrm{n}_2 + \lambda_3 \mathrm{n}_3 \otimes \mathrm{n}_3$, where $\{\mathrm{n}_i\}$ is an othonormal 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

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

$$\mathcal{A}_{\mathbb{Q}} = \left\{ \rho : S^2 \to [0, \infty) \ \middle| \ \int_{S^2} \rho(\mathrm{p})\, \mathrm{dp} = 1; \mathbb{Q} = \int_{S^2} \left(\mathrm{p} \otimes \mathrm{p} - \frac{1}{3} \mathbb{I} \right) \rho(\mathrm{p})\, \mathrm{dp} \right\}.$$

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

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

Energy and dissipation

- 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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- The dissipation pseudo-potential is given by

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

  - 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 $\operatorname{div} \boldsymbol{v} = 0$, $+\infty$ otherwise

$\mathbb{Q}$-tensor equation

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We assume that the driving force governing the dynamics of the director $\mathbb{Q}$ is of "gradient type" $\partial_{\mathbb{Q}}\mathcal{F}$:

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

- The left hand side is the "generalized material derivative" $D_t\mathbb{Q} = \partial_t \mathbb{Q} + \mathbf{v} \cdot \nabla \mathbb{Q} - \mathbb{S}(\nabla \mathbf{v}, \mathbb{Q})$
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- The right hand side is of "gradient type" $-\mathbb{H} = \partial_{\mathbb{Q}}\mathcal{F}$, i.e.
- $\mathbb{H} = \Delta\mathbb{Q} - \theta\frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} - \frac{\partial G(\mathbb{Q})}{\partial \mathbb{Q}} = \Delta\mathbb{Q} - \theta\frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} + \lambda\mathbb{Q}$, $\lambda \geq 0$
- $\Gamma(\theta)$ represents a collective rotational viscosity coefficient
- The function f represents a convex singular potential of [Ball-Majumdar] type

The Ball-Majumdar potential

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

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

$$\mathcal{A}_{\mathbb{Q}} = \left\{ \rho : S^2 \to [0, \infty) \ \Big| \ \int_{S^2} \rho(\mathrm{p})\, \mathrm{dp} = 1; \mathbb{Q} = \int_{S^2} \left(\mathrm{p} \otimes \mathrm{p} - \frac{1}{3}\mathbb{I} \right) \rho(\mathrm{p})\, \mathrm{dp} \right\}.$$

$\Longrightarrow$ 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

Entropy inequality

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The evolution of temperature is prescribed by stating the entropy inequality

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

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

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

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

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

Main result: the "Entropic formulation"

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

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

Outline

The damage phenomena

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We prove

- the existence of "entropic weak solutions"
- Our global-in-time existence result is obtained by passing to the limit in a carefully devised time-discretization scheme by means of proper compactness and lower-semincontinuity arguments

The state variables and the PDEs

- the absolute temperature θ
- the (small) displacement variables $\boldsymbol{u}$ ($\epsilon_{ij}(\boldsymbol{u}) := (\boldsymbol{u}_{i,j} + \boldsymbol{u}_{j,i})/2$, $i, j = 1, 2, 3$)
- the damage parameter $z \in [0, 1]$: $z = 0$ (completely damaged), $z = 1$ (completely undamaged)
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with the initial-boundary conditions

$$\theta(0) = \theta^0, \quad \boldsymbol{u}(0) = \boldsymbol{u}^0, \quad \boldsymbol{u}_t(0) = \mathrm{v}^0, \quad z(0) = z^0, \quad c(0) = c^0 \quad \text{a.e. in } \Omega$$

$$\mathsf{K}(\theta)\nabla\theta\cdot\boldsymbol{n} = h, \quad \boldsymbol{u} = \boldsymbol{d}, \quad \nabla z\cdot\boldsymbol{n} = 0, \quad \nabla c\cdot\boldsymbol{n} = 0, \quad m(c,z)\nabla\mu\cdot\boldsymbol{n} = 0 \quad \text{a.e. on } \partial\Omega\times(0,T)$$

Nonlinearities and data

$$\theta_t + c_t\theta + z_t\theta + \rho\theta\,\mathrm{div}(\boldsymbol{u}_t) - \mathrm{div}(\mathsf{K}(\theta)\nabla\theta) = g + |c_t|^2 + |z_t|^2 + a(c,z)\epsilon(\boldsymbol{u}_t) : \mathbb{V}\epsilon(\boldsymbol{u}_t) + m(c,z)|\nabla\mu|^2$$

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- $\rho \rightsquigarrow$ thermal expansion coefficient;
- $\mathsf{K} \rightsquigarrow$ continuous heat conductivity: $\exists\,\kappa > 1$: $c_0(1+\theta^\kappa) \le \mathsf{K}(\theta) \le c_1(1+\theta^\kappa)$;
- $m \rightsquigarrow$ mobility is a smooth function bounded from below by a positive constant;
- $\mathbb{C} \rightsquigarrow$ elasticity tensor and $\mathbb{V} \rightsquigarrow$ viscosity tensor, $\mathbb{V} = \omega\mathbb{C}$, $\omega > 0$;
- $a \rightsquigarrow$ bounded away from zero and from above as well as a_z and a_c,
- $b \in \mathrm{C}^1([0,1];[0,+\infty))$;
- $\sigma \rightsquigarrow$ regular;
- $\phi = \widehat{\beta} + \gamma \rightsquigarrow$ mixing potential with $\widehat{\beta}$ convex possibly non-smooth and γ λ-concave, e.g. $\widehat{\beta}(c) = (1+c)\log(1+c) + (1-c)\log(1-c)$ or $\widehat{\beta}(c) = I_{[-1,1]}(c)$ and $\gamma(c) = -c^2$;
- $\boldsymbol{f}$ volume force and g heat source

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Our approach is based on a gradient theory of phase separation and damage processes due to M. Frémond (2012), M. Gurtin (1996) and J.W. Cahn and J.E. Hilliard (1958).

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- presence of the quadratic dissipative terms on the right-hand side in the internal energy balance;

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$$\boldsymbol{u}_{tt} - \mathrm{div}\left(a(c,z)\mathbb{V}\epsilon(\boldsymbol{u}_t) + b(c,z)\mathbb{C}(\epsilon(\boldsymbol{u}) - \epsilon^*(c)) - \rho\theta\mathbb{1}\right) = \boldsymbol{f}$$

$$z_t + \partial I_{(-\infty,0]}(z_t) - \Delta_p(z) + \partial I_{[0,\infty)}(z) + \sigma'(z) \ni -\frac{1}{2}b_{,z}(c,z)\mathbb{C}(\epsilon(\boldsymbol{u}) - \epsilon^*(c)) : (\epsilon(\boldsymbol{u}) - \epsilon^*(c)) + \theta$$

$$c_t = \mathrm{div}(m(c,z)\nabla\mu)$$

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- presence of the quadratic dissipative terms on the right-hand side in the internal energy balance;
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Other approaches to treat PDE systems with an L^1-right-hand side are available in the literature: resorting to the notion of *renormalized solution*, and or by means of *Boccardo-Galloüet* type techniques for example

The literature

Several contributions on systems coupling

- rate-dependent damage and thermal processes (cf., e.g. works by Bonetti, Bonfanti, E.R., Rossi, etc.) as well as
- rate-dependent damage and phase separation (cf., e.g., [Heinemann, Kraus, 2011, 2013, 2015]) are available in the literature

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- the evolution of the damage process is therein considered *rate-independent*, which clearly affects the weak solution concept
- dealing with a *rate-dependent* flow rule for the damage variable is one of the challenges of our own analysis, due to the presence of the quadratic nonlinearity in $\epsilon(\boldsymbol{u})$ on the right-hand side of the damage equation

The "entropic" formulation of the heat equation

We restate the heat equation

$$\theta_t + c_t\theta + z_t\theta + \rho\theta\,\mathrm{div}(\boldsymbol{u}_t) - \mathrm{div}(\mathsf{K}(\theta)\nabla\theta) = g + |c_t|^2 + |z_t|^2 + a(c,z)\epsilon(\boldsymbol{u}_t) : \mathbb{V}\epsilon(\boldsymbol{u}_t) + m(c,z)|\nabla\mu|^2 \quad \text{as}$$

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the weak entropy inequality (for a.a. $0 \le s \le t \le T$ and $s = 0$, and for sufficiently regular and positive tests φ)

$$\int_s^t \int_\Omega (\log(\theta) + c + z)\varphi_t \,\mathrm{d}x\,\mathrm{d}r - \rho\int_s^t \int_\Omega \mathrm{div}(\boldsymbol{u}_t)\varphi\,\mathrm{d}x\,\mathrm{d}r - \int_s^t \int_\Omega \mathsf{K}(\theta)\nabla\log(\theta)\cdot\nabla\varphi\,\mathrm{d}x\,\mathrm{d}r$$
$$\le \left(\int_\Omega (\log(\theta(r)) + c(r) + z(r))\varphi(r)\,\mathrm{d}x\right)\Big|_{r=s}^{r=t} - \int_s^t \int_\Omega \mathsf{K}(\theta)|\nabla\log(\theta)|^2\varphi\,\mathrm{d}x\,\mathrm{d}r$$
$$-\int_s^t \int_\Omega \left(g + |c_t|^2 + |z_t|^2 + a(c,z)\varepsilon(\boldsymbol{u}_t) : \mathbb{V}\varepsilon(\boldsymbol{u}_t) + m(c,z)|\nabla\mu|^2\right)\frac{\varphi}{\theta}\,\mathrm{d}x\,\mathrm{d}r - \int_s^t \int_{\partial\Omega} h\frac{\varphi}{\theta}\,\mathrm{d}S\,\mathrm{d}r$$

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coupled with the total energy inequality (for a.a. $0 \le s \le t \le T$ and $s = 0$)

$$\mathcal{E}(t) \le \mathcal{E}(s) + \int_s^t \int_\Omega g \,\mathrm{d}x\,\mathrm{d}r + \int_s^t \int_{\partial\Omega} h \,\mathrm{d}S\,\mathrm{d}r + \int_s^t \int_\Omega \mathrm{f}\cdot\mathrm{u}_t \,\mathrm{d}x\,\mathrm{d}r + \int_s^t \int_{\partial\Omega} (\boldsymbol{\sigma}\mathrm{n})\cdot\boldsymbol{d}_t \,\mathrm{d}S\,\mathrm{d}r$$

where

$$\mathcal{E} = \int_\Omega \frac{1}{p}|\nabla c|^p + \frac{1}{p}|\nabla z|^p + W(c,\epsilon(\boldsymbol{u}),z) + \phi(c) + \sigma(z) + I_{[0,+\infty)}(z) + \theta + \frac{1}{2}|\boldsymbol{u}_t|^2 \,\mathrm{d}x$$

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Main tool: apply upper semicontinuity arguments for the limit passage in the time-discrete approximation of system

The weak formulation of the damage flow rule

We replace the damage inclusion

$$z_t + \partial I_{(-\infty,0]}(z_t) - \Delta_p(z) + \partial I_{[0,\infty)}(z) + \sigma'(z) \ni -\partial z(c, \epsilon(\boldsymbol{u}), z) + \theta \quad \text{by}$$

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the damage energy-dissipation inequality (for all $t \in (0,T]$, $s = 0$, and a.a. $0 < s \le t$)

$$\int_s^t \int_\Omega |z_t|^2 \,\mathrm{d}x\,\mathrm{d}r + \int_\Omega \left(\frac{1}{p} |\nabla z(t)|^p + \sigma(z(t)) \right) \mathrm{d}x \\ \le \int_\Omega \left(\frac{1}{p} |\nabla z(s)|^p + \sigma(z(s)) \right) \mathrm{d}x + \int_s^t \int_\Omega z_t \left(-W_{,z}(c, \epsilon(\boldsymbol{u}), z) + \theta \right) \mathrm{d}x\,\mathrm{d}r$$

and the one-sided variational inequality for the damage process

$$\int_\Omega \left(z_t\zeta + |\nabla z|^{p-2}\nabla z \cdot \nabla\zeta + \xi\zeta + \sigma'(z(t))\zeta + W_{,z}(c, \epsilon(\boldsymbol{u}), z)\zeta - \theta\zeta \right) \mathrm{d}x \ge 0 \quad \text{a.e. in } (0, T$$

for all sufficiently regular test functions ζ, where $\xi \in \partial I_{[0,+\infty)}(z)$ a.e. in Q, and $z(x,t) \in [0,1]$, $z_t(x,t) \in (-\infty, 0]$ a.e. in Q

Consistency with the standard solution notion

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- Concerning the weak formulation of the damage flow rule, the two previous inequalities on z yield the *damage variational inequality* (with $\xi \in \partial I_{[0,+\infty)}(z)$)

$$\int_s^t \int_\Omega |\nabla z|^{p-2} \nabla z \cdot \nabla \zeta \,\mathrm{d}x\,\mathrm{d}r - \int_\Omega \frac{1}{p} |\nabla z(t)|^p \,\mathrm{d}x + \int_\Omega \frac{1}{p} |\nabla z(s)|^p \,\mathrm{d}x$$
$$+ \int_s^t \int_\Omega \Big(z_t(\zeta - z_t) + \sigma'(z)(\zeta - z_t) + \xi(\zeta - z_t) \Big) \,\mathrm{d}x\,\mathrm{d}r$$
$$\geq \int_s^t \int_\Omega \Big(- W_{,z}(c, \epsilon(\boldsymbol{u}), z)(\zeta - z_t) + \theta(\zeta - z_t) \Big) \,\mathrm{d}x\,\mathrm{d}r$$

$\forall\, t \in (0, T]$, $s = 0$, for a.a. $0 < s \leq t$ and for all $\zeta \in L^p(0, T; W^{1,p}_{-}(\Omega)) \cap L^\infty(0, T; L^\infty(\Omega))$

The "Entropic" weak formulation

We call a quintuple $(c, \mu, z, \theta, \boldsymbol{u})$ an entropic weak solution to the PDE system if

$$c \in L^\infty(0,T;W^{1,p}(\Omega)) \cap H^1(0,T;L^2(\Omega)),\ \Delta_p(c) \in L^2(0,T;L^2(\Omega))$$
$$\mu \in L^2(0,T;H^2_N(\Omega))$$
$$z \in L^\infty(0,T;W^{1,p}(\Omega)) \cap H^1(0,T;L^2(\Omega)),$$
$$\theta \in L^2(0,T;H^1(\Omega)) \cap L^\infty(0,T;L^1(\Omega)), \quad \theta^{\frac{\kappa+\alpha}{2}} \in L^2(0,T;H^1(\Omega)) \text{ for all } \alpha \in (0,1),$$
$$\boldsymbol{u} \in H^1(0,T;H^2(\Omega;\mathbb{R}^d)) \cap W^{1,\infty}(0,T;H^1(\Omega;\mathbb{R}^d)) \cap H^2(0,T;L^2(\Omega;\mathbb{R}^d)),$$

the initial-boundary conditions

$$c(0)=c^0,\ z(0)=z^0,\ \boldsymbol{u}(0)=\boldsymbol{u}^0,\ \boldsymbol{u}_t(0)=\boldsymbol{v}^0 \quad \text{a.e. in } \Omega, \quad \boldsymbol{u}=\boldsymbol{d} \quad \text{a.e. on } \partial\Omega \times (0,T)$$

and

- the "entropic" heat formulation
- the weak damage flow rule
- the a.e. Cahn-Hilliard equation

are satisfied

Existence of "Entropic" solutions

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Theorem Under the previous hypotheses and assuming that

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

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

$$h \in L^1(0,T;L^2(\partial\Omega)), \quad h \geq 0 \quad \text{a.e. in } \partial\Omega \times (0,T)$$

and that the initial data fulfill

$$c^0 \in W^{1,p}(\Omega), \quad \widehat{\beta}(c^0) \in L^1(\Omega), \quad m(c^0) \text{ belongs to the interior of } \mathrm{dom}(\beta)$$

$$z^0 \in W^{1,p}(\Omega), \quad 0 \leq z^0 \leq 1 \text{ in } \Omega$$

$$\theta^0 \in L^1(\Omega), \quad \log\theta^0 \in L^1(\Omega), \quad \exists\, \theta_* > 0 : \ \theta^0 \geq \theta_* > 0 \text{ a.e. in } \Omega$$

$$\boldsymbol{u}^0 \in H^2(\Omega;\mathbb{R}^d) \text{ with } \boldsymbol{u}^0 = \boldsymbol{d}(0) \ \text{ a.e. on } \partial\Omega, \quad \boldsymbol{v}^0 \in H^1(\Omega;\mathbb{R}^d)$$

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then there exists an entropic weak solution $(c,\mu,z,\theta,\boldsymbol{u})$ to the PDE system such that

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

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If in addition in the heat conductivity $\kappa \in (1,5/3)$ if $d=3$ and $\kappa \in (1,2)$ if $d=2$, then we have

$$\theta \in \mathrm{BV}([0,T];W^{2,d+\epsilon}(\Omega)') \qquad \text{for every } \epsilon > 0$$

and the total energy inequality holds for all $t \in [0,T]$, for $s=0$, and for almost all $s \in (0,t)$

Sketch of the estimates at a continuum level

- From the total energy balance, being the total energy

$$\mathcal{E} = \int_\Omega \frac{1}{p}|\nabla c|^p + \frac{1}{p}|\nabla z|^p + W(c, \epsilon(\boldsymbol{u}), z) + \phi(c) + \sigma(z) + I_{[0,+\infty)}(z) + \theta + \frac{1}{2}|\boldsymbol{u}_t|^2 \,\mathrm{d}x\,,$$

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- We resort to higher elliptic regularity results to gain a uniform bound on $\|\mu\|_{L^2(0,T;H^2(\Omega))}$

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is only L^1, because $|z_t|^2 \in L^1$ $\Rightarrow$ "entropic" formulation still needed

Rigorous proof

- All the estimates can be made rigorous via time-discretization
- Time-discrete scheme carefully tailored to nonlinear estimates of heat equation
  - fully implicit $\rightsquigarrow$ essential for strict positivity
  - eqns. tightly coupled $\Rightarrow$ existence via fixed point theorem
  - discrete versions of total energy inequality & entropy inequality hold $\rightarrow$ estimates & passage to the limit $\Rightarrow$ conclusion of existence proof
- Compactness
- Limit passage via lower semicontinuity + maximal monotone operator techniques
- Note that the fact that the inqualities can be proved at a discrete level could be useful for numerics

Outline

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  - it can be applied in different contexts: damage, liquid crystals [Feireisl-R.-Schimperna-Zarnescu], two phase fluids [Eleuteri-R.-Schimperna] (Giulio will talk about that on Thursday!), porous media with hysteresis [Detmann-Krejci-R.] etc.

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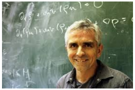

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      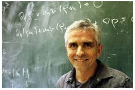

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     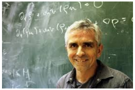

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BUT LET ME CONCLUDE WITH ...

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