Some results on phase change models with microscopic movements

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7th AIMS International Conference on
Dyn. Systems, Diff. Equations and Applications

Arlington Texas USA – May 18 - 21, 2008

Plan of the Talk

- Derivation of Frémond's model of phase transitions and the comparison with other models

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- Related open problems and perspectives

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with a proper choice of the **internal energy functional** (depending on the state variables) and of the **pseudo-potential of dissipation** (depending on the dissipative variables).

The free-energy functional

We take into account of elasticity effects by choosing

$$\underline{\Psi(\vartheta, \varepsilon(\mathbf{u}), \chi, \nabla\chi)} = c_V \vartheta(1 - \log \vartheta) - \frac{\lambda}{\vartheta_c}(\vartheta - \vartheta_c)\chi + \frac{(1-\chi)\varepsilon(\mathbf{u})\mathcal{R}_e\varepsilon(\mathbf{u})}{2} + W(\chi) + \frac{\nu}{2}|\nabla\chi|^2$$

- $\varepsilon(\mathbf{u})$ the linearized symmetric strain tensor, namely $\varepsilon_{ij}(\mathbf{u}) := (u_{i,j} + u_{j,i})/2, \ i, j = 1, 2, 3$
- $(1 - \chi)$ the local proportion of the non viscous phase, e.g. the solid phase in solid-liquid phase transitions
- $\mathcal{R}_e$ a symmetric positive definite elasticity tensor (set $\mathcal{R}_e \equiv \mathbb{I}$)
- c_V, ϑ_c, λ and $\nu(> 0)$ the specific heat, the equilibrium temperature, the latent heat of the system, and the interfacial energy coefficient (set $c_V = \lambda/\vartheta_c = 1$)
- $W(\chi) + (\nu/2)|\nabla\chi|^2$ a mixture or interaction free-energy

The Pseudo-Potential of dissipation

Following the line of [MOREAU, '71], we include dissipation by means of the following functional

$$\Phi(\chi_t, \varepsilon(\mathbf{u}_t), \nabla\vartheta) = \frac{\mu}{2}|\chi_t|^2 + \frac{\chi}{2}\varepsilon(\mathbf{u}_t)\mathcal{R}_v\varepsilon(\mathbf{u}_t) + \frac{h(\vartheta)|\nabla\vartheta|^2}{2\vartheta},$$

where

- $\mathcal{R}_v$ is a symmetric and positive definite viscosity matrix (set $\mathcal{R}_v \equiv \mathbb{I}$);
- χ represents the local proportion of the viscous phase, e.g. the liquid phase in solid-liquid phase transitions;
- $h(\vartheta) \geq h_0 > 0$ stands for the heat conductivity of the process;
- $\mu > 0$ is a relaxation parameter

The equation of macroscopic motion

The **equation of macroscopic motion** is the following stress-strain relation, taking into account of accelerations:

$$\boxed{\mathbf{u}_{tt} - \operatorname{div}\sigma = \mathbf{0} \quad \text{in } \Omega \times (0, T)}$$

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$$\sigma = \sigma^{nd} + \sigma^{d} = \frac{\partial \Psi}{\partial \varepsilon(\mathbf{u})} + \frac{\partial \Phi}{\partial \varepsilon(\mathbf{u}_t)},$$

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However, our analysis carries over to other kinds of boundary conditions on $\mathbf{u}$ like a *pure traction* problem or a *displacement-traction* problem.

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If the volume amount of mechanical energy provided by the external actions is zero, the **generalized principle of virtual power by** [Frémond, '02] gives

$$\boxed{B - \operatorname{div} \mathbf{H} = 0 \quad \text{in } \Omega \times (0,T), \qquad \mathbf{H} \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega \times (0,T)}$$

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$$B = \frac{\partial\Psi}{\partial\chi} + \frac{\partial\Phi}{\partial\chi_t} = -\vartheta + \vartheta_c - \frac{|\varepsilon(\mathbf{u})|^2}{2} + W'(\chi) + \mu\chi_t$$

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we derive **the phase equation**

$$\boxed{\mu\chi_t - \nu\Delta\chi + W'(\chi) = \vartheta - \vartheta_c + \frac{|\varepsilon(\mathbf{u})|^2}{2} \quad \text{in } \Omega \times (0,T)}$$

coupled with the B.C. $\partial_{\mathbf{n}}\chi = 0$ on $\partial\Omega \times (0,T)$.

The internal energy balance

The first principle of thermodynamics can be expressed as

$$\boxed{e_t + \operatorname{div} \mathbf{q} = \sigma : \varepsilon(\mathbf{u}_t) + B\chi_t + \mathbf{H} \cdot \nabla\chi_t}$$

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- e is the (density of) internal energy:

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- the heat flux is $\mathbf{q} = -\vartheta \dfrac{\partial \Phi}{\partial \nabla\vartheta} = -h(\vartheta)\nabla\vartheta\,;$
- on the right-hand side: the mechanically induced heat sources, related to macroscopic and microscopic stresses:

$$\sigma : \varepsilon(\mathbf{u}_t) + B\chi_t + \mathbf{H} \cdot \nabla\chi_t = \chi|\varepsilon(\mathbf{u}_t)|^2 + (1-\chi)\varepsilon(\mathbf{u})\varepsilon(\mathbf{u}_t) - \vartheta\chi_t$$
$$+\mu|\chi_t|^2 + \lambda\chi_t - \frac{|\varepsilon(\mathbf{u})|^2\chi_t}{2} + W'(\chi)\chi_t + \nu\nabla\chi\nabla\chi_t\,.$$

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Due to the cancellations of the *blue* terms, we get

$$\vartheta_t + \vartheta\chi_t - \operatorname{div}(h(\vartheta)\nabla\vartheta) = \chi|\varepsilon(\mathbf{u}_t)|^2 + \mu|\chi_t|^2$$

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- It is sufficient to note that the internal energy balance can be expressed in terms of the entropy $s = -\frac{\partial \Psi}{\partial \vartheta}$ in this way:

$$\vartheta\left(s_t + \operatorname{div}\left(\frac{\mathbf{q}}{\vartheta}\right)\right) = \sigma^{\mathrm{d}} : \varepsilon(\mathbf{u}_t) + B^{\mathrm{d}}\chi_t - \frac{\mathbf{q}}{\vartheta} \cdot \nabla\vartheta$$

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- The right-hand side turns out to be non negative because $(\sigma^{\mathrm{d}}, B^{\mathrm{d}}, -\mathbf{q}/\vartheta) \in \partial\Phi(\mathbf{u}_t, \chi_t, \nabla\vartheta)$, and Φ is convex in all of its variables

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- Therefore, the Clausius-Duhem inequality ensues from the positivity of ϑ

The resulting PDE system

The PDE system in $\Omega \times (0, T)$ turns out to be:

$$\vartheta_t + \chi_t \vartheta - \operatorname{div}(h(\vartheta)\nabla\vartheta) = \mu|\chi_t|^2 + \chi|\varepsilon(\mathbf{u}_t)|^2$$

$$\mu\chi_t - \nu\Delta\chi + W'(\chi) = \vartheta - \vartheta_c + \frac{|\varepsilon(\mathbf{u})|^2}{2}$$

$$\mathbf{u}_{tt} - \operatorname{div}\,((1-\chi)\varepsilon(\mathbf{u}) + \chi\varepsilon(\mathbf{u}_t)) = \mathbf{0}$$

coupled with the following initial and boundary conditions:

$$\vartheta(0) = \vartheta_0\,, \quad \chi(0) = \chi_0\,, \quad \mathbf{u}(0) = \mathbf{u}_0, \quad \mathbf{u}_t(0) = \mathbf{v}_0 \quad \text{in } \Omega$$

$$\partial_{\mathbf{n}}\vartheta = 0, \quad \partial_{\mathbf{n}}\chi = 0, \quad \mathbf{u} = \mathbf{0} \quad \text{on } \partial\Omega \times (0, T)$$

The literature on the full phase change system

✓ The corresponding 3D problem was solved (locally in time) in [E.R., R. Rossi, J. Differential Equations (2008)] under the *small perturbation assumptions*, i.e. with

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- ✓ Degenerating stress-strain relations appear in models for damaging phenomena coupling χ and $\mathbf{u}$ equations (cf., e.g., [Bonetti, Schimperna, Segatti (2004–2005)]). The phase variable χ is related to the local proportion of damaged material ($\chi = 0$ when the body is completely damaged). Local (in time) well-posedness is proved

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- ✓ Due to the presence of the term $\chi_t\,\vartheta$ in the internal energy balance, no global-in-time well-posedness result has yet been obtained for Frémond's phase-field model in the 3D case, even neglecting the **u**-equation and the higher order dissipative contributions on the r.h.s. in the internal energy balance

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- ✓ A 1D global result is proved in [Luterotti, Stefanelli, ZAA (2002)]

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3a) existence of regular solutions in case of a superlinear heat conductivity h in the heat flux law

3b) existence of weak solutions for the standard Fourier heat flux law (i.e. $h \equiv 1$)

Formulation of Problem 1 (The case $h \equiv 1$ – Fourier heat flux)

Find functions $\vartheta, \chi : \Omega \times [0, T] \to \mathbb{R}$ such that

$$\chi(x,t) \in \mathrm{dom}(W) \text{ and } \vartheta(x,t) > 0 \text{ a.e. in } \Omega \times (0,T)$$

and $\mathbf{u} : \Omega \times [0, T] \to \mathbb{R}^3$ fulfilling the initial conditions:

$$\vartheta(0) = \vartheta_0\,, \quad \chi(0) = \chi_0\,, \quad \mathbf{u}(0) = \mathbf{u}_0, \quad \mathbf{u}_t(0) = \mathbf{v}_0 \quad \text{in } \Omega\,, \tag{IC1}$$

the equations a.e. in $\Omega \times (0, T)$:

$$\vartheta_t + \chi_t \vartheta - \Delta\vartheta = \mu|\chi_t|^2 + \chi|\varepsilon(\mathbf{u}_t)|^2 \tag{P1a}$$

$$\mu\chi_t - \nu\Delta\chi + W'(\chi) = \vartheta - \vartheta_c + \frac{|\varepsilon(\mathbf{u})|^2}{2} \tag{P1b}$$

$$\mathbf{u}_{tt} - \mathrm{div}\,((1-\chi)\varepsilon(\mathbf{u}) + \chi\varepsilon(\mathbf{u}_t)) = \mathbf{0} \tag{P1c}$$

and the boundary conditions:

$$\partial_{\mathbf{n}}\vartheta = 0, \quad \partial_{\mathbf{n}}\chi = 0, \quad \mathbf{u} = \mathbf{0} \quad \text{on } \partial\Omega \times (0,T)\,. \tag{BC1}$$

Formulation of Problem 2 (The case $\varepsilon(\mathbf{u}) = \mathrm{const}$)

Find functions $\vartheta, \chi : \Omega \times [0, T] \to \mathbb{R}$ such that

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Relations between Problem 2 and the "classical" models

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The global results

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- existence of *weak* solutions in case $h(\vartheta) = h_0$ (Fourier heat flux law), obtained as a limit for $\varepsilon \searrow 0$ of the previous one and satisfying (P2b–BC2), an *entropy inequality* and the *total energy conservation* in a suitable sense.

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(iii) $\mathrm{dom}(\widehat{\beta}) = [0,1]$

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$$\mathbf{u}_0 \in H_0^2(0, \ell), \quad \mathbf{v}_0 \in H_0^1(0, \ell),$$

$$\vartheta_0 \in H^1(0, \ell) \quad \text{and} \quad \min_{x \in [0, \ell]} \vartheta_0(x) > 0, \qquad \chi_0 \in H_N^2(\Omega)$$

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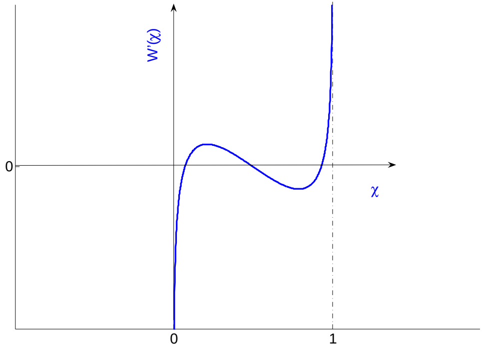
(iv) the datum χ_0 is "separated from the potential barriers":

$$\min_{x \in \overline{\Omega}} \chi_0(x) > 0, \qquad \max_{x \in \overline{\Omega}} \chi_0(x) < 1.$$

✓ The coercivity condition on β rules out the case in which $\widehat{\beta}$ is the indicator function of $[0,1]$, but is fulfilled, e.g., in the case of the logarithmic potential:

$$W'(r) = \ln(r) - \ln(1-r) - c_1 r - c_2, \quad \text{for } r \in (0,1)$$



Theorem 1 (Well-posedness for Problem 1 on $[0, T]$)

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- there exist $\delta \in (0,1)$ - depending on the potential W and on the initial datum χ_0,
- there exist $\zeta_T \in (0,1)$ - depending on the potential W, on the initial datum χ_0, and on the final time T,
- there exist $\theta_T^* > 0$ - depending on T and on the problem data,
- and there exist a unique triple $(\vartheta, \chi, \mathbf{u})$ solving Problem 1 and complying with

$$\vartheta \in L^2(0,T;H^2_N(\Omega)) \cap L^\infty(0,T;H^1(0,\ell)) \cap H^1(0,T;L^2(\Omega)) \cap W^{1,\infty}(0,T;H^1(0,\ell)')$$

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

$$\mathbf{u} \in H^1(0,T;H^2_0(0,\ell)) \cap W^{1,\infty}(0,T;H^1_0(0,\ell)) \cap H^2(0,T;L^2(\Omega))$$

and such that the following separation inequalities hold true:

$$\vartheta(x,t) \geq \theta_T^*, \quad \delta \leq \chi(x,t) \leq \zeta_T \quad \forall (x,t) \in [0,\ell] \times [0,T].$$

Remarks on Theorem 1

✓ The two *separation inequalities* for χ:

$$\chi(x,t) \geq \delta > 0 \quad \text{and} \quad \chi(x,t) \leq \zeta_T < 1$$

have a different character:

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- the second one has a *quantitative nature*, i.e. it holds with a constant ζ_T depending on the $L^\infty(0,T;L^\infty(0,\ell))$-norm of the right-hand side of (P1b), and thus, ultimately, on the time interval in which (P1b) is considered

Theorem 2 (Long-time behavior of solution to Problem 1)

We consider Problem 1, where (P1a) is replaced (within the framework of *small perturbation assumptions*) with

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Then, the nonempty ω-limit set:

$$\omega(\vartheta_0,\chi_0,\mathbf{u}_0) := \{(\vartheta_\infty,\chi_\infty,\mathbf{u}_\infty) \in H^1(0,\ell)\times H^1(0,\ell)\times H^1_0(0,\ell) \ : \ \exists\, t_n \nearrow \infty \ : \ (\vartheta(t_n),\chi(t_n),\mathbf{u}(t_n)) \to (\vartheta_\infty,\chi_\infty,\mathbf{u}_\infty) \text{ in } H^{1-\nu}(0,\ell)\times H^{1-\nu}(0,\ell)\times H^{1-\nu}_0(0,\ell)\ \forall \nu \in (0,1)\}$$

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is compact and connected in $H^{1-\nu}(0,\ell)\times H^{1-\nu}(0,\ell)\times H^{1-\nu}_0(0,\ell)$ for all $\nu \in (0,1)$. Moreover, $\exists\,\zeta_\infty \in (0,1)$: all $(\vartheta_\infty,\chi_\infty,\mathbf{u}_\infty) \in \omega(\vartheta_0,\chi_0,\mathbf{u}_0)$ solves the stationary problem in $(0,\ell)$:

$$-\Delta\vartheta_\infty = 0, \qquad -\Delta\chi_\infty + \beta(\chi_\infty) + \gamma(\chi_\infty) = \vartheta_\infty, \qquad \mathbf{u}_\infty = 0$$

and fulfils

$$\vartheta_\infty(x) \geq 0\,, \qquad \min_{x\in[0,\ell]} \chi_\infty(x) \geq \delta\,, \qquad \max_{x\in[0,\ell]} \chi_\infty(x) \leq \zeta_\infty\,.$$

In particular, $\exists\,\bar\vartheta_\infty \in [0,+\infty)$: $\vartheta_\infty(x) = \bar\vartheta_\infty$ for all $x \in [0,\ell]$.

Remarks on Theorem 2

✓ In addition to Theorem 2, if

$$W' = \beta + \gamma \text{ is strictly increasing in } (0,1),$$

for every $(\vartheta_\infty, \chi_\infty, 0) \in \omega(\vartheta_0, \chi_0, \mathbf{u}_0)$, the component χ_∞ is also constant on $(0,\ell)$ and

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Instead, the separation from 1 does not hold globally on $(0,+\infty)$.

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✓ In order to prove the existence of the *global attractor* for bundle of trajectories we would need to strengthen our large-time a priori estimates on $\mathbf{u}$. However, it seems to us that better large-time estimates on $\mathbf{u}$ cannot be obtained, if one relies on the sole (Sep0). The same technical drawback makes it difficult to implement *Łojasiewicz-Simon procedures* to prove the convergence as $t \to +\infty$ of the whole trajectories $(\vartheta(t), \chi(t), u(t))_{t\in(0,+\infty)}$ to the elements of their ω-limit.

Recall: Problem 2 (The case $\varepsilon(\mathbf{u}) = \mathrm{const}$)

Find functions $\vartheta, \chi : \Omega \times [0, T] \to \mathbb{R}$ such that

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We fix two positive constants c_k, c_w, an three exponents $p \in [3, +\infty)$, $q \in (5, +\infty)$, $\alpha \in (0, 1)$, and assume that

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(iv) $\chi_0 \in [L^q(\Omega), W^{2,q}_N(\Omega)]_{1-1/q,q}$, $W(\chi_0) \in L^1(\Omega)$.

Theorem 3 (Well-posedness for Problem 2 in case $\varepsilon > 0$).

Fix $T > 0$ and assume Hypothesis 2. Suppose that W, satisfies

- either the regularity assumption

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Then, there exist a unique solution (ϑ, χ) to Problem 2 such that it complies with the following regularity properties:

$$\vartheta \in C^{0,\sigma}(\overline{Q}_T) \cap C^0((0,T]; H^2(\Omega)) \cap C^1((0,T]; C^{0,\sigma}(\overline{\Omega}))$$
$$\chi \in C^{0,\sigma}(\overline{Q}_T) \cap C^0((0,T]; H^2(\Omega)) \cap C^1((0,T]; C^{0,\sigma}(\overline{\Omega}))\,.$$

Theorem 4 (Existence for Problem 2 in case $\varepsilon = 0$)

Fix $T > 0$ and assume Hypothesis 2. Let $s \in (13/8, 11/6)$ in the 3D case, $s \in (5/3, 2)$ in the 2D case.

Theorem 4 (Existence for Problem 2 in case $\varepsilon = 0$)

Fix $T > 0$ and assume Hypothesis 2. Let $s \in (13/8, 11/6)$ in the 3D case, $s \in (5/3, 2)$ in the 2D case. Then there exists at least one pair (ϑ, χ) with the regularities

$$
\begin{aligned}
&\vartheta \in L^\infty(0,T;L^1(\Omega)) \cap L^s(Q_T)\\
&\qquad \vartheta(x,t) > 0 \quad \text{a.e. in } Q_T\\
&\log(\vartheta) \in L^\infty(0,T;L^1(\Omega)) \cap L^2(0,T;H^1(\Omega))\\
&\chi \in C^0([0,T];H^1(\Omega)) \cap L^s(0,T;W^{2,s}(\Omega)), \qquad \chi_t \in L^s(Q_T)
\end{aligned}
$$

satisfying the *entropy inequality* $(\forall \varphi \in \mathcal{D}(\overline{Q}_T),\ \varphi \geq 0)$:

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

equation (P2b), initial and boundary conditions (BC2–IC2), and the *total energy conservation*

$$
E(t) = E(0) \quad \text{a.e. in } [0,T], \quad \text{where } E \equiv \int_\Omega \left(\vartheta + W(\chi) + \frac{\nu}{2} |\nabla \chi|^2 \right) dx\,.
$$

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- The crucial estimate leading to the existence of *strong solutions* (cf. Theorem 3) is (P2a) $\times 1/\vartheta$ leading to

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- It is easy to check that the *entropy inequality* and the *energy conservation* in Theorem 4, together with equation (P2b) give rise to the standard energy balance (P2a) in case the solution is sufficiently smooth