ADMAT2012

PDEs for multiphase advanced materials

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Recent results on a singular and possibly degenerate Cahn-Hilliard type system

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1 - The equations

Model by P. Podio Guidugli (Ric. Mat. 2006)

- $\Omega = \text{body} \subset \mathbb{R}^3$ and $\Gamma = \text{boundary of } \Omega$
- Ω open, bounded, connected, and smooth
- $\mu = $ chemical potential and $\rho = $ order parameter

$$2\rho\partial_t\mu + \mu\partial_t\rho - \kappa\Delta\mu = 0 \quad \text{and} \quad \mu \geq 0 \quad \text{in } \Omega \times (0, T)$$

$$0 < \rho < 1 \quad \text{and} \quad -\Delta\rho + f'(\rho) = \mu \quad \text{in } \Omega \times (0, T)$$

$$\partial_n\mu = \partial_n\rho = 0 \quad \text{on } \Gamma \times (0, T)$$

$$\mu|_{t=0} = \mu_0 \quad \text{and} \quad \rho|_{t=0} = \rho_0 \quad \text{in } \Omega$$

- $f = f_1 + f_2$ double well potential on $(0,1)$
  f_1 convex singular at end-points, f_2 smooth in $[0,1]$

2 - The equations (cont'd)

Two "viscosity terms" have been added

- $\varepsilon > 0$ and $\delta > 0$

$$(\varepsilon + 2\rho)\partial_t \mu + \mu \partial_t \rho - \kappa \Delta \mu = 0$$
$$\delta \partial_t \rho - \Delta \rho + f'(\rho) = \mu$$

- The case $\varepsilon = 0$ could be considered with some care while $\delta = 0$ leads to ill-posedness, namely
- infinitely many (even smooth) solutions
- no uniqueness and no control on time regularity
- the Cauchy condition for μ should be reformulated
- think of suitably selected solutions
- completely open problem !!!
- From now on, $\delta = 1$

3 - History

Series of papers with P. Colli, J. Sprekels, P. Podio-Guidugli
[1] SIAM-JAM'11 - [2] DCDS-S t.a. - [3] CMT t.a. - [4] MJM t.a.

- Main assumption on the potential: $f = f_1 + f_2$ with

$$f_1 \text{ convex and smooth in } (0,1), \ f_2 \text{ smooth on } [0,1]$$

$$\lim_{\rho \searrow 0} f_1'(\rho) = -\infty \quad \text{and} \quad \lim_{\rho \nearrow 1} f_1'(\rho) = +\infty$$

e.g., the logarithmic double well potential

or an even more singular multiple well potential

- Existence for fixed $\varepsilon > 0$ [1]
- Uniqueness for $\varepsilon > 0$: provided μ, $f'(\rho)$ are bdd [1]
- Sufficient conditions for such a boundedness [1]

4 - History (cont'd)

- Asymptotics as $\varepsilon \to 0$: suitable reformulation for $\varepsilon = 0$ [2]

- Longtime behavior for both cases $\varepsilon > 0$ and $\varepsilon = 0$ [1-2]

- Distributed optimal control problem with $\varepsilon > 0$ [3]

$$(\varepsilon + 2\rho)\partial_t \mu + \mu \partial_t \rho - \kappa \Delta \mu = \underset{\uparrow}{u}$$

Neumann BC as before

- Boundary optimal control problem with $\varepsilon > 0$ [4]

$$(\varepsilon + 2\rho)\partial_t \mu + \mu \partial_t \rho - \kappa \Delta \mu = 0$$

3rd type BC: $\partial_n \mu = \alpha(\underset{\uparrow}{u} - \mu), \quad \alpha > 0$

5 - Fresh news and plan of the talk

Three new papers with P. Colli, J. Sprekels, P. Podio-Guidugli on well-posedness: generalizations in several directions $* * *$

- 1st paper, the most important one: submitted $*$
- 2nd paper: to appear in BUMI, in memory of E. Magenes $*$
- 3rd paper: in preparation $*$

More papers in preparation involving P. Krejčí as a new co-author

- Time discretization (future $\rightarrow$ full discretization and numerics)
- Asyptotics as $\sigma \rightarrow 0$ in the modified 2nd equation

$$\partial_t \rho - \sigma \Delta \rho + f'(\rho) = \mu \quad \text{(in fact a more general full problem)}$$

and relations with hysteresis

Plan of the talk

- the above generalizations $* * *$

6 - First generalization

- The above system with a fixed $\varepsilon > 0$, thus $\varepsilon = 1$

$$\begin{aligned}(1+2\rho)\partial_t\mu + \mu\partial_t\rho - \kappa\Delta\mu &= 0\\ \partial_t\rho - \Delta\rho + f'(\rho) &= \mu\end{aligned}$$

becomes

$$\begin{aligned}(1+2g(\rho))\partial_t\mu + \mu\partial_t g(\rho) - \kappa\Delta\mu &= 0\\ \partial_t\rho - \Delta\rho + f'(\rho) &= \mu g'(\rho)\end{aligned}$$

with $g : \mathbb{R} \to \mathbb{R}$ nonnegative on $\mathrm{dom\,f}$ $\quad$ $(+$ something else)
(in the above situation we had $\mathrm{g}(\rho) = \rho$ and $\mathrm{dom\,f} = (0,1)$).

7 - First generalization (cont'd)

Easy generalization from the mathematical point of view !
However, interesting in modeling.

For a given μ, the equation for ρ reads Allen-Cahn

$$\partial_{\mathrm{t}}\rho - \Delta\rho + \frac{\partial}{\partial\rho}\mathrm{F}_{\mu}(\rho) = 0 \quad \text{with} \quad \mathrm{F}_{\mu}(\rho) := \mathrm{f}(\rho) - \mu\,\mathrm{g}(\rho)$$

- Already with $\mathrm{g}(\rho) = \rho$, F_{μ} is not symmetric for a symmetric f (the preferred well depends on μ).
- In the more general case we consider, new situations occur.

For instance, the choice $\mathrm{f}_2 = \mu_{\mathrm{c}}\,\mathrm{g}$ with some critical value μ_{c} leads to

$$\mathrm{F}_{\mu}(\rho) = \mathrm{f}_1(\rho) + (\mu_{\mathrm{c}} - \mu)\,\mathrm{g}(\rho)$$

and one can construct double-well/convex potentials F_{μ} according to the sign of $\mu_{\mathrm{c}} - \mu$.

8 - Second generalization: general potentials

Aim: replace f by a much more general double well potential, e.g.,

$$f(\rho) = I(\rho) - \rho^2$$

where I is the indicator function of $[-1, 1]$

or a smooth potential on the whole of $\mathbb{R}$, like $f(\rho) = (1 - \rho^2)^2$.

- OK for existence, while trouble for uniqueness !

Preliminary observation on the old uniqueness proof.

$$(1) \qquad (1 + 2\rho)\partial_t \mu + \mu \partial_t \rho - \kappa \Delta \mu = 0$$

$$(2) \qquad \partial_t \rho - \Delta \rho + f_1'(\rho) + f_2'(\rho) = \mu$$

Pick two solutions (μ_i, ρ_i), $i = 1, 2$.

Natural trial: use monotonicity of f_1', i.e.,

$$\int_{Q_t} ((2)_1 - (2)_2) \times (\rho_1 - \rho_2) + \int_{Q_t} ((1)_1 - (1)_2) \times (?_1 - ?_2)$$

where $?_i$ are suitably chosen and $Q_t = \Omega \times (0, t)$.

9 - Second generalization: general potentials (cont'd)

- Natural test functions $?_i$, e.g., μ_i
  led to mess and we got lost !!!
- New trial:

$$\int_{Q_t} ((1)_1 - (1)_2) \times (\mu_1 - \mu_2) + \int_{Q_t} ((2)_1 - (2)_2) \times (\partial_t \rho_1 - \partial_t \rho_2).$$

Thus the whole of $f'(\rho)$ moved to the right hand side.

- This uses just the regularity of f' and might work only if

$$|(f'(\rho_1) - f'(\rho_2))(\rho_1 - \rho_2)| \le c|\rho_1 - \rho_2|^2 \quad \text{i.e.}$$

ρ_i bounded away from 0 and 1

- This is true for logarithmic-type potentials
  and false if f = indicator + concave

10 - Second generalization: general potentials (cont'd)

- Now: new uniqueness proof that makes the natural trial work (hence, with any multiple well potential)
- **Trick:** rewrite eq'n (1) for μ in a different form

- **Assumptions on the potential:**

$$
\begin{aligned}
&\mathrm{f} = \mathrm{f}_1 + \mathrm{f}_2 \\
&\mathrm{f}_1 : \mathbb{R} \to [0, +\infty] \quad \text{convex, proper, l.s.c.} \\
&\mathrm{f}_2 : \mathbb{R} \to \mathbb{R} \quad \text{smooth with } \mathrm{f}_2' \text{ Lipschitz}
\end{aligned}
$$

Examples

all the above log-type potentials, $\mathrm{f}(\rho) = (1-\rho^2)^2$

$\mathrm{f}(\rho) = \mathrm{I}(\rho) - \rho^2$, I = indicator funct' of $[-1, 1]$, etc

11 - Second generalization: general potentials (cont'd)

Recall 1st eq'n (with $\kappa = 1$ w.l.o.g.)

$$(1) \qquad (1 + 2\mathrm{g}(\rho))\partial_{\mathrm{t}}\mu + \mu\partial_{\mathrm{t}}\mathrm{g}(\rho) - \Delta\mu = 0$$

Multiply (1) by $\alpha(\rho)$, look for a Leibniz rule in the first two terms, get an ODE for α, and see that $\alpha = (1 + 2\mathrm{g})^{-1/2}$ works.

Hence, we rewrite (1) in the new form

$$\partial_{\mathrm{t}}\big(\mu/\alpha(\rho)\big) - \alpha(\rho)\Delta\mu = 0 \quad \text{where} \quad \alpha(\rho) := \big(1 + 2\mathrm{g}(\rho)\big)^{-1/2}$$

and $\mu/\alpha(\rho)$ is the new unkonwn function in place of μ, i.e.,

$$\partial_{\mathrm{t}}\mathrm{z} - \alpha(\rho)\Delta\big(\alpha(\rho)\,\mathrm{z}\big) = 0 \quad \text{and} \quad \mu := \alpha(\rho)\,\mathrm{z}$$

More precisely, we account for the Neumann BC as follows

$$(1') \qquad \int_\Omega (\partial_{\mathrm{t}}\mathrm{z})\mathrm{v} + \int_\Omega \nabla\big(\alpha(\rho)\,\mathrm{z}\big) \cdot \nabla\big(\alpha(\rho)\,\mathrm{v}\big) = 0$$

for every $\mathrm{v} \in \mathrm{H}^1(\Omega)$ and a.e. in $(0, \mathrm{T})$

12 - Second generalization: general potentials (cont'd)

New system

$$(1') \qquad \int_\Omega (\partial_t z) v + \int_\Omega \nabla\big(\alpha(\rho)\, z\big) \cdot \nabla\big(\alpha(\rho)\, v\big) = 0$$

for every $v \in H^1(\Omega)$ and a.e. in $(0, T)$

$$(2) \qquad \partial_t \rho - \Delta\rho + f'(\rho) = \mu g'(\rho) \qquad + \text{ Neumann BC}$$

and Cauchy conditions, where $\mu := \alpha(\rho)\, z$ in (2).

Pick two sol's (z_i, ρ_i) and set $z := z_1 - z_2$ and $\rho := \rho_1 - \rho_2$. Then

$$\int_0^t \Big((1')_1 - (1')_2\Big) \,\Big|_{v\,=\,z} \, ds + M \int_{Q_t} \Big((2)_1 - (2)_2\Big)\, \rho$$

where M is suitably big and chosen later on in the proof.

13 - Second generalization: general potentials (cont'd)

Then everything works.

However, the proof is rather technical !
In particular, it uses some further regularity of μ
(and of z as a consequence), like

$$(*) \qquad \mu \in W^{1,4}(0,T;L^2(\Omega)) \cap L^4(0,T;W^{1,6}(\Omega))$$

besides boundedness.
More generally, we have proved that

$$\mu \in W^{1,p}(0,T;L^2(\Omega)) \cap L^p(0,T;H^2(\Omega)) \quad \text{for } p \in [1,+\infty)$$

This implies $(*)$ since $H^1(\Omega) \subset L^6(\Omega)$, whence $H^2(\Omega) \subset W^{1,6}(\Omega)$.

14 - Third generalization: nonlinear const' law

The equation for μ

$$(1 + 2\mathrm{g}(\rho))\partial_{\mathrm{t}}\mu + \mu\partial_{\mathrm{t}}\mathrm{g}(\rho) - \kappa\Delta\mu = 0$$

becomes

$$(1) \qquad (1 + 2\mathrm{g}(\rho))\partial_{\mathrm{t}}\mu + \mu\partial_{\mathrm{t}}\mathrm{g}(\rho) - \mathrm{div}\big(\kappa(\mu,\rho)\nabla\mu\big) = 0$$

where $\kappa : \mathbb{R}^2 \to \mathbb{R}$ is smooth enough.
Main assumption: uniform parabolicity and bdd'ness, i.e.,

$$0 < \kappa_* \le \kappa(\mu,\rho) \le \kappa^* \quad \text{for every } \mu \text{ and } \rho$$

15 - Third generalization: nonlinear const' law (cont'd)

Theorem. *Existence of a solution in a proper space.*

- No uniqueness proof (we didn't try: too complicated)
- but **uniqueness** (and a continuous dependence inequality) if $\kappa = \kappa(\mu)$ with κ Lipschitz
  (1st eq'n rewritten, same trick as before)

16 - Fourth generalization: degeneracy

This with $\kappa = \kappa(\mu)$ (independent of ρ) and existence, only

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- Aim: to allow $\kappa = \mu^{\mathrm{m}-1}$ with any exponent $\mathrm{m} \geq 1$
  so that $\mathrm{div}(\kappa \nabla \mu) \approx \Delta \mu^{\mathrm{m}}$ like in the porous media eq'n

Too difficult due to unboundedness of κ !

- New aim: to allow a bdd version like $\kappa = \tanh \mu^{\mathrm{m}-1}$ with any exponent $\mathrm{m} \geq 1$
  (slow diffusion only where μ is small)

- **It works**, provided that. . . . . (see below)
  Precisely, more degeneracy for small values of μ can be allowed

17 - Fourth generalization: degeneracy (cont'd)

Precise assumptions:

i) $\kappa : [0, +\infty) \to \mathbb{R}$ is continuous

ii) there exist $\kappa_*, \kappa^* > 0$ and $\mu_* \geq 0$ such that

$$\kappa(\mu) \leq \kappa^* \quad \forall \mu \geq 0 \quad \text{and} \quad \kappa(\mu) \geq \kappa_* \quad \forall \mu \geq \mu_*$$

iii) the function $[0, +\infty) \ni \mu \mapsto \mathrm{K}(\mu) := \int_0^\mu \kappa(\mathrm{s})\,\mathrm{ds}$

is strictly increasing

Examples

- $\mu_* = 0$: uniform parabolicity
- $\kappa(\mu) = \tanh \mu^{\mathrm{m}-1}$, $\mathrm{m} > 1$: e.g., $\mu_* = 1$ and $\kappa_* = \tanh 1$

Remarks: no monotonicity for κ, and iii) is equivalent to:

$\kappa \geq 0$ and the set $\{\mu \in [0, \mu_*] : \kappa(\mu) = 0\}$ has an empty interior

(i.e., a lot of degeneracy for small values of μ is possible)

18 - Fourth generalization: degeneracy (cont'd)

Trouble

$$(1) \quad (1+2\mathrm{g}(\rho))\partial_{\mathrm{t}}\mu + \mu\partial_{\mathrm{t}}\mathrm{g}(\rho) - \mathrm{div}\big(\kappa(\mu)\nabla\mu\big) = 0 \quad + \text{BC}$$

- Due to degeneracy, lack of information on $\nabla\mu$ where μ is small
- Consequence: lack of information on both $\partial_{\mathrm{t}}\mu$ and $\partial_{\mathrm{n}}\mu|_{\Gamma}$

- **Remedy**: rewrite (1) in different form
  use $\nabla\mathrm{K}(\mu)$ (recall $\mathrm{K}' = \kappa$) instead of $\kappa(\mu)\nabla\mu$ in eq'n and BC
  and change the first part of (1) and the IC, namely

$$\begin{array}{ll} (1') & \partial_{\mathrm{t}}\big((1+2\mathrm{g}(\rho))\,\mu\big) - \mu\partial_{\mathrm{t}}\mathrm{g}(\rho) - \Delta\mathrm{K}(\mu) = 0 \\ \mathrm{BC}' & \partial_{\mathrm{n}}\mathrm{K}(\mu)|_{\Gamma} = 0 \qquad \text{(in the variational sense)} \\ \mathrm{IC}' & \big((1+2\mathrm{g}(\rho))\,\mu\big)|_{\mathrm{t}=0} = (1+2\mathrm{g}(\rho_0))\,\mu_0 \end{array}$$

19 - Fourth generalization: degeneracy (cont'd)

Full problem (+ BC + IC):

$$(1') \qquad \partial_t \left((1 + 2g(\rho))\, \mu \right) - \mu \partial_t g(\rho) - \Delta K(\mu) = 0$$

$$(2) \qquad \partial_t \rho - \Delta \rho + f'(\rho) = \mu g'(\rho)$$

Then, the expected regularity of $K(\mu)$ is something like

$$K(\mu) \in L^2(0,T; H^1(\Omega))$$

(since $v = K(\mu)$ should be an admissible test function)
whence, we can ask that

$$\partial_t \left((1 + 2g(\rho))\, \mu \right) \in L^2(0,T; (H^1(\Omega))^*)$$

Theorem. *There exists a solution in a proper space.*

- Recall: **uniqueness** OK if $\mu_* = 0$ (uniform parab) and κ Lip

20 - Fourth generalization: degeneracy (cont'd)

A small detail on the existence proof
parabolic regularization + time delay

$$(1')_\tau \qquad \partial_t\big((1+2g(\rho))\,\mu\big) - \mu\partial_t g(\rho) - \Delta\widetilde{K}(\mu) = 0$$

$$(2)_\tau \qquad \partial_t\rho - \Delta\rho + f'(\rho) = g'(\rho)\,\mathcal{T}_\tau\mu$$

where
$$\widetilde{K}(\mu) := \int_0^\mu \big(\kappa(|s|)+\tau\big)\,ds$$
$$\mathcal{T}_\tau\mu(t) := \mu(t-\tau) \quad \text{for } t > \tau$$
$$\mathcal{T}_\tau\mu(t) := \mu_0 \quad \text{for } t < \tau$$

- existence for the approximating problem
- a priori estimates
- convergence as $\tau \searrow 0$ via compactness and monotonicity

Thank you for your attention

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Coordinates & info's: Google $\longrightarrow$ gianni gilardi $\longrightarrow$ $1^{\rm st}$ result is

http://www-dimat.unipv.it/gilardi