

**The Caginalp phase-field system
with singular potentials
and dynamic boundary conditions**

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Study of the asymptotic behavior of the system

$$\eta \frac{\partial w}{\partial t} - \Delta w = -\frac{\partial u}{\partial t}, \quad \eta > 0$$

$$\delta \frac{\partial u}{\partial t} - \Delta u + f(u) = w, \quad \delta > 0$$

in a bounded regular domain $\Omega \subset R^3$

Proposed by G. Caginalp to model melting-solidification phenomena

w: (relative) temperature

u: order parameter

Other motivations:

- Singular perturbation of the Cahn-Hilliard equation:

$\eta = 0$: Cahn-Hilliard equation with viscosity

$$\frac{\partial u}{\partial t} - \delta \frac{\partial}{\partial t} \Delta u + \Delta^2 u - \Delta f(u) = 0$$

$\eta = \delta = 0$: Cahn-Hilliard equation

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) = 0$$

- Nonisothermal Allen-Cahn model

One has satisfactory results for classical boundary conditions (Neumann, Dirichlet, mixed)

- Regular potentials (typically, $f(s) = s^3 - s$):

- Well-posedness: G. Caginalp; C.-M. Elliott, S. Zheng

- Existence of finite dimensional attractors: P.W. Bates, S. Zheng; D. Brochet, X. Chen, D. Hilhorst; A. Miranville, S. Zelik; ...

- Convergence of solutions to steady states: S. Aizicovici, E. Feireisl, F. Issard-Roch; Z. Zhang; ...

- Generalizations:

Memory effects: S. Aizicovici, E. Feireisl; C. Giorgi, M. Grasselli, V. Pata; ...

Hyperbolic relaxation: M. Grasselli, H. Petzeltová, G. Schimperna; H. Wu, M. Grasselli, S. Zheng

- Singular potentials:

Thermodynamically relevant singular potential:

$$f(s) = -2\kappa_0 s + \kappa_1 \ln \frac{1+s}{1-s}, \quad s \in (-1, 1)$$

$$0 < \kappa_0 < \kappa_1$$

- Well-posedness: M. Grasselli, A. Miranville, V. Pata, S. Zelik; M. Grasselli, H. Petzeltová, G. Schimperna
- Existence of finite dimensional attractors: M. Grasselli, A. Miranville, V. Pata, S. Zelik; L. Cherfils, A. Miranville
- Convergence of solutions to steady states: M. Grasselli, H. Petzeltová, G. Schimperna; L. Cherfils, A. Miranville
- Hyperbolic relaxation: M. Grasselli, A. Miranville, V. Pata, S. Zelik

Dynamic boundary condition:

$$\frac{\partial u}{\partial t} - \Delta_{\Gamma} u + \lambda u + g(u) + \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma, \lambda > 0$$

$$\Gamma = \partial\Omega$$

Δ_{Γ} : Laplace-Beltrami operator

ν : unit outer normal to Γ

Proposed in the context of the Cahn-Hilliard equation to account for interactions with the walls for confined systems

Original derivation: $g(s) \equiv c = \text{Const.}$

c : characterizes the preferential attraction of one of the phases by the walls

$c = 0$: no preferential attraction

Remark: One expects w and u to be coupled in the dynamic boundary conditions (for regular potentials: C.G. Gal, M. Grasselli, A. Miranville)

Initial and boundary value problem:

$$\begin{aligned} \frac{\partial w}{\partial t} - \Delta w &= -\frac{\partial u}{\partial t} \\ \frac{\partial u}{\partial t} - \Delta u + f(u) &= w \\ \frac{\partial w}{\partial \nu} &= 0 \text{ on } \Gamma \\ \frac{\partial u}{\partial t} - \Delta_{\Gamma} u + \lambda u + g(u) + \frac{\partial u}{\partial \nu} &= 0 \text{ on } \Gamma \\ w|_{t=0} &= w_0 \\ u|_{t=0} &= u_0 \end{aligned}$$

We rewrite the system in the equivalent form

$$\begin{aligned} \frac{\partial w}{\partial t} - \Delta w &= -\frac{\partial u}{\partial t} \\ \frac{\partial u}{\partial t} - \Delta u + f(u) &= w \\ \frac{\partial w}{\partial \nu} &= 0 \text{ on } \Gamma \\ \frac{\partial \psi}{\partial t} - \Delta_{\Gamma} \psi + \lambda \psi + g(\psi) + \frac{\partial u}{\partial \nu} &= 0 \text{ on } \Gamma, \quad \psi = u|_{\Gamma} \\ w|_{t=0} &= w_0 \\ u|_{t=0} = u_0, \quad \psi|_{t=0} &= \psi_0 \quad (\psi_0 = u_0|_{\Gamma}) \end{aligned}$$

Regular potentials (f and g):

- Well-posedness: R. Chill, E. Fašangová, J. Prüss; A. Miranville, S. Gatti; C.G. Gal, M. Grasselli
- Existence of finite dimensional attractors: A. Miranville, S. Gatti; C.G. Gal, M. Grasselli; C.G. Gal, M. Grasselli, A. Miranville
- Convergence of solutions to steady states: R. Chill, E. Fašangová, J. Prüss; C.G. Gal, M. Grasselli
- Coupled boundary conditions: C.G. Gal, M. Grasselli, A. Miranville

Singular potential f : an essential difficulty is to prove that u remains in $(-1, 1)$

→ We have to prove that u is separated from -1 and 1

Remark: For regular potentials, we cannot prove in general that $u \in [-1, 1]$

The case $g \equiv 0$

We can more generally assume that

$$\lambda > \max(-g(1), g(-1))$$

Assumptions on f :

$$\begin{aligned} f &\in \mathcal{C}^3(-1, 1), \quad \lim_{s \rightarrow \pm 1} f(s) = \pm\infty \\ \lim_{s \rightarrow \pm 1} f'(s) &= +\infty \end{aligned}$$

Assumptions on $z_0 = (w_0, u_0, \psi_0)$:

$$\begin{aligned} E(z_0) &= D(u_0) + \|w_0\|_{H^2}^2 + \|u_0\|_{H^2}^2 \\ &+ \|\psi_0\|_{H^2(\Gamma)}^2 < +\infty, \quad D(u_0) > 0 \\ \|\psi_0\|_{L^\infty(\Gamma)} &< 1 \\ u_0|_\Gamma &= \psi_0 \\ D(\varphi) &= \frac{1}{1 - \|\varphi\|_{L^\infty}} \end{aligned}$$

$$\rightarrow \|u_0\|_{L^\infty} < 1$$

- Uniqueness:

Theorem: For any 2 solutions z_1 and z_2 with initial data $z_{1,0}$ and $z_{2,0}$ satisfying the above assumptions,

$$\begin{aligned} & \|w_1 - w_2\|_{L^2}^2 + \|u_1 - u_2\|_{L^2}^2 + \|\psi_1 - \psi_2\|_{L^2(\Gamma)}^2 \\ & \leq c_1 e^{c_2 t} (\|w_{1,0} - w_{2,0}\|_{L^2}^2 + \|u_{1,0} - u_{2,0}\|_{L^2}^2 \\ & \quad + \|\psi_{1,0} - \psi_{2,0}\|_{L^2(\Gamma)}^2) \end{aligned}$$

where c_1 and c_2 depend on the H^2 -norms of the initial data and on $D(u_{0,i})$, $i = 1, 2$.

- Existence:

Essential step: prove that

$$\|u(t)\|_{L^\infty} < 1, \quad t \geq 0$$

We a priori assume that

$$\|u\|_{L^\infty(\Omega \times \mathbb{R}^+)} < 1$$

a) We have

$$\begin{aligned} & \|w(t)\|_{H^2}^2 + \|u(t)\|_{H^1}^2 + \|\psi(t)\|_{H^1(\Gamma)}^2 \\ & + \int_0^t e^{-\alpha(t-s)} \left(\left\| \frac{\partial u}{\partial t}(s) \right\|_{H^1}^2 + \left\| \frac{\partial \psi}{\partial t}(s) \right\|_{H^1(\Gamma)}^2 \right) ds \\ & \leq Q(E(z_0))e^{-\alpha t} + c_{I_0} \end{aligned}$$

where Q monotone increasing and $\alpha > 0$ are independent of z_0 and c_{I_0} only depends on $I_0 = \langle w_0 + u_0 \rangle$

Remark: The quantity $\langle w(t) + u(t) \rangle$ is conserved

b) Separation property

$\exists \beta > 0$ s.t.

$$\|w(t)\|_{L^\infty} \leq c \|w(t)\|_{H^2} \leq \beta, \quad t \geq 0$$

We fix $\delta \in (0, 1)$ s.t.

$$\begin{aligned} \|u_0\|_{L^\infty} &\leq \delta \\ f(\delta) &\geq \beta \end{aligned}$$

We set $v = u - \delta$ and $\phi = \psi - \delta$:

$$\begin{aligned}\frac{\partial v}{\partial t} - \Delta v + f(u) - f(\delta) &= w - f(\delta) \\ \frac{\partial \phi}{\partial t} - \Delta_{\Gamma} \phi + \lambda \phi + \frac{\partial v}{\partial \nu} &= -\lambda \delta \text{ on } \Gamma\end{aligned}$$

Since

$$\begin{aligned}w - f(\delta) &\leq 0, \quad t \geq 0 \\ -\lambda \delta &\leq 0 \\ v|_{t=0} = u_0 - \delta &\leq 0\end{aligned}$$

We have

$$\begin{aligned}u(t, x) &\leq \delta, \quad t \geq 0, \text{ a.e. } x \in \Omega \\ \psi(t, x) &\leq \delta, \quad t \geq 0, \text{ a.e. } x \in \Omega\end{aligned}$$

We proceed similarly for a lower bound

→ $\exists \delta \in (0, 1)$ s.t.

$$\begin{aligned}\|u(t)\|_{L^\infty} &\leq \delta, \quad t \geq 0 \\ \|\psi(t)\|_{L^\infty(\Gamma)} &\leq \delta, \quad t \geq 0\end{aligned}$$

c) We rewrite the equations for u and ψ as an elliptic system:

$$\begin{aligned}-\Delta u &= h_1 \equiv w - \frac{\partial u}{\partial t} - f(u) \\ -\Delta_\Gamma \psi + \lambda \psi + \frac{\partial u}{\partial \nu} &= h_2 \equiv -\frac{\partial \psi}{\partial t} \text{ on } \Gamma \\ u|_\Gamma &= \psi\end{aligned}$$

$$h_1 \in L^2(\Omega), \quad h_2 \in L^2(\Gamma)$$

Elliptic regularity theorem (A. Miranville, S. Zelik):

$$\|u(t)\|_{H^2} + \|\psi(t)\|_{H^2(\Gamma)} \leq M, \quad t \geq 0$$

$$M = M(D(u_0), \|w_0\|_{H^2}, \|u_0\|_{H^2}, \|\psi_0\|_{H^2(\Gamma)})$$

d) $\exists t_1 > 0$ s.t.

$$\|w(t)\|_{H^3} + \|u(t)\|_{H^3} + \|\psi(t)\|_{H^3(\Gamma)} \leq M_1, \quad t \geq t_1$$

$$M_1 = M_1(D(u_0), \|w_0\|_{H^2}, \|u_0\|_{H^2}, \|\psi_0\|_{H^2(\Gamma)})$$

If, furthermore,

$$\|w_0\|_{H^3} + \|u_0\|_{H^3} + \|\psi_0\|_{H^3(\Gamma)} < +\infty$$

then

$$\|w(t)\|_{H^3} + \|u(t)\|_{H^3} + \|\psi(t)\|_{H^3(\Gamma)} \leq M_2, \quad t \geq 0$$

$$M_2 = M_2(D(u_0), \|w_0\|_{H^3}, \|u_0\|_{H^3}, \|\psi_0\|_{H^3(\Gamma)})$$

e) Existence of a solution

- We regularize f s.t. the above estimates hold with the same constants
- We prove the existence of a local solution
- This solution is in fact global
- We pass to the limit in the regularized problem

Remark: We can consider initial data which contain the pure states (i.e., u_0 can take the values -1 and 1): we set

$$\Phi = \{z = (w, u, \psi) \in H^2(\Omega) \times H^2(\Omega) \times H^2(\Gamma), \\ u|_{\Gamma} = \psi, \frac{\partial w}{\partial \nu}|_{\Gamma} = 0, \|u\|_{L^\infty} < 1, \|\psi\|_{L^\infty(\Gamma)} < 1\}$$

We have the existence and uniqueness of solutions in the closure $L = \{z \in L^2(\Omega) \times L^\infty(\Omega) \times L^\infty(\Gamma), \|u\|_{L^\infty} \leq 1, \|\psi\|_{L^\infty(\Gamma)} \leq 1\}$ of Φ in $L^2(\Omega) \times L^2(\Omega) \times L^2(\Gamma)$

Dissipativity

Phase space:

$$\Phi_M = \{z \in \Phi, |I_0| \leq M\}$$

$$I_0 = \langle w + u \rangle$$

Dissipative estimate for w : if $D(u_0) + \|z_0\|_{\Phi}^2 \leq R_0^2$,

$$\|w(t)\|_{H^2} \leq Q(R_0)e^{-\alpha t} + c_{I_0}, \quad t \geq 0, \quad \alpha > 0$$

$\rightarrow \exists t_0 = t_0(R_0, M)$ s.t., if $t \geq t_0$,

$$\|w(t)\|_{L^\infty} \leq c_M$$

c_M independent of R_0

We choose $\delta_M \in (0, 1)$ (δ_M is independent of R_0) and $t_1 \geq t_0$ s.t.

$$(i) f(\delta_M) \geq c_M + 1$$

$$(ii) \alpha = \frac{1-\delta_M}{t_1} \text{ is small enough } (\leq 1) \text{ s.t.}$$

$$f(\mu) \equiv f(1 - \alpha t_0) \geq \beta_M + 1$$

$$\|w(t)\|_{L^\infty} \leq \beta_M = \beta_M(R_0), \quad t \geq 0, \quad c_M \leq \beta_M$$

$$\alpha \leq \lambda \delta_M$$

We set

$$y_+(t) = \begin{cases} 1 - \alpha t, & 0 \leq t \leq t_1 \\ \delta_M, & t \geq t_1 \end{cases}$$

We set $v = u - y_+$ and $\phi = \psi - y_+$:

$$\begin{aligned}\frac{\partial v}{\partial t} - \Delta v + f(u) - f(y_+) &= H(t) \\ \frac{\partial \phi}{\partial t} - \Delta_{\Gamma} \phi + \frac{\partial v}{\partial t} + \lambda \phi &= G(t)\end{aligned}$$

$$H(t) = w(t) - f(y_+(t)) - \frac{\partial y_+}{\partial t}(t)$$

$$G(t) = -\lambda y_+(t) - \frac{\partial y_+}{\partial t}(t) \leq -\lambda \delta_M + \alpha \leq 0$$

Furthermore,

$$\begin{aligned}H(t) &\leq \beta_M + 1 - f(\mu) \leq 0, \quad 0 \leq t \leq t_0 \\ c_M + 1 - f(\delta_M) &\leq 0, \quad t \geq t_0\end{aligned}$$

This yields

$$u(t) \leq y_+(t), \quad t \geq 0$$

$$\rightarrow u(t) \leq \delta_M, \quad t \geq t_1$$

Theorem: The problem possesses the finite dimensional global attractor \mathcal{A}_M in Φ_M .

Remarks: a) \mathcal{A}_M is the smallest compact set which is invariant and attracts all bounded sets of initial data as $t \rightarrow +\infty$

b) Dimension: covering dimensions (Hausdorff or fractal dimension)

c) Even though the initial phase space is infinite dimensional, the limit dynamics is finite dimensional and can be described by a finite number of parameters

The general case

We are not able to consider constants (or solutions to ODEs) as upper- and lower-solutions

We will consider space-dependent upper- and lower-solutions

We set $v = u - y_+$ and $\phi = \psi - y_+|_{\Gamma}$, $y_+ = y_+(x)$ regular enough:

$$\begin{aligned} \frac{\partial v}{\partial t} - \Delta v + f(v) - f(y_+) &= w - f(y_+) - \Delta y_+ \\ \frac{\partial \phi}{\partial t} - \Delta_{\Gamma} \phi + g(\psi) - g(y_+|_{\Gamma}) + \frac{\partial v}{\partial \nu} + \lambda \phi \\ &= -g(y_+|_{\Gamma}) - \Delta_{\Gamma} y_+|_{\Gamma} - \lambda y_+|_{\Gamma} - \frac{\partial y_+}{\partial \nu}|_{\Gamma} \end{aligned}$$

No a priori information on the sign of $g(y_+|_{\Gamma}) + \Delta_{\Gamma} y_+|_{\Gamma} + \lambda y_+|_{\Gamma}$

→ One solution is to have $\frac{\partial y_+}{\partial \nu}|_{\Gamma}$ positive and large

→ We need stronger assumptions on f

Further assumptions on f :

$f(1 - s)$ behaves like $\frac{c_+}{s^p}$ in the neighborhood of 0^+ , $c_+ > 0$, $p > 1$

$f(-1 + s)$ behaves like $\frac{c_-}{s^q}$ in the neighborhood of 0^+ , $c_- < 0$, $q > 1$

Remark: These assumptions are natural and do not seem to be related with the choice of upper- and lower-solutions: consider the "best" upper-solution

$$\begin{aligned} -\Delta y_+ + f(y_+) &= \beta \\ y_+|_{\Gamma} &= 1 \end{aligned}$$

Then, close to the boundary,

$$y_+(x) \leq 1 - cd(x)^{\frac{2}{1+p}}, \quad c > 0, \quad d(x) = \text{dist}(x, \Gamma)$$

→ We need the condition $p > 1$ to have $\frac{\partial y_+}{\partial \nu}$ large close to Γ

Assumptions on g :

$$g \in \mathcal{C}^2(\mathbb{R})$$

$$\liminf_{|s| \rightarrow +\infty} g'(s) \geq 0$$

$$\text{either } g \equiv \text{Const. or } g(s)s \geq \mu s^2 - \mu',$$

$$s \in \mathbb{R}, \mu > 0, \mu' \geq 0$$

Construction of a super-solution:

We set, for $\epsilon > 0$ small enough, $\Omega_\epsilon = \{x \in \Omega, d(x) > \epsilon\}$, $d(x) = \text{dist}(x, \Gamma)$

We consider the thin domain

$$\Omega - \bar{\Omega}_\epsilon = \{x \in \Omega, 0 < d(x) < \epsilon\}$$

We set, for ϵ small enough,

$$\theta_\epsilon(s) = \frac{1}{\epsilon^{2-r}}s^2 - \frac{2}{\epsilon^{1-r}}s + 1 - \epsilon^r$$
$$0 < r < 1, \quad (p+1)r > 2$$

Remark: For p given, $p > 1$, $\exists r$ such that the above are satisfied

We set $\eta_\epsilon = \theta_\epsilon(d(x))$, $x \in \Omega - \overline{\Omega}_\epsilon$

The function η_ϵ satisfies, for ϵ small enough,

$$\eta_\epsilon \in [1 - 2\epsilon^r, 1 - \epsilon^r]$$
$$\eta_\epsilon = 1 - \epsilon^r \text{ on } \Gamma$$
$$\eta_\epsilon = 1 - 2\epsilon^r \text{ on } \Gamma_\epsilon = \partial\Omega_\epsilon$$
$$\frac{\partial\eta_\epsilon}{\partial\nu} = \frac{2}{\epsilon^{1-r}} \text{ on } \Gamma$$
$$\frac{\partial\eta_\epsilon}{\partial\nu} = 0 \text{ on } \Gamma_\epsilon$$

$$-\Delta\eta_\epsilon + f(\eta_\epsilon) \geq \beta \text{ a.e. } x \in \Omega - \overline{\Omega}_\epsilon$$
$$\|w(t)\|_{L^\infty} \leq \beta, \quad t \geq 0$$

We finally set

$$y_\epsilon^+ = \begin{cases} \eta_\epsilon & \text{in } \Omega - \overline{\Omega_\epsilon} \\ 1 - 2\epsilon^r & \text{in } \Omega_\epsilon \end{cases}$$

The function y_ϵ^+ satisfies

$$\begin{aligned} y_\epsilon^+ &\in H^2(\Omega) \\ -\Delta y_\epsilon^+ + f(y_\epsilon^+) &\geq \beta \text{ a.e. } x \in \Omega \\ y_\epsilon^+ &\in [1 - 2\epsilon^r, 1 - \epsilon^r] \text{ a.e. } x \in \Omega \\ y_\epsilon^+|_\Gamma &= 1 - \epsilon^r \\ \frac{\partial y_\epsilon^+}{\partial \nu}|_\Gamma &= \frac{2}{\epsilon^{1-r}} \rightarrow +\infty \text{ as } \epsilon \rightarrow 0^+ \end{aligned}$$

$\rightarrow y_\epsilon^+$ is a super-solution if ϵ is small enough:

$$u(t, x) \leq y_\epsilon^+(x) \leq 1 - \epsilon^r, \quad t \geq 0, \text{ a.e. } x \in \Omega$$

We proceed similarly for a lower bound

→ Existence and uniqueness of solutions

Open questions:

(i) $p = 1$ and logarithmic potentials

(ii) Dissipative estimates