# Weak solutions for a degenerating PDE system for phase transitions and damage

E. Rocca

Università degli Studi di Milano

joint work with Riccarda Rossi (Università di Brescia, Italy)



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- The application of the generalization of the principle of virtual powers to the damage phenomena:
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- Introduce the nonlinear PDE system arising in thermomechanics we deal with
- The main key ideas in order to handle nonlinearities + degeneracy ⇒ entropic formulation + generalization of the principle of virtual powers
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- Other possible applications of these formulations to: phase separation, liquid crystals, immiscible fluids.

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Concentrate on damage phenomena accounting for

- the absolute temperature heta
- the evolution of the (small) displacement variables **u**
- the damage parameter  $\chi \in [0,1]$ :  $\chi = 0$  (completely damaged),  $\chi = 1$  (completely undamaged)

where the internal energy balance display nonlinear dissipation and the momentum equation contains  $\chi$ -dependent elliptic operators, degenerating at the *pure phase*  $\chi=0$ 

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

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

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

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- Unidirectional:  $I_{(-\infty,0]}(\chi_t) = 0$  if  $\chi_t \in (-\infty,0]$ ,  $I_{(-\infty,0]}(\chi_t) = +\infty$  otherwise
- Nonlocal:  $A_s$  the s-Laplacian ( $s = 1: -\Delta$ )
- $W = \widehat{\beta} + \widehat{\gamma}$ ,  $\widehat{\gamma} \in C^2(\mathbb{R})$ ,  $\widehat{\beta}$  proper, convex, l.s.c.,  $\overline{\mathrm{dom}(\widehat{\beta})} = [0,1]$  (e.g.  $\widehat{\beta} = I_{[0,1]}$ )

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- 1. a suitable *energy conservation* and *entropy inequality* inspired by:
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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, WIAS preprint 1569 and Adv. Math. Sci. Appl. (2011)] for non-degenerating isothermal diffuse interface models for phase separation and damage \iff weak formulation of the phase equation
  - 2.2. 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 complete damage \(\infty\) weak formulation of the momentum balance

The generalized	principle	of virtual	powers:	damage	phenomena

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 $\Rightarrow$  neglect the nonlinear terms  $\chi |\varepsilon(\mathbf{u}_t)|^2 + |\chi_t|^2$  on the r.h.s (using the small perturbations assumption) in the internal energy balance

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give a weak formulation of the (degenerate) momentum balance and the phase equation (principle of virtual powers)

$$\begin{aligned} \mathbf{u}_{tt} - \operatorname{div}(\chi \varepsilon(\mathbf{u}_t) + \chi \varepsilon(\mathbf{u}) - \rho \theta \mathbf{1}) &= \mathbf{f} \\ \chi_t + \partial I_{(-\infty,0]}(\chi_t) + A_s \chi + W'(\chi) &\ni -\frac{|\varepsilon(\mathbf{u})|^2}{2} + \theta \end{aligned}$$

in order to handle the degeneracy and the nonlinearities in the  $\mathbf{u}+\chi$ -equations.

The non-degenerating approximation

# The non-degenerating approximation

 $\underline{\text{Main aim:}}$  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  $\chi$ 

# The non-degenerating approximation

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

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

[FIRST RESULT.] Local in time well-posedness for a suitable formulation of the reversible problem, using in

$$\theta_t + \chi_t \theta - \Delta \theta = g \underbrace{ + \chi \varepsilon (\mathbf{u}_t)|^2 + |\chi_t|^2}_{= 0}$$
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[SECOND RESULT.] Global well-posedness in the 1D case without small perturbations assumption [E.R., Rossi, Appl. Math., Special Volume (2008)]

<u>Note:</u> in both these results we assumed  $\chi_0$  separated from the thresholds 0 and 1 and we prove (via coercivity condition on W at the thresholds 0 and 1) that the solution  $\chi$  of

$$\chi_t - \Delta \chi + W'(\chi) \ni -\frac{|\varepsilon(\mathbf{u})|^2}{2} + \theta$$

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The last result [E.R., R. Rossi, preprint arXiv:1205.3578v1 (2012)]: global existence result in 3D using a suitable notion of solution and without enforcing the separation property, i.e. allowing for degeneracy  $\implies$  we need a s-Laplacian or a p-Laplacian

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

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

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

- the stiffness of the material decreases as  $\chi \searrow 0$
- f is a concave function, a primitive of the specific heat is  $\hat{c}(\theta) = f(\theta) \theta f'(\theta)$
- $a_s(z_1, z_2) := \int_{\Omega} \int_{\Omega} \frac{\left(\nabla z_1(x) \nabla z_1(y)\right) \cdot \left(\nabla z_2(x) \nabla z_2(y)\right)}{|x y|^{d + 2(s 1)}} \, \mathrm{d}x \, \mathrm{d}y$  is the bilinear form associated to the nonlocal fractional s-Laplacian  $A_s$  (or  $a_p(\chi, \chi) = |\nabla \chi|^p/p$ )
- s>d/2 (or p>d): 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.,  $\overline{\mathrm{dom}(\widehat{\beta})}=[0,1]$  (e.g.  $\widehat{\beta}=\emph{I}_{[0,1]})$
- we can include the thermal expansion term  $-\rho\theta {\rm tr}(\varepsilon({\bf u}))$  (neglect it in this presentation)

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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 is the heat conductivity
- $I_{(-\infty,0]}(\chi_t)=0$  if  $\chi_t\in(-\infty,0],\ I_{(-\infty,0]}(\chi_t)=+\infty$  otherwise

## The modelling

The momentum equation

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

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The "standard" principle of virtual powers

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

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



# The technique

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• We replace the momentum equation with a non-degenerating one

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

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as the enthalpy equation

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

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We assume that

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

$$\exists c_2, c_3 > 0 \ \forall \theta \in [0, +\infty) : c_2 \mathsf{c}(\theta) \le k(\theta) \le c_3 (\mathsf{c}(\theta) + 1)$$

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

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

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

## 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

$$w \in L^{r}(0, T; W^{1,r}(\Omega)) \cap L^{\infty}(0, T; L^{1}(\Omega)) \cap BV([0, T]; W^{1,r'}(\Omega)^{*})$$

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

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

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

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

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

$$\int_{\Omega} \varphi(t) w(t) (\mathrm{d}x) - \int_{0}^{t} \int_{\Omega} w \varphi_{t} \, \mathrm{d}x + \int_{0}^{t} \int_{\Omega} \chi_{t} \Theta(w) \varphi \, \mathrm{d}x + \int_{0}^{t} \int_{\Omega} K(w) \nabla w \nabla \varphi \, \mathrm{d}x$$

$$= \int_{0}^{t} \int_{\Omega} g \varphi + \int_{\Omega} w_{0} \varphi(0) \, \mathrm{d}x$$

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

and the subdifferential inclusion "in a suitable sense"

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

[Theorem 1] ( $\delta>0$ ) Under the previous assumptions on the data ( $W=I_{[0,+\infty)}+\widehat{\gamma}$ ), 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:

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

[Theorem 1]  $(\delta > 0)$  Under the previous assumptions on the data  $(W = I_{[0,+\infty)} + \widehat{\gamma})$ , 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** 

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

$$\begin{split} & \int_{\tau}^{t} \int_{\Omega} |\chi_{t}|^{2} dx dr + \frac{1}{2} a_{s}(\chi(t), \chi(t)) + \int_{\Omega} W(\chi(t)) dx \\ & \leq \frac{1}{2} a_{s}(\chi(\tau), \chi(\tau)) + \int_{\Omega} W(\chi(\tau)) dx + \int_{\tau}^{t} \int_{\Omega} \chi_{t} \left( -\frac{|\varepsilon(\mathbf{u})|^{2}}{2} + \Theta(w) \right) dx dr \end{split}$$

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[2.] Suppose in addition that  $g(x,t) \ge 0$ ,  $\theta_0 > \underline{\theta}_0 \ge 0$  a.e. Then  $\theta(x,t) := \Theta(w(x,t)) \ge \underline{\theta}_0 \ge 0$  a.e.

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$$\leq \frac{1}{2} a_{s}(\chi(\tau), \chi(\tau)) + \int_{\Omega} W(\chi(\tau)) dx + \int_{\tau}^{t} \int_{\Omega} \chi_{t} \left( -\frac{|\varepsilon(\mathbf{u})|^{2}}{2} + \Theta(w) \right) dx dr$$

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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

## Generalized principle of virtual powers vs classical phase inclusion

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

$$\int_0^T \int_\Omega \chi_t \varphi + \mathsf{a}_s(\chi,\varphi) + \xi \varphi + \gamma(\chi) \varphi + \frac{|\varepsilon(\mathsf{u})|^2}{2} \varphi - \Theta(w) \varphi \ge 0 \qquad \qquad \text{(one-sided)}$$

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

$$\int_{\tau}^{t} \int_{\Omega} |\chi_{t}|^{2} dx dr + \frac{1}{2} a_{s}(\chi(t), \chi(t)) + \int_{\Omega} W(\chi(t)) dx 
\leq \frac{1}{2} a_{s}(\chi(\tau), \chi(\tau)) + \int_{\Omega} W(\chi(\tau)) dx + \int_{\tau}^{t} \int_{\Omega} \chi_{t} \left( -\frac{|\varepsilon(\mathbf{u})|^{2}}{2} + \Theta(w) \right) dx dr$$
(energy)

• "Differentiating in time" the energy inequality (energy) and using the chain rule, we conclude that  $(w, \mathbf{u}, \chi, \xi)$  comply with

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

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

$$\chi_t + A_s \chi + \xi(t) + \gamma(\chi) + \frac{|\varepsilon(\mathbf{u})|^2}{2} - \Theta(w) \in -\partial I_{(-\infty,0]}(\chi_t) \text{ in } H^{-s}(\Omega)$$

• We pass to the limit in a carefully designed time-discretization scheme

- We pass to the limit in a carefully designed time-discretization scheme
- Any weak solution  $(w, \mathbf{u}, \chi)$  fulfills the **total energy inequality** for all  $t \in (0, T]$ , for  $\tau = 0$ , and for almost all  $0 < \tau < t$

$$\int_{\Omega} w(t)(\mathrm{d}x) + \frac{1}{2} \int_{\Omega} |\mathbf{u}_{t}(t)|^{2} \, \mathrm{d}x + \int_{\tau}^{t} \int_{\Omega} |\chi_{t}|^{2} \, \mathrm{d}x \, \mathrm{d}r + \int_{\tau}^{t} \int_{\Omega} (\chi + \delta) |\varepsilon(\mathbf{u}_{t})|^{2} \, \mathrm{d}x \, \mathrm{d}r \\
+ \frac{1}{2} \int_{\Omega} (\chi + \delta) |\varepsilon(\mathbf{u}(t))|^{2} \, \mathrm{d}x + a_{s}(\chi(t), \chi(t)) + \int_{\Omega} W(\chi(t)) \, \mathrm{d}x \\
\leq \int_{\Omega} w(\tau)(\mathrm{d}x) + \frac{1}{2} \int_{\Omega} |\mathbf{u}_{t}(\tau)|^{2} \, \mathrm{d}x + \frac{1}{2} \int_{\Omega} (\chi + \delta) |\varepsilon(\mathbf{u}(\tau))|^{2} \, \mathrm{d}x + a_{s}(\chi(\tau), \chi(\tau)) \\
+ \int_{\Omega} W(\chi(\tau)) \, \mathrm{d}x + \int_{\tau}^{t} \int_{\Omega} \mathbf{f} \cdot \mathbf{u}_{t} \, \mathrm{d}x \, \mathrm{d}r + \int_{\tau}^{t} \int_{\Omega} \mathbf{g} \, \mathrm{d}x \, \mathrm{d}r.$$

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• The presence of the s-Laplacian with  $s>d/2\Longrightarrow$  an estimate for  $\chi$  in  $L^\infty(0,T;H^s(\Omega))$  (from the total energy balance)  $\Longrightarrow$  we can now test the momentum balance by  $-\operatorname{div}(\varepsilon(\mathbf{u}_t))\Longrightarrow$  an  $L^\infty(0,T;L^2(\Omega))$ -bound on the quadratic nonlinearity  $|\varepsilon(\mathbf{u})|^2$  on the right-hand side of

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

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

• A BOCCARDO-GALLOUËT-type estimate + Gagliardo-Nirenberg inequality lead to an  $L^r(0, T; W^{1,r}(\Omega))$ -estimate on the enthalpy w (and hence on  $\Theta(w)$ ).

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

Rewrite the momentum equation

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

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

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

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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

$$\begin{split} &\int_{\Omega} w_{\delta}(t)(\mathrm{d}x) + \frac{1}{2} \int_{\Omega} |\partial_{t}\mathbf{u}_{\delta}(t)|^{2} \, \mathrm{d}x + \int_{\tau}^{t} \int_{\Omega} |\partial_{t}\chi_{\delta}|^{2} \, \mathrm{d}x + \frac{1}{2} \int_{\tau}^{t} \int_{\Omega} |\mu_{\delta}|^{2} \, \mathrm{d}x \\ &+ \frac{|\eta_{\delta}(t)|^{2}}{2} + \frac{1}{2} a_{s}(\chi_{\delta}(t), \chi_{\delta}(t)) + \int_{\Omega} W(\chi_{\delta}(t)) \, \mathrm{d}x \\ &\leq \int_{\Omega} w_{\delta}(\tau)(\mathrm{d}x) + \frac{1}{2} \int_{\Omega} |\partial_{t}\mathbf{u}_{\delta}(\tau)|^{2} \, \mathrm{d}x + \frac{|\eta_{\delta}(\tau)|^{2}}{2} + \frac{1}{2} a_{s}(\chi_{\delta}(\tau), \chi_{\delta}(\tau)) \\ &+ \int_{\Omega} W(\chi_{\delta}(\tau)) \, \mathrm{d}x + \int_{\tau}^{t} \int_{\Omega} \mathbf{f} \cdot \partial_{t}\mathbf{u}_{\delta} \, \mathrm{d}x + \int_{\tau}^{t} \int_{\Omega} \mathbf{g} \, \mathrm{d}x \end{split}$$

[Theorem 2] ( $\delta=0$ ) Under the previous assumptions, there exist

$$\begin{aligned} \mathbf{u} &\in W^{1,\infty}(0,T;L^2(\Omega)) \cap H^2(0,T;H^{-1}(\Omega)), \ \boldsymbol{\mu} \in L^2(0,T;L^2(\Omega)), \ \boldsymbol{\eta} \in L^\infty(0,T;L^2(\Omega)), \\ w &\in L^r(0,T;W^{1,r}(\Omega)) \cap L^\infty(0,T;L^1(\Omega)) \cap \mathrm{BV}([0,T];W^{1,r'}(\Omega)^*) \\ \chi &\in L^\infty(0,T;H^s(\Omega)) \cap H^1(0,T;L^2(\Omega)), \quad \chi(x,t) \geq 0, \quad \chi_t(x,t) \leq 0 \text{ a.e.} \end{aligned}$$

such that

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$$\mu = \sqrt{\chi} \, \varepsilon(\mathbf{u}_t), \,\, \boldsymbol{\eta} = \sqrt{\chi} \, \varepsilon(\mathbf{u}) \,,$$

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such that it holds true (a.e. in any open set  $A \subset \Omega \times (0,T)$ :  $\chi > 0$  a.e. in A)

$$\mu = \sqrt{\chi} \, \varepsilon(\mathbf{u}_t), \ \boldsymbol{\eta} = \sqrt{\chi} \, \varepsilon(\mathbf{u}),$$

the weak enthalpy equation and the weak momentum and phase relations

$$\begin{split} \partial_t^2 \mathbf{u} - \operatorname{div}(\sqrt{\chi}\,\boldsymbol{\mu}) - \operatorname{div}(\sqrt{\chi}\,\boldsymbol{\eta})) &= \mathbf{f} \quad \text{in } H^{-1}(\Omega;\mathbb{R}^d), \text{ a.e. in } (0,T)\,, \\ \int_0^T \int_\Omega \left(\partial_t \chi + \gamma(\chi)\right) \varphi \, \mathrm{d}x + \int_0^T a_{\mathfrak{s}}(\chi,\varphi) &\leq \int_0^T \int_\Omega \left(-\frac{1}{2\chi}|\boldsymbol{\eta}|^2 + \Theta(w)\right) \varphi \, \mathrm{d}x \\ &\text{for all } \varphi \in L^2(0,T;H^s_+(\Omega)) \cap L^\infty(Q) \text{ with } \operatorname{supp}(\varphi) \subset \{\chi > 0\}, \end{split}$$

[Theorem 2] ( $\delta = 0$ ) Under the previous assumptions, there exist

$$\mathbf{u} \in W^{1,\infty}(0,T;L^{2}(\Omega)) \cap H^{2}(0,T;H^{-1}(\Omega)), \ \mu \in L^{2}(0,T;L^{2}(\Omega)), \ \eta \in L^{\infty}(0,T;L^{2}(\Omega)), \ w \in L^{r}(0,T;W^{1,r}(\Omega)) \cap L^{\infty}(0,T;L^{1}(\Omega)) \cap \mathrm{BV}([0,T];W^{1,r'}(\Omega)^{*}) \ \chi \in L^{\infty}(0,T;H^{s}(\Omega)) \cap H^{1}(0,T;L^{2}(\Omega)), \ \chi(x,t) \geq 0, \ \chi_{t}(x,t) \leq 0 \text{ a.e.}$$

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the weak enthalpy equation and the weak momentum and phase relations

$$\partial_t^2 \mathbf{u} - \operatorname{div}(\sqrt{\chi}\,\boldsymbol{\mu}) - \operatorname{div}(\sqrt{\chi}\,\boldsymbol{\eta})) = \mathbf{f} \quad \text{in } H^{-1}(\Omega;\mathbb{R}^d), \text{ a.e. in } (0,T),$$

$$\int_0^T \int_{\Omega} \left( \partial_t \chi + \gamma(\chi) \right) \varphi \, \mathrm{d}x + \int_0^T \mathsf{a}_{\mathsf{s}}(\chi, \varphi) \le \int_0^T \int_{\Omega} \left( -\frac{1}{2\chi} |\boldsymbol{\eta}|^2 + \Theta(w) \right) \varphi \, \mathrm{d}x$$

for all  $\varphi \in L^2(0, T; H^s_+(\Omega)) \cap L^\infty(Q)$  with  $\operatorname{supp}(\varphi) \subset \{\chi > 0\}$ ,

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

$$\begin{split} \int_{\Omega} w(t)(\mathrm{d}x) + \int_{0}^{t} \int_{\Omega} |\chi_{t}|^{2} \, \mathrm{d}x + \frac{1}{2} \int_{0}^{t} \int_{\Omega} |\mu|^{2} \, \mathrm{d}x + \int_{\Omega} W(\chi(t)) \, \mathrm{d}x + \mathcal{J}(t) &\leq \int_{\Omega} w_{0} \, \mathrm{d}x \\ + \frac{1}{2} \int_{\Omega} |\mathbf{v}_{0}|^{2} \, \mathrm{d}x + \frac{1}{2} \chi_{0} |\varepsilon(\mathbf{u}_{0})|^{2} + \frac{1}{2} a_{s}(\chi_{0}, \chi_{0}) + \int_{\Omega} W(\chi_{0}) \, \mathrm{d}x + \int_{0}^{t} \int_{\Omega} \mathbf{f} \cdot \mathbf{u}_{t} \, \mathrm{d}x \mathrm{d}r + \int_{0}^{t} \int_{\Omega} \mathbf{g} \, \mathrm{d}x \\ & \text{with } \int_{0}^{t} \mathcal{J}(r) \, \mathrm{d}r \geq \frac{1}{2} \int_{0}^{t} \left( \int_{\Omega} |\mathbf{u}_{t}(r)|^{2} \, \mathrm{d}x + |\eta(r)|^{2} + a_{s}(\chi(r), \chi(r)) \right) \end{split}$$

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$$\begin{split} \int_0^T \int_\Omega \left( \partial_t \chi + \gamma(\chi) \right) \varphi \, \mathrm{d}x + \int_0^T a_s(\chi, \varphi) & \leq \int_0^T \int_\Omega \left( -\frac{1}{2\chi} |\eta|^2 \varphi + \Theta(w) \varphi \right) \, \mathrm{d}x \\ \text{for all } \varphi \in L^2(0, T; H^s_+(\Omega)) \cap L^\infty(Q) \text{ with } \mathrm{supp}(\varphi) \subset \{\chi > 0\}, \end{split}$$

coincides with the one-sided inequality

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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:

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

### Work in progress: avoid the small perturbation assumptions

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

$$\theta_t + \chi_t \theta - \Delta \theta = |\chi_t|^2 + \chi |\varepsilon(\mathbf{u}_t)|^2$$

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Our next aim: to couple the weak equations for  ${\bf u}$  and  $\chi$  with a suitable formulation of the internal energy balance:

a weak energy conservation and entropy inequality

inspired by 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

Entropic formulation: a phase transitions model

## A first application of the entropic formulation: solid-liquid phase transitions

In order to show the potential power of this idea we

... give a description of the method stating more precisely the content of this recent work [E. Feireisl, H. Petzeltovà, E.R., Existence of solutions to some models of phase changes with microscopic movements, Math. Meth. Appl. Sci. (2009)] in which this notion of solution has been firstly applied to phase transition models

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⇒ a new weaker notion of solution is needed



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Finally, couple these relations to a suitable phase dynamics.

Assuming the system is thermally isolated, the entropy balance results

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$$\int_0^T \int_{\Omega} s_t \varphi - \int_0^T \int_{\Omega} \frac{\mathbf{q}}{\theta} \cdot \nabla \varphi = \int_0^T \int_{\Omega} r \varphi \quad \forall \varphi \in \mathcal{D}(\overline{Q}_T),$$

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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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$$\int_{0}^{T} \int_{\Omega} \left( (\log \theta + \chi) \, \partial_{t} \varphi - \nabla \log \theta \cdot \nabla \varphi \right) dx dt$$

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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

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

where

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Finally, the phase dynamics results as

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

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

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

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

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

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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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the phase equation

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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, damage phenomena

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✓ the energy conservation E(t) = E(0) for a.e.  $t \in [0, T]$ , where

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



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for every test function  $\varphi \in \mathcal{D}(\overline{Q}_T)$ ,  $\varphi \geq 0$  and

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$$E \equiv \int_{\Omega} \left( heta + W(\chi) + rac{1}{2} a_s(\chi, \chi) + rac{|\mathbf{u}_t|^2}{2} + \chi rac{|arepsilon(\mathbf{u})|^2}{2} 
ight) dx \,.$$

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

Finally, with C. Heinemann, C. Kraus and R. Rossi, we would like to study the case of non-isothermal phase separation and damage.

### A further application to liquid crystals

 In [E. Feireisl, M. Frémond, E.R., G. Schimperna, ARMA 2012] we have coupled the incompressible Nevier-Stokes equation

$$\begin{aligned} &\operatorname{div} \mathbf{v} = 0, \quad \mathbf{v}_t + \mathbf{v} \cdot \nabla_x \mathbf{v} + \nabla_x p = \operatorname{div} \mathbb{S} + \operatorname{div} \sigma^{nd} + \mathbf{g} \\ \mathbb{S} &= \nu(\theta) \left( \nabla_x \mathbf{v} + \nabla_x^t \mathbf{v} \right), \quad \sigma^{nd} = -\nabla_x d \odot \nabla_x d + (\partial_d W(d) - \Delta d) \otimes d \end{aligned}$$

and the evolution of the director field d, representing preferred orientation of molecules in a neighborhood of any point of a reference domain



$$d_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} d - d \cdot \nabla_{\mathbf{x}} \mathbf{v} = \Delta d - \partial_d W(d)$$

with an entropic formulation of the inernal energy balance displaying higher order nonlinearities on the right hand side:

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

• In [E. Feireisl, E.R., G. Schimperna, A. Zarnescu, preprint arXiv: 1207.1643v1 2012] we have extended it to the tensorial Ball-Majumdar model for liquid crystals

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$$\operatorname{div} \mathbf{v} = 0, \quad \partial_t \mathbf{v} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) + \nabla p = \operatorname{div} \mathbb{S} - \mu \nabla_x \chi, \quad \mathbb{S} = \nu(\theta, \chi) \left( \nabla_x \mathbf{v} + \nabla_x^t \mathbf{v} \right)$$
 (1)

$$\partial_t \theta + \operatorname{div}(\theta \mathbf{v}) + \operatorname{div} \mathbf{q} = \mathbb{S} : \nabla_x \mathbf{v} + |\nabla_x \mu|^2$$
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$$\partial_t \chi + \mathbf{v} \cdot \nabla_{\mathbf{x}} \chi = \Delta \mu \,, \quad \mu = -\Delta \chi + W'(\chi) - \lambda(\theta)$$
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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/