Phase transition systems with dynamic boundary conditions

Maurizio Grasselli

Dipartimento di Matematica “F. Brioschi”
Politecnico di Milano, ITALY
maurizio.grasselli@polimi.it

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Phase-field systems

- bdd domain $\Omega \subset \mathbb{R}^3$ with smooth bdry Γ
- two-phase stress-free material occupying Ω, $\forall\, t \geq 0$
- θ (relative) temperature
- χ order parameter (or phase-field)

$$\boxed{(\varepsilon\theta + \lambda\chi)_t - k\Delta\theta = 0}$$

$$\boxed{\chi_t - \alpha\Delta\chi + F'(\chi) - \lambda\theta = 0}$$

- k, α, ε positive coefficients, $\lambda \in \mathbb{R}$
- F nonconvex potential

A naive derivation

- bulk free energy functional

$$E_\Omega(\chi,\theta) = \int_\Omega \left[\frac{\alpha}{2}|\nabla\chi|^2 + F(\chi) - \lambda\chi\theta - \frac{\varepsilon}{2}\theta^2\right] dx$$

- equation for the temperature

$$(-\partial_\theta E_\Omega(\chi,\theta))_t + \nabla\cdot\mathbf{q} = 0, \qquad \mathbf{q} = -k\nabla\theta$$

- equation for the order parameter

$$\chi_t = -\partial_\chi E_\Omega(\chi,\theta)$$

Mathematical results

Main topics

- well-posedness and longtime behavior of solutions
- nature of stationary states
- existence and smoothness of global attractors
- existence of exponential attractors
- construction of inertial manifolds (one or two spatial dim.)
- convergence of trajectories to single equilibria

Some contributors: *S.Aizicovici, P.W.Bates, G.Caginalp, Chen Xinfu, L.Cherfils, P.Colli, C.M.Elliott, M.Fabrizio, G.J.Fix, E.Feireisl, S.Gatti, G.Gilardi, C.Giorgi, D.Hilhorst, K.-H.Hoffmann, N.Kenmochi, P.Kreičí, Ph.Laurençot, A.Miranville, A.Novick-Cohen, V.Pata, H.Petzeltová, E.Rocca, G.Schimperna, J.Sprekels, S.Zelik, Zheng Songmu, . . .*

Dynamic boundary conditions

Most papers are devoted to DN, NN or RN bdry conditions:

$$\boxed{b\partial_{\mathbf{n}}\theta + c\theta = \partial_{\mathbf{n}}\chi = 0}$$

more recently, dynamic bdry conditions have been considered for χ (see *Maass et al.* for separation processes, *Qian et al.* for immiscible two-phase flows)

$$\boxed{\partial_{\mathbf{n}}\theta = 0, \quad \chi_t = \beta\Delta_\Gamma\chi - \alpha\partial_{\mathbf{n}}\chi - G'(\chi)}$$

- $\beta > 0$
- Δ_Γ Laplace-Beltrami operator
- G bdry (nonconvex) potential

Dynamic bdry conditions: known results

Chill, Fašangová & Prüss (2006)

- F polynomially controlled growth of degree 6
- $G \equiv 0$
- $\exists$ smooth solutions
- convergence to single equilibria via Łojasiewicz-Simon inequality (F real analytic)

Gatti & Miranville (2006)

- F and G smooth potentials (no growth restrictions)
- construction of a s-continuous dissipative semigroup
- $\exists$ global attractor $\mathcal{A}_\varepsilon$ upper semicontinuous at $\varepsilon = 0$
- $\exists$ exponential attractors $\mathcal{E}_\varepsilon$

Dynamic bdry conditions: known results

Cherfils & Miranville (2007)

- F singular potential defined on $(-1, 1)$
- G smooth potential (sign restrictions)
- construction of a s-continuous dissipative semigroup
- $\exists$ global attractor of finite fractal dimension
- convergence to single equilibria via Ł-S method (F real analytic, $G \equiv 0$)

Gatti, Cherfils & Miranville (2007 and 2008)

- F singular potential defined on $(-1, 1)$
- G smooth potential (sign restrictions are removed)
- separation property and existence of global solutions
- existence of global and exponential attractors

Dynamic bdry conditions: known results

Gal & G. (2007)

- F and G smooth potential (more general than *Gatti & Miranville*)
- more general bdry condition for θ

$$\boxed{a\theta_t + b\partial_{\mathbf{n}}\theta + c\theta = 0}$$

  with $a, b, c \geq 0$ (not all $= 0$)
- construction of a dissipative semigroup (larger phase spaces w.r.t. *Gatti & Miranville*)
- $\exists$ global attractor, $\exists$ exponential attractors

Gal, G. & Miranville (2007)

- $\exists$ family of exponential attractors $\{\mathcal{E}_\varepsilon\}$ stable as $\varepsilon \searrow 0$ in the case $a = c = 0$, $b = 1$

Coupled dynamic bdry conditions

Gal, G. & Miranville (2008)

dynamic bdry conditions for $\theta \Rightarrow$ coupling effects on Γ

[cf. also *Savaré & Visintin* (1997) and *Schimperna* (1999) for concentrated capacity pbs]

- surface free energy functional

$$E_\Gamma(\chi,\theta) = \int_\Omega \left[\frac{\beta}{2}|\nabla_\Gamma \chi|^2 + G(\chi) - \delta\chi\theta - \frac{a}{2}\theta^2 \right] dS$$

where $\delta > 0$ and $a > 0$

- dynamic bdry condition for χ

$$\chi_t = -\partial_\chi E_\Gamma(\chi,\theta) - \alpha\partial_{\mathbf{n}}\chi = \beta\Delta_\Gamma\chi - \alpha\partial_{\mathbf{n}}\chi - G'(\chi) + \delta\theta$$

Coupled dynamic bdry conditions

- first Law of Thermodynamics

$$\int_\Omega (e_\Omega)_t dx + \int_\Gamma (e_\Gamma)_t dS = -\int_\Omega \nabla \cdot \mathbf{q} + \int_\Gamma \Phi(x,t,\theta,\nabla\theta) dS$$

where

$$e_\Omega = -\partial_\theta E_\Omega(\chi,\theta) = \varepsilon\theta + \lambda\chi, \quad e_\Gamma = -\partial_\theta E_\Gamma(\chi,\theta) = a\theta + \delta\chi$$

- dynamic bdry condition for θ

$$(a\theta + \delta\chi)_t = \Phi(x,t,\theta,\nabla\theta)$$

- our choice

$$\Phi(x,t,\theta,\nabla\theta) = -k\partial_{\mathbf{n}}\theta - c\theta, \qquad c \geq 0$$

Phase-field system with coupled dyn. bdry conditions

- equations in $\Omega \times (0, \infty)$

$$\begin{cases} (\varepsilon\theta + \lambda\chi)_t - k\Delta\theta = 0 \\ \chi_t - \alpha\Delta\chi + F'(\chi) - \lambda\theta = 0 \end{cases}$$

- equations on $\Gamma \times (0, \infty)$

$$\begin{cases} (a\theta + \delta\chi)_t + k\partial_{\mathbf{n}}\theta + c\theta = 0 \\ \chi_t - \beta\Delta_\Gamma\chi + \alpha\partial_{\mathbf{n}}\chi + G'(\chi) - \delta\theta = 0 \end{cases}$$

- initial conditions

$$\theta(0) = \theta_0, \qquad \chi(0) = \chi_0$$

Assumptions on F and G

- well-posedness ($\Rightarrow \exists$ continuous semigroup): we suppose

$$\begin{cases} F, G \in C^2(\mathbb{R}) \\ \liminf_{|y|\to\infty} F''(y) > 0, \quad \liminf_{|y|\to\infty} G''(y) > 0 \end{cases}$$

- dissipativity and $\exists$ global attractor: if $c = 0$ we also require

$$F'(y)y \geq k_1 y^2 - k_2, \quad G'(y)y \geq k_3 y^2 - k_4, \quad \forall\, y \in \mathbb{R}, \; k_i > 0$$

- $\exists$ exponential attractors: we add

$$F'', \, G'' \in C^{0,1}_{loc}(\mathbb{R})$$

- convergence to single equilibria: we must require F and G to be real analytic

Interpreting the bdry conditions for θ

- $\mathbb{X} = L^2\left(\bar{\Omega}, dx \oplus adS\right)$
- $\|\boldsymbol{\Theta}\|^2_{\mathbb{X}} = \|\Theta_1\|^2_{2,\Omega} + a\|\Theta_2\|^2_{2,\Gamma}$

$$\boxed{A = -\Delta : \mathcal{D}(A) \subset \mathbb{X} \to \mathbb{X}}$$

- $\mathcal{D}(A)$ is contained in

$$\{u \in H^2_{loc}(\Omega) \,:\, \Delta u \in \mathbb{X}, \quad a(\Delta u)|_\Gamma + k\partial_{\mathbf{n}} u + cu = 0\}$$

Remark

A is nonnegative, self-adjoint and generates an analytic semigroup on $\mathbb{X}$ [see Favini et al. (2002)]

The phase space for θ

$$\boxed{Z_c = H^1(\Omega)}$$

endowed with the norms

- $\|u\|_{Z_c}^2 = k\|\nabla u\|_{2,\Omega}^2 + c\|u|_\Gamma\|_{2,\Gamma}^2 \quad [c > 0]$
- $\|u\|_{Z_0}^2 = k\|\nabla u\|_{2,\Omega}^2 + |\langle\langle u\rangle\rangle|^2 \quad [c = 0]$

where

$$\langle\langle u\rangle\rangle = \frac{1}{|\Omega| + a|\Gamma|}\left(\int_\Omega \varepsilon u\,dx + \int_\Gamma au\,dS\right)$$

The phase space for χ

- $\mathbb{V}_s = \overline{(C^s(\bar{\Omega}))}^{\|\cdot\|_s}$
- $\|v\|_0 = \|v\|_{2,\Omega}^2 + \|v|_\Gamma\|_{2,\Gamma}^2$
- $\|v\|_1 = \alpha\|\nabla v\|_{2,\Omega}^2 + \beta\|\nabla_\Gamma v|_\Gamma\|_{2,\Gamma}^2 + \|v|_\Gamma\|_{2,\Gamma}^2$
- $\mathbb{V}_s \equiv H^s(\Omega) \oplus H^s(\Gamma)$

$$\boxed{\mathbb{V}_2 \equiv H^2(\Omega) \oplus H^2(\Gamma)}$$

with norm $\|\boldsymbol{\Psi}\|_{\mathbb{V}_2}^2 = \|\Psi_1\|_{H^2(\Omega)}^2 + \|\Psi_2\|_{H^2(\Gamma)}^2$

Problem $\mathbf{P}_c$

Problem $\mathbf{P}_c$ For any given $(\theta_0, \chi_0) \in Z_c \times \mathbb{V}_2$ find

$$\boxed{(\theta, \chi) \in C([0, \infty); Z_c \times \mathbb{V}_2)}$$

s.t.

$$(\theta(0), \chi(0)) = (\theta_0, \chi_0), \quad (\theta_t, \chi_t) \in L^2((0, \infty); \mathbb{X} \times \mathbb{V}_1)$$

and

$$\boxed{\begin{cases} (\varepsilon\theta + \lambda\chi)_t - k\Delta\theta = 0 \\ \chi_t - \alpha\Delta\chi + F'(\chi) - \lambda\theta = 0 \\ (a\theta + \delta\chi)_t + k\partial_{\mathbf{n}}\theta + c\theta = 0 \\ \chi_t - \beta\Delta_\Gamma\chi + \alpha\partial_{\mathbf{n}}\chi + G'(\chi) - \delta\theta = 0 \end{cases}}$$

Existence result

Theorem

$\mathbf{P}_c$ *has a solution s.t.* $\theta \in L^2_{loc}([0,\infty);\mathcal{D}(A))$ *and,* $\forall\, t \geq 0$,

$$\boxed{\mathbb{I}(\theta(t),\chi(t)) = \mathbb{I}(\theta_0,\chi_0) \quad \textit{if } c = 0}$$

where

$$\mathbb{I}(u,v) = \frac{1}{|\Omega| + a|\Gamma|}\left(\int_\Omega (\varepsilon u + \lambda v)\,dx + \int_\Gamma au\,dS\right)$$

Remark

Fixed-point argument to get a local smooth solution which satisfies suitable a priori bounds

The solution semigroup

Theorem

Let $(\theta_i(t), \chi_i(t))$ *be solutions corresponding to* $(\theta_{0i}, \chi_{0i}) \in Z_c \times \mathbb{V}_2$, $i = 1, 2$. *Then*

$$\|(\theta_1 - \theta_2)(t)\|_{\mathbb{X}} + \|(\chi_1 - \chi_2)(t)\|_{\mathbb{V}_1}$$
$$\leq C_1 e^{C_2 t} \left(\|\theta_{01} - \theta_2\|_{\mathbb{X}} + \|\chi_{01} - \chi_{02}\|_{\mathbb{V}_1}\right)$$

$\forall\, t \geq 0$, *where* $C_i = C_i \left(\|(\theta_{0i}, \chi_{0i})\|_{Z_K \times \mathbb{V}_2}\right) > 0$

Remark

$S_c(t) : Z_c \times \mathbb{V}_2 \to Z_c \times \mathbb{V}_2$ *defined by*

$$(\theta(t), \chi(t)) = S_c(t)(\theta_0, \chi_0), \quad \forall\, t \geq 0$$

is a closed semigroup

Compact absorbing sets

- if $c > 0$
$$\mathbb{Y}_c = Z_c \times \mathbb{V}_2$$
- if $c = 0$
$$\mathbb{Y}_c = \{(u, v) \in Z_0 \times \mathbb{V}_2 \; : \; |\mathbb{I}(u, v)| \leq M\}$$
for some $M \geq 0$
- $\mathbb{Y}_c$ is a complete metric space

Theorem

$S_c(t)$ has an absorbing set bdd in $H^2 \times \mathbb{V}_3$

Global and exponential attractors

- $\exists$ compact absorbing set
- $S_c(t)$ is a closed semigroup

then, thanks to *Pata & Zelik* (2007), we deduce

Theorem

$S_c(t)$ has the global connected attractor $\mathcal{A}_c$ which is bdd in $H^2(\Omega) \times \mathbb{V}_3$

we can also prove (via smoothing property)

Theorem

$S_c(t)$ has an exponential attractor $\mathcal{E}_c$

which yields as a by-product

Corollary

$\mathcal{A}_c$ has finite fractal dimension

Proposition

$(\mathbb{Y}_c, S_c(t))$ is a gradient system with Lyapunov functional

$$\mathcal{L}_c(u,v) = \|u\|^2_{2,\Omega} + a\|u|_\Gamma\|^2_{2,\Gamma} + \alpha\|\nabla v\|^2_{2,\Omega} + \beta\|\nabla_\Gamma v|_\Gamma\|^2_{2,\Gamma} + 2F(v) + 2G(v)$$

so that, if Σ_c is the set of equilibria, then

- *$\mathcal{A}_c$ coincides with the unstable manifold of Σ_c*
- *$\omega(\theta_0, \chi_0) \subset \Sigma_c$ is nonempty, connected and compact in $\mathbb{Y}_c$ for any $(\theta_0, \chi_0) \in \mathbb{Y}_c$*

Convergence to single equilibria

Theorem

If F and G are real analytic, then, for any given $(\theta_0, \chi_0) \in \mathbb{Y}_c$, $\exists\, (\theta_\infty, \chi_\infty)$ *solution to the stationary problem s.t.*

$$\omega(\theta_0, \chi_0) = \{(\theta_\infty, \chi_\infty)\}$$

and $\exists\, \xi \in (0, 1/2)$ *and* $C > 0$ *s.t.,* $\forall\, t \geq 0$,

$$\|\chi(t) - \chi_\infty\|_{\mathbb{V}_2} + \|\theta(t) - \theta_\infty\|_{H^1(\Omega)} \leq C(1+t)^{-\frac{\xi}{1-2\xi}}$$

Remark

The argument is based on a suitable version of the Łojasiewicz-Simon inequality

Enlarging the phase space

- F with polynomially controlled growth of degree 4
- G with polynomially controlled growth of degree 2 if $\beta = 0$ (i.e., no diffusion on Γ)
- $c > 0$

$$\mathbb{Y}_c = \mathbb{X} \times \mathbb{V}_1$$

- $c = 0$

$$\mathbb{Y}_c = \{(u, v) \in \mathbb{X} \times \mathbb{V}_1 \ : \ |\mathbb{I}(u, v)| \le M\}$$

- $S_c(t)$ can be extended to the phase space $\mathbb{Y}_c$

Remark

ALL THE PREVIOUS RESULTS STILL HOLD

Nonlinear coupling

- equations in $\Omega \times (0, \infty)$

$$\begin{cases} (\varepsilon\theta + \lambda(\chi))_t - k\Delta\theta = 0 \\ \chi_t - \alpha\Delta\chi + F'(\chi) - \lambda'(\chi)\theta = 0 \end{cases}$$

- equations on $\Gamma \times (0, \infty)$

$$\begin{cases} (a\theta + \delta(\chi))_t + k\partial_{\mathbf{n}}\theta + c\theta = 0 \\ \chi_t - \beta\Delta_\Gamma\chi + \alpha\partial_{\mathbf{n}}\chi + G'(\chi) - \delta'(\chi)\theta = 0 \end{cases}$$

- initial conditions

$$\theta(0) = \theta_0, \qquad \chi(0) = \chi_0$$

Nonlinear coupling in the bulk only

Problem P Find θ and χ s.t.

$$\begin{cases} (\varepsilon\theta + \lambda(\chi))_t - k\Delta\theta = 0 \\ \chi_t - \alpha\Delta\chi + F'(\chi) - \lambda'(\chi)\theta = 0 \\ \theta = 0 \\ \chi_t - \beta\Delta_\Gamma\chi + \alpha\partial_{\mathbf{n}}\chi + G'(\chi) = 0 \\ \theta(0) = \theta_0, \qquad \chi(0) = \chi_0 \end{cases}$$

Results [Cavaterra, Gal, G. & Miranville, in preparation]

- well-posedness
- existence of the global attractor
- existence of an exponential attractor
- convergence to single equilibria (F, G real analytic)

Well-posedness

Basic assumptions

- $F, G, \lambda \in C^2(\mathbb{R})$
- $|F''(y)| \leq c_0(1 + |y|^2)$
- $F'(y)y \geq c_1|y|^4 - c_2$
- $G'(y)y \geq c_3|y|^2 - c_4$
- λ'' bdd

Theorem

For any given $(\theta_0, \chi_0) \in L^2 \times \mathbb{V}_1$, $\exists\,!\,(\theta, \chi) \in C([0, \infty); L^2 \times \mathbb{V}_1)$ *which solves* **P** *and satisfies*

- $\chi_t \in L^2((0, \infty); \mathbb{V}_0)$
- $\theta \in L^2((0, \infty); H_0^1)$
- $\chi \in L^2_{loc}((0, \infty); \mathbb{V}_2)$

Attractors

We can define a s-continuous dissipative semigroup

$$S(t) : L^2 \times \mathbb{V}_1 \to L^2 \times \mathbb{V}_1$$

by setting

$$(\theta(t), \chi(t)) = S(t)(\theta_0, \chi_0), \quad \forall\, t \geq 0$$

Theorem

$S(t)$ has the global attractor $\mathcal{A}$ bdd in $H_0^1 \times \mathbb{V}_2$

Theorem

If F'' and G'' are loc. Lip., then $S(t)$ has an exponential attractor $\mathcal{E}$ bdd in $H_0^1 \times \mathbb{V}_2$ ($\Rightarrow \mathcal{A}$ has finite fractal dimension)

Work in progress and future issues

G., Miranville & Schimperna (in progress)

- bdry coupling with singular F (and, possibly, G) of the form

$$\boxed{F(s) = \gamma_1[(1+s)\ln(1+s) + (1-s)\ln(1-s)] - \gamma_2 s^2}$$

[see G., Petzeltová & Schimperna (2006) for DN case]

future issues

- nonlinear coupling in the bulk and on the bdry
- memory effects (hyperbolic behavior)
- Penrose-Fife systems with dynamic bdry conditions

Memory and dynamic bdry conditions: an example

$$
\begin{cases}
(\varepsilon\theta + \lambda\chi)_t - \displaystyle\int_0^\infty k(s)\Delta\theta(t-s)ds = 0 \\
\chi_t + \displaystyle\int_0^\infty h(s)(-\Delta\chi + f(\chi) - \lambda\theta)(t-s)ds = 0 \\
\chi_t + \displaystyle\int_0^\infty \ell(s)(-\Delta_\Gamma\chi + \chi + g(\chi) + \partial_{\mathbf{n}}\chi)(t-s)ds = \theta = 0 \\
\theta(s) = \tilde{\theta}_0(-s),\ \chi(s) = \tilde{\chi}_0(-s) \quad \text{in } \ \Omega,\ s \geq 0
\end{cases}
$$

- $h, k, \ell \geq 0$ smooth exp. decreasing relaxation kernels
- DN and NN cases: G. & Rotstein (2001), Rotstein et al. (2001), Novick-Cohen (2002), G. & Pata (2004, 2005), Grinfeld & Novick-Cohen (2006), Vergara (2007), G. (2008)