Weak formulation of a nonlinear PDE system arising from models of phase transitions and damage

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- Introduce the nonlinear PDE system coupling
  - an internal energy balance
  - a (possibly degenerating) momentum balance
  - an order parameter equation

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

where the internal energy balance displays nonlinear dissipation and the momentum equation contains χ-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:** $A_s : H^s(\Omega) \to H^s(\Omega)^*$ the fractional $s-$Laplacian ($s > d/2$)
- $W = \widehat{\beta} + \widehat{\gamma}$, $\widehat{\gamma} \in C^2(\mathbb{R})$, $\widehat{\beta}$ 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:

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 $\Longrightarrow$ **weak** formulation of the **internal energy balance**

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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 $\Longrightarrow$ **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 $\Longrightarrow$ **weak** formulation of the **momentum balance**

Weak formulation of the χ+u-equations: the generalized principle of virtual powers

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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

$$c(\theta)\theta_t + \chi_t\theta + \rho\theta \operatorname{div} \mathbf{u}_t - \operatorname{div}(k(\theta)\nabla\theta) = g \quad \underbrace{+\chi\varepsilon(\mathbf{u}_t)|^2 + |\chi_t|^2}_{=0}$$

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

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

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

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

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

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Note that *both* the coefficients need to be truncated when taking the degenerate limit in the momentum equation:

- the truncation in front of $\varepsilon(\mathbf{u}_t)$ allows us to deal with the *main part* of the elliptic operator but
- in order to pass to the limit in the quadratic term on the right-hand side of χ-eq., we also need to truncate the coefficient of $\varepsilon(\mathbf{u})$

Our results

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[First result] **Local in time well-posedness** for a suitable formulation of the reversible problem, using in

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the *small perturbations assumption* in the **3D** (in space) setting [E.R., Rossi, J. Differential Equations, 2008]

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Note: in both these results we assumed χ_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 χ 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** $\Longrightarrow$ we need a s-Laplacian or a p-Laplacian on χ

The free-energy

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

$$\mathcal{F} = \int_\Omega \Big(f(\theta) + \chi \frac{|\varepsilon(\mathbf{u})|^2}{2} + \frac{a_s(\chi,\chi)}{2} + W(\chi) - \theta\chi \Big)\,\mathrm{d}x$$

- **the stiffness of the material decreases as $\chi \searrow 0$**
- f is a concave function, the heat capacity is $c(\theta) = -\theta f''(\theta)$
- $a_s(z_1, z_2) := \int_\Omega \int_\Omega \frac{(\nabla z_1(x) - \nabla z_1(y)) \cdot (\nabla z_2(x) - \nabla z_2(y))}{|x-y|^{d+2(s-1)}}\,\mathrm{d}x\,\mathrm{d}y$ 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 compact 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. $\widehat{\beta} = I_{[0,1]}$)
- we can include the thermal expansion term $-\rho\theta\mathrm{tr}(\varepsilon(\mathbf{u}))$ (neglected in this presentation)

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The pseudo-potential

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

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

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

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

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The internal energy balance

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

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

$$\mathbf{u}_{tt} - \mathrm{div}((\chi + \delta)\varepsilon(\mathbf{u}_t) + (\chi + \delta)\varepsilon(\mathbf{u})) = \mathbf{f}, \quad \delta > 0 \tag{1}$$

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- A major difficulty stems from the simultaneous presence in (2) of $\partial I_{(-\infty,0]}(\chi_t)$ and $W'(\chi)$ and from the low regularities of $-\frac{|\varepsilon(\mathbf{u})|^2}{2} + \theta$ on the r.h.s. $\Longrightarrow$ follow the approach of [Heinemann, Kraus, Adv. Math. Sci. Appl. (2011)] and consider a suitable weak formulation of (2) consisting of a one-sided variational inequality + an energy inequality $\Longrightarrow$ **generalized principle of virtual powers**

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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 χ, also coupled with the temperature equation

Energy vs Enthalpy

In order to deal with the low regularity of θ, rewrite the internal energy equation

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

as the enthalpy equation

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

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

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We assume that

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

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

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

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

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

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

The approximating non-degenerate Problem $[\mathrm{P}_\delta]$

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

$$w \in L^r(0,T;W^{1,r}(\Omega)) \cap L^\infty(0,T;L^1(\Omega)) \cap \mathrm{BV}([0,T];W^{1,r'}(\Omega)^*)$$
$$\mathbf{u} \in H^1(0,T;H^2(\Omega;\mathbb{R}^d)) \cap W^{1,\infty}(0,T;H^1_0(\Omega)) \cap H^2(0,T;L^2(\Omega;\mathbb{R}^d))$$
$$\chi \in L^\infty(0,T;H^s(\Omega)) \cap H^1(0,T;L^2(\Omega))$$

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

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

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

$$\int_\Omega \varphi(t)\, w(t)(\mathrm{d}x) - \int_0^t \int_\Omega w\varphi_t \,\mathrm{d}x + \int_0^t \int_\Omega \chi_t \Theta(w)\varphi \,\mathrm{d}x + \int_0^t \int_\Omega K(w)\nabla w \nabla\varphi \,\mathrm{d}x$$
$$= \int_0^t \int_\Omega g\varphi + \int_\Omega w_0 \varphi(0)\,\mathrm{d}x$$

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

and the subdifferential inclusion **"in a suitable sense"**

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

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 ($W = I_{[0,+\infty)} + \widehat{\gamma}$), then,

[1.] Problem [P_δ] admits a *weak solution* $(w, \mathbf{u}, \chi)$, which, beside fulfilling the enthalpy and momentum equations, satisfies $\chi_t(x,t) \le 0$ 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**

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

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

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

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

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

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

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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 χ 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 $(\forall \varphi \in L^2(0,T; H^s_-(\Omega)) \cap L^\infty(Q))$:

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

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

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

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

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

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

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

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

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- 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

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

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

$$\begin{aligned}
&\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 |\boldsymbol{\mu}_\delta|^2\,\mathrm{d}x \\
&\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))\,\mathrm{d}x \\
&\le \int_\Omega w_\delta(\tau)(\mathrm{d}x) + \frac{1}{2}\int_\Omega |\partial_t \mathbf{u}_\delta(\tau)|^2\,\mathrm{d}x + \frac{|\boldsymbol{\eta}_\delta(\tau)|^2}{2} + \frac{1}{2}a_s(\chi_\delta(\tau),\chi_\delta(\tau)) \\
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[Theorem 2] **($\delta = 0$)** Under the previous assumptions, there exist

$$\mathbf{u} \in W^{1,\infty}(0,T;L^2(\Omega)) \cap H^2(0,T;H^{-1}(\Omega)),\ \boldsymbol{\mu} \in L^2(0,T;L^2(\Omega)),\ \boldsymbol{\eta} \in L^\infty(0,T;L^2(\Omega)),$$

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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)

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the weak enthalpy equation

$$\int_\Omega \varphi(t)\, w(t)(\mathrm{d}x) - \int_0^t \int_\Omega w\varphi_t\,\mathrm{d}x + \int_0^t \int_\Omega \chi_t \Theta(w)\varphi\,\mathrm{d}x + \int_0^t \int_\Omega K(w)\nabla w \nabla\varphi\,\mathrm{d}x$$
$$= \int_0^t \int_\Omega g\varphi + \int_\Omega w_0\varphi(0)\,\mathrm{d}x \quad \forall\,\varphi \in \mathrm{C}^0([0,T];W^{1,r'}(\Omega)) \cap W^{1,r'}(0,T;L^{r'}(\Omega)),\ t \in (0,T]$$

the *weak* momentum balance

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

and phase relations

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

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

Degenerate total energy inequality

For almost all $t \in (0, T]$ we obtain

$$\mathcal{H}(t) + \int_0^t \int_\Omega |\chi_t|^2 \,\mathrm{d}x + \frac{1}{2}\int_0^t \int_\Omega |\boldsymbol{\mu}|^2 \,\mathrm{d}x \le \int_\Omega w_0 \,\mathrm{d}x + \frac{1}{2}\int_\Omega |\mathbf{v}_0|^2 \,\mathrm{d}x + \frac{1}{2}\chi_0|\varepsilon(\mathbf{u}_0)|^2$$

$$+ \frac{1}{2}a_s(\chi_0, \chi_0) + \int_\Omega W(\chi_0) \,\mathrm{d}x + \int_0^t \int_\Omega \mathbf{f} \cdot \mathbf{u}_t \,\mathrm{d}x\mathrm{d}r + \int_0^t \int_\Omega g \,\mathrm{d}x$$

with $\mathcal{H}(t) \ge \int_\Omega w(t)(\mathrm{d}x) + \frac{1}{2}\int_\Omega |\partial_t \mathbf{u}(t)|^2 \,\mathrm{d}x + \frac{1}{2}a_s(\chi(t), \chi(t)) + \int_\Omega W(\chi(t)) \,\mathrm{d}x + \mathcal{J}(t)$

where $\mathcal{J}(t) := \frac{1}{2}\liminf_{\delta_k \downarrow 0} \int_\Omega |\boldsymbol{\eta}_{\delta_k}(t)|^2 \,\mathrm{d}x$

with $(\boldsymbol{\eta}_{\delta_k})$ a suitable subsequence of $(\boldsymbol{\eta}_\delta)$ from the approximated problem.
And for all $0 \le t_1 \le t_2 \le T$ there holds

$$\int_{t_1}^{t_2} \mathcal{H}(r) \,\mathrm{d}r \ge \int_{t_1}^{t_2} \left(\int_\Omega w(r)(\mathrm{d}x) + \frac{1}{2}a_s(\chi(r), \chi(r)) \,\mathrm{d}r \right)$$

$$+ \int_{t_1}^{t_2} \left(\int_\Omega \left(\frac{1}{2}|\partial_t \mathbf{u}(r)|^2 + W(\chi(r)) + \frac{1}{2}|\boldsymbol{\eta}(r)|^2 \right) \mathrm{d}x \right) \mathrm{d}r \,.$$

A comparison between the solution notions

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

coincides with the **one-sided inequality**

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

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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** for χ

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

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:

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Our **next aim**: to couple the weak equations for $\mathbf{u}$ and χ 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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$\Longrightarrow$ a new weaker notion of solution is needed

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Finally, couple these relations to a suitable phase dynamics

The entropy production

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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 $[0, T] \times \overline{\Omega} =: \overline{Q}_T$;

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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

$$E \equiv \int_\Omega \left(\theta + W(\chi) + \frac{|\nabla \chi|^2}{2} \right) dx\,.$$

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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

$\widehat{\beta} : \mathbb{R} \to [0, +\infty]$ 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 $r \in \mathrm{dom}(\widehat{\beta})$

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

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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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- **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**

Work in progress: an entropic formulation for the damage phenomena

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

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

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$$\leq \int_0^T \int_\Omega \frac{1}{\theta}\left(-|\chi_t|^2 - \chi|\varepsilon(\mathbf{u}_t)|^2 - \nabla\log\theta\cdot\nabla\theta\right)\varphi dxdt$$

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

- ✓ the energy conservation $E(t) = E(0)$ 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 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**

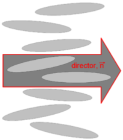
A further application to liquid crystals

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

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

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

where $\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d}$ is the 3×3 matrix given by $\nabla_i\mathbf{d}\cdot\nabla_j\mathbf{d}$, $(\mathbf{a}\otimes\mathbf{b})_{ij}:=a_i b_j$, $1\le i,j\le 3$, and the evolution of the director field $\mathbf{d}$, representing preferred orientation of molecules in a neighborhood of any point of a reference domain



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

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

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

- 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

A further application to two phase fluids

- A fluid-mechanical theory for **two-phase mixtures of fluids** faces a well known mathematical difficulty:
  - the movement of the interfaces $\Longrightarrow$ Lagrangian description
  - the bulk fluid flow $\Longrightarrow$ Eulerian framework

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

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

$$\partial_t\chi+\mathbf{v}\cdot\nabla_x\chi=\Delta\mu\,,\quad \mu=-\Delta\chi+W'(\chi)-\lambda(\theta) \tag{3}$$

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

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

$$\partial_t \chi + \mathbf{v} \cdot \nabla_x \chi = \Delta \mu\,, \quad \mu = -\Delta \chi + W'(\chi) - \lambda(\theta) \tag{3}$$

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/