THE CAHN-HILLIARD EQUATION WITH A LOGARITHMIC POTENTIAL AND DYNAMIC BOUNDARY CONDITIONS

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Cahn-Hilliard system :

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

Equivalently :

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

Describes the phase separation process in a binary alloy : spinodal decomposition, coarsening

u : order parameter
w : chemical potential
κ : mobility
α : related to the surface tension at the interface

f : derivative of a double-well potential F

Typical choice :

$$F(s) = \frac{1}{4}(s^2 - 1)^2$$
$$f(s) = s^3 - s$$

Thermodynamically relevant potential :

$$F(s) = -\theta_0 s^2 + \theta_1((1+s)\ln(1+s)$$
$$+(1-s)\ln(1-s))$$
$$f(s) = -2\theta_0 s + \theta_1 \ln \frac{1+s}{1-s}$$
$$s \in (-1,1),\ 0 < \theta_1 < \theta_0$$

Remark : κ should more generally depend on u and degenerate :

$$\frac{\partial u}{\partial t} = \mathrm{div}(\kappa(u)\nabla u)$$

$\kappa(s) = 1 - s^2$
Restricts the diffusion process to the interfacial region
Is observed when the movements of atoms are confined to this region

Usual boundary conditions :

$$\frac{\partial w}{\partial \nu} = 0 \text{ on } \Gamma$$
$$\frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma$$

$\Omega \subset R^N,\ N \leq 3$: domain occupied by the material
$\Gamma = \partial\Omega$
ν : unit outer normal vector

Equivalently :

$$\frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = 0 \text{ on } \Gamma$$

Regular potentials :

• Well-posedness, regularity : C.M. Elliott-S. Zheng, B. Nicolaenko-B. Scheurer, D. Li-C. Zhong, ...

• Existence of finite-dimensional attractors : B. Nicolaenko-B. Scheurer-R. Temam, D. Li-C. Zhong, ...

• Convergence of solutions to steady states : S. Zheng, P. Rybka-K.-H. Hoffmann

Logarithmic (singular) potentials :

Main difficulty : prove that u remains in $(-1, 1)$

Remark : Not true for regular potentials

• Well-posedness, regularity : C.M. Elliott-S. Luckhaus, C.M. Elliott-H. Garcke, A. Debussche-L. Dettori, A. Miranville-S. Zelik

• Existence of finite-dimensional attractors : A. Debussche-L. Dettori, A. Miranville-S. Zelik

• Convergence of solutions to steady states : H. Abels-M. Wilke

Dynamic boundary conditions :

Influence of the walls for confined systems

Mainly studied for polymer mixtures

Technological applications

Problem : define the boundary conditions (we need 2 boundary conditions)

First boundary condition : no mass flux at the boundary :

$$\frac{\partial w}{\partial \nu} = 0 \text{ on } \Gamma$$

Different approach : G.R. Goldstein-A. Miranville-G. Schimperna

Second boundary condition : we consider, in addition to the Ginzburg-Landau free energy

$$\Psi_{\mathrm{GL}}(u, \nabla u) = \int_{\Omega} (\frac{\alpha}{2} |\nabla u|^2 + F(u)) dx$$

the surface free energy

$$\Psi_{\Gamma}(u, \nabla u) = \int_{\Gamma} (\frac{\alpha_{\Gamma}}{2} |\nabla_{\Gamma} u|^2 + G(u)) dx$$

$\alpha_{\Gamma} > 0$
∇_{Γ} : surface gradient

Original surface potential : $G(s) = \frac{1}{2} a_{\Gamma} s^2 - b_{\Gamma} s$

$a_{\Gamma} > 0$: accounts for a modification of the effective interaction between the components
b_{Γ} : characterizes the preferential attraction of one of the components by the walls

Total energy : $\Psi = \Psi_{\text{GL}} + \Psi_\Gamma$

The system tends to minimize the excess surface energy :

$$\frac{1}{d}\frac{\partial u}{\partial t} - \alpha_\Gamma \Delta_\Gamma u + g(u) + \alpha \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma$$

$d > 0$: relaxation parameter
Δ_Γ : Laplace-Beltrami operator
$g = G'$

$\rightarrow$ Dynamic boundary condition

Regular potentials : the system is well understood

Contributors : R. Chill, C.G. Gal, E. Fašangová, A. Miranville, J. Pruess, R. Racke, H. Wu, S. Zelik, S. Zheng, ...

Singular potentials : more complicated and less understood

First existence and uniqueness result : G. Gilardi-A. Miranville-G. Schimperna

For f singular and g regular : sign assumptions on g near the singular points of f :

$$g(1) > 0, \; g(-1) < 0$$

Forces the order parameter to stay away from ± 1 on Γ

Question :

• What happens when the sign conditions are not satisfied ?

Nonexistence of classical solutions :

When the sign conditions are not satisfied, we can have nonexistence of classical solutions

We consider the scalar ODE

$$y'' - f(y) = 0, \; x \in (-1, 1)$$
$$y'(\pm 1) = K > 0$$

Assumptions :

• f is singular at ± 1
• $F(\pm 1) < +\infty$ $(F' = f)$
• f is odd

Satisfied by the usual logarithmic potentials

When K is small : existence and uniqueness of a solution which is separated from the singular values ($\|y\|_{L^\infty(-1,1)} < 1$) and is odd

Standard interior regularity estimates yield

$$|y'(x)| \leq c_0, \ |y(x)| \leq 1 - \delta$$

$x \in (-\frac{1}{2}, \frac{1}{2})$, $\delta > 0$, c_0 independent of K

Multiply the equation by y' and integrate over $(0, 1)$:

$$|\frac{1}{2}K^2 - F(y(1))| \leq c_1$$

c_1 (and $F(\pm 1)$) independent of K

This inequality cannot hold when K is large

$\rightarrow$ We do not have a classical solution

Since y is odd, the ODE can be rewritten as

$$y'' - f(y) =< y'' - f(y) >$$

$< . >= \frac{1}{\mathrm{Vol}(\cdot)} \int_\Omega .dx$

$\rightarrow$ 1-D stationary Cahn-Hilliard system with dynamic BCs

Numerical results :

$\Omega = (0, 10) \times (0, 4)$

Periodicity in the x-direction, dynamic boundary conditions in the y-direction

u_0 : uniformly distributed random fluctuations of amplitude ± 0.5

$f(s) = -3s + \ln(\frac{1+s}{1-s})$, g affine

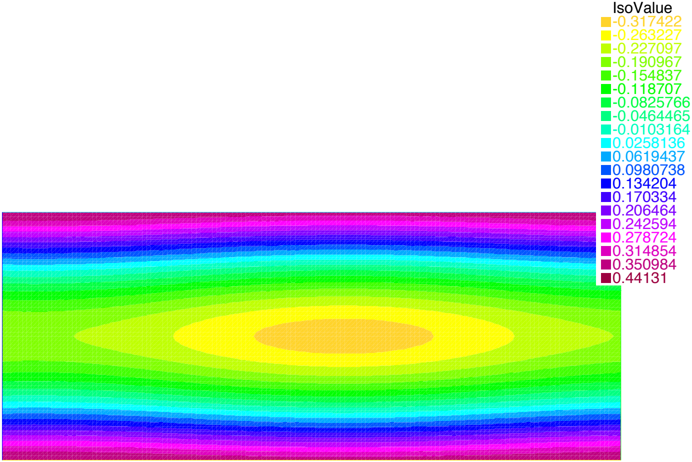

FIGURE: Isovalues of u, at time $t = 20$, $g(s) = s - 0.8$.

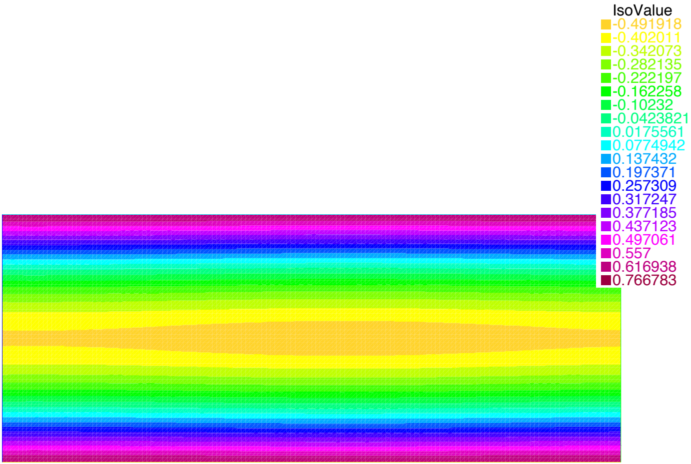

FIGURE: Isovalues of u, at time $t = 20$, $g(s) = s - 1.5$.

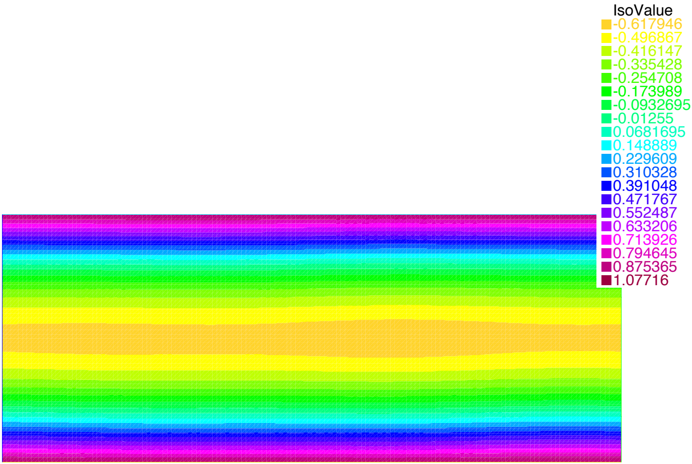

FIGURE: Isovalues of u, at time $t = 0.72$, $g(s) = s - 3$.

FIGURE: Isovalues of u_0.

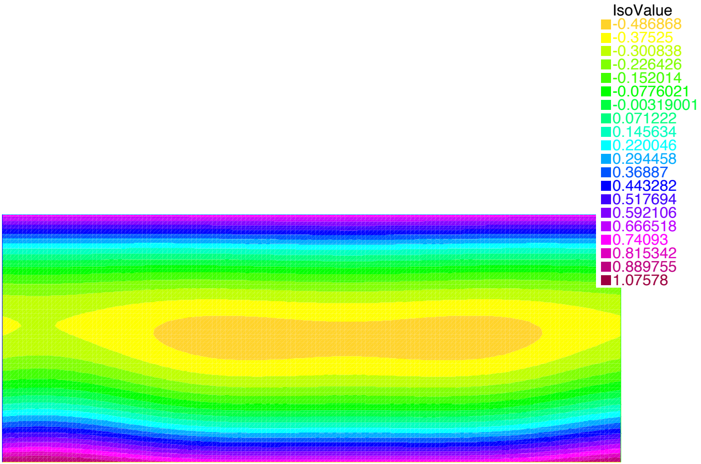

FIGURE: Isovalues of u, at time $t = 0.46$, $g(s) = s - 3$.

Convergence of a sequence of solutions to regularized problems :

$$
\begin{aligned}
&\frac{\partial u}{\partial t} = \Delta w \\
&w = -\Delta u + f_0(u) + \lambda u,\ \lambda \in R \\
&\frac{\partial w}{\partial \nu} = 0 \text{ on } \Gamma \\
&\frac{\partial \psi}{\partial t} - \Delta_\Gamma \psi + g_0(\psi) + \psi + \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma \\
&\psi = u|_\Gamma
\end{aligned}
$$

$$f(s) = f_0(s) + \lambda s,\ g(s) = g_0(s) + s$$

Assumptions :

- $f_0 \in \mathcal{C}^2(-1,1),\ f_0(0) = 0$
- $\lim_{s\to\pm 1} f_0(s) = \pm\infty,\ \lim_{s\to\pm 1} f_0'(s) = +\infty$
- $f_0' \geq 0,\ \mathrm{sgn}(s) f_0''(s) \geq 0$
- $g_0 \in \mathcal{C}^2(R),\ \|g_0\|_{\mathcal{C}^2(R)} \leq c$

Regularized potential :

$$f_{0,n}(s) = f_0(s),\ |s| \le 1 - \frac{1}{n}$$
$$f_{0,n}(s) = f_0(1 - \frac{1}{n}) + f_0'(1 - \frac{1}{n})(s - 1 + \frac{1}{n})$$
$$s > 1 - \frac{1}{n}$$
$$f_{0,n}(s) = f_0(-1 + \frac{1}{n}) + f_0'(-1 + \frac{1}{n})(s + 1 - \frac{1}{n})$$
$$s < -1 + \frac{1}{n}$$

Regularized problem : f_0 replaced by $f_{0,n}$

Existence and uniqueness of the solution u_n to the regularized problem

Satisfies, for n large enough

$$\|u_n(t)\|^2_{\mathcal{C}^\alpha(\Omega)} + \|u_n(t)\|^2_{H^2(\Gamma)} + \|u_n(t)\|^2_{H^2(\Omega_\epsilon)} + \|u_n(t)\|^2_{H^1(\Omega)} +$$
$$\|\frac{\partial u_n}{\partial t}(t)\|^2_{H^{-1}(\Omega)} + \|\frac{\partial u_n}{\partial t}(t)\|^2_{L^2(\Gamma)} +$$
$$\|\nabla D_\tau u_n(t)\|^2_{L^2(\Omega)^{2N}} + \|f_{0,n}(u_n(t))\|_{L^1(\Omega)} +$$
$$\int_t^{t+1}(\|\frac{\partial u_n}{\partial t}(s)\|^2_{H^{-1}(\Omega)} + \|\frac{\partial u_n}{\partial t}(s)\|^2_{L^2(\Gamma)})ds \leq$$
$$ce^{-\beta t}(1 + \|u_n(0)\|^2_{H^1(\Omega)} + \|u_n(0)\|^2_{H^1(\Gamma)} +$$
$$\|\frac{\partial u_n}{\partial t}(0)\|^2_{H^{-1}(\Omega)} + \|\frac{\partial u_n}{\partial t}(0)\|^2_{L^2(\Gamma)})^2 + c'$$

$\Omega_\epsilon = \{x \in \Omega,\ d(x,\Gamma) > \epsilon\},\ \epsilon > 0$
$D_\tau u_n = \nabla u_n - \frac{\partial u_n}{\partial \nu}\nu$
$\alpha > 0,\ \beta > 0,\ c,\ c'$ independent of n

Remark : Actually, $u_n(t) \in H^2(\Omega)$, but this regularity does not pass to the limit

Smoothing property :

$$\|\frac{\partial u_n}{\partial t}(t)\|^2_{H^{-1}(\Omega)} + \|\frac{\partial u_n}{\partial t}(t)\|^2_{L^2(\Gamma)} \leq \frac{c}{t}(1 + \|u_n(0) - < u_n(0) > \|^2_{H^{-1}(\Omega)} + \|u_n(0)\|^2_{L^2(\Gamma)})$$

$t \in (0,1],\ c$ independent of n

Lipschitz estimate :

$$\|u_1(t) - u_2(t)\|_{H^{-1}(\Omega)} + \|u_1(t) - u_2(t)\|_{L^2(\Gamma)} \leq ce^{c't}(\|u_1(0) - u_2(0)\|_{H^{-1}(\Omega)} + \|u_1(0) - u_2(0)\|_{L^2(\Gamma)})$$
$$< u_1(0) >=< u_2(0) >= m,\ t \geq 0$$

$c,\ c'$ independent of $t,\ n,\ u_1,\ u_2$

u_n converges to some function u

We wish to call u the "generalized" solution to the singular problem

Variational solutions :

We set

$$B(u,v) = (\nabla u, \nabla v)_\Omega + \lambda(u,v)_\Omega + \\ +L((-\Delta)^{-1}\overline{u}, \overline{v})_\Omega + (\nabla_\Gamma u, \nabla_\Gamma v)_\Gamma$$

$u,\ v \in H^1(\Omega) \otimes H^1(\Gamma) = \{w,\ w \in H^1(\Omega), w|_\Gamma \in H^1(\Gamma)\}$

$L > 0$ chosen s.t.

$$\|\nabla u\|^2_{L^2(\Omega)^3} + \lambda\|u\|^2_{L^2(\Omega)} + L\|u\|^2_{H^{-1}(\Omega)} \geq \\ \frac{1}{2}\|u\|^2_{H^1(\Omega)},\ u \in H^1(\Omega),\ < u >= 0$$

$\overline{u} = u- < u >$

$(.,.)_\Omega, (.,.)_\Gamma$: scalar products in $L^2(\Omega)$ and $L^2(\Gamma)$

We rewrite the problem as

$$
\begin{aligned}
&(-\Delta)^{-1}\frac{\partial u}{\partial t} - \Delta u + \\
&f_0(u) + \lambda u - < w >= 0 \\
&w = -\Delta u + f_0(u) + \lambda u \\
&\frac{\partial \psi}{\partial t} - \Delta_\Gamma \psi + g(\psi) + \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma \\
&\psi = u|_\Gamma \\
&u|_{t=0} = u_0,\ \psi|_{t=0} = \psi_0
\end{aligned}
$$

We multiply the first equation by $u - v$, $v = v(x)$ s.t.

$$
< u(t) - v >= 0,\ t \geq 0 :
$$

$$
\begin{aligned}
&((-\Delta)^{-1}\frac{\partial u}{\partial t}, u - v)_\Omega + (\frac{\partial u}{\partial t}, u - v)_\Gamma + \\
&B(u, u - v) + (f_0(u), u - v)_\Omega = \\
&L(u, (-\Delta)^{-1}(u - v))_\Omega - (g(u), u - v)_\Gamma
\end{aligned}
$$

Positivity of B and monotonicity of f_0 :

$$\begin{array}{l}((-\Delta)^{-1}\frac{\partial u}{\partial t}, u-v)_\Omega + (\frac{\partial u}{\partial t}, u-v)_\Gamma + \\ B(v, u-v) + (f_0(v), u-v)_\Omega \leq \\ L(u, (-\Delta)^{-1}(u-v))_\Omega - (g(u), u-v)_\Gamma\end{array}$$

Variational inequality (VI)

We set

$$\begin{array}{l}\Phi = \{(u,\psi) \in L^\infty(\Omega) \times L^\infty(\Gamma), \\ \|u\|_{L^\infty(\Omega)} \leq 1,\ \|\psi\|_{L^\infty(\Gamma)} \leq 1\}\end{array}$$

Definition : Let $(u_0, \psi_0) \in \Phi$. Then, (u, ψ) is a variational solution if

(i) $u(t)|_\Gamma = \psi(t)$ a.e. $t > 0$, $u(0) = u_0$, $\psi(0) = \psi_0$;

(ii) $-1 < u(t, x) < 1$ a.e. $(t, x) \in R^+ \times \Omega$;

(iii) $(u, \psi) \in \mathcal{C}([0, +\infty); H^{-1}(\Omega) \times L^2(\Gamma)) \cap L^2(0, T; H^1(\Omega) \times H^1(\Gamma))$, $T > 0$;

(iv) $f(u) \in L^1((0, T) \times \Omega),\ T > 0$;

(v) $(\frac{\partial u}{\partial t}, \frac{\partial \psi}{\partial t}) \in L^2(\tau, T; H^{-1}(\Omega) \times L^2(\Gamma)), T > \tau > 0$;

(vi) $< u(t) >=< u_0 >,\ t \geq 0$;

(vii) the variational inequality (VI) is satisfied for a.e. $t > 0$ and every test function $v = v(x)$ s.t. $v \in H^1(\Omega) \otimes H^1(\Gamma), f(v) \in L^1(\Omega), < v >=< u_0 >$.

Remark : $u(t)|_\Gamma = \psi(t)$ only for $t > 0$

• A variational solution, if it exists is unique

• $\forall (u_0, \psi_0) \in \Phi$, $\exists$ a variational solution and $(u_n, \psi_n = u_n|_\Gamma)$ converges (for a subsequence) to a variational solution

• The variational solutions satisfy the a priori estimates mentioned earlier

• The variational solutions satisfy the smoothing and Lipschitz properties

A variational solution does not necessarily solve the equations in the usual sense

True if $u(t) \in H^2(\Omega)$

A variational solution solves the first equation

$$(-\Delta)^{-1}\frac{\partial u}{\partial t} - \Delta u + \\ f_0(u) + \lambda u - < w > = 0 \text{ in } \mathcal{D}'$$

Does not necessarily satisfy the dynamic boundary condition

More precisely, the trace

$$\frac{\partial u}{\partial \nu} = [\frac{\partial u}{\partial \nu}]_{\text{int}}$$

exists in $L^\infty(\tau, T; L^1(\Gamma))$, $0 < \tau < T$

(u_n, ψ_n) satisfies

$$\frac{\partial \psi_n}{\partial t} - \Delta_\Gamma \psi_n + g(\psi_n) + \frac{\partial u_n}{\partial \nu} = 0 \text{ on } \Gamma$$

in $L^\infty(\tau, T; L^2(\Gamma))$, $T > \tau > 0$, and the limit

$$[\frac{\partial u}{\partial \nu}]_{\text{ext}} = \lim_{n \to +\infty} \frac{\partial u_n}{\partial \nu}$$

exists in $L^\infty(\tau, T; L^2(\Gamma))$ weak star

$$\to \frac{\partial \psi}{\partial t} - \Delta_\Gamma \psi + g(\psi) + [\frac{\partial u}{\partial \nu}]_{\text{ext}} = 0 \text{ on } \Gamma$$

$\to$ A variational solution is a classical one if

$$[\frac{\partial u}{\partial \nu}]_{\text{int}} = [\frac{\partial u}{\partial \nu}]_{\text{ext}} \text{ a.e. } (t, x) \in R^+ \times \Gamma$$

Remark : Scalar ODE

$$\begin{aligned} & y'' - f(y) = 0, \; x \in (-1,1) \\ & y'(\pm 1) = K > 0 \end{aligned}$$

There exists a critical value K_0 s.t., if $K > K_0$, there is no classical solution

However, there exists a variational solution which is solution to

$$\begin{aligned} & y'' - f(y) = 0, \; x \in (-1,1) \\ & y(\pm 1) = \pm 1 \end{aligned}$$

$$y'|_{x=\pm 1} \neq K$$

Existence of classical solutions :

Related to the H^2-regularity and the separation from the singularities of f_0

Theorem : Let (u,ψ) be a variational solution and set, for $\delta > 0$ and $T > 0$,

$$\Omega_\delta(T) = \{x \in \Omega,\ |u(T,x)| < 1-\delta\}.$$

Then, $u(T) \in H^2(\Omega_\delta(T))$ and

$$\|u(T)\|_{H^2(\Omega_\delta(T))} \leq Q_{\delta,T},$$

where $Q_{\delta,T}$ is independent of u.

Consequence : if

$$|u(t,x)| < 1 \text{ a.e. } (t,x) \in R^+ \times \Gamma$$

then

$$[\frac{\partial u}{\partial \nu}]_{\text{int}} = [\frac{\partial u}{\partial \nu}]_{\text{ext}} \text{ a.e. } (t,x) \in R^+ \times \Gamma$$

and u is a classical solution

$\rightarrow$ The existence of classical solutions is related to the separation property on the boundary

True if f_0 has sufficiently strong singularities

Theorem : We assume that

$$\lim_{s \to \pm 1} F_0(s) = +\infty, \; F_0' = f_0.$$

Then, the separation property on the boundary holds and a variational solution is a classical one.

True if f_0 behaves like $\frac{s}{(1-s^2)^p}$, $p > 1$

Not true for logarithmic potentials

In that case, we can have $|u(t,x)| = 1$ on a set with nonzero measure on the boundary (possibly, on the whole boundary)

Theorem : We assume that

$$\pm g(\pm 1) > 0.$$

Then, a variational solution is a classical one.

Existence of finite-dimensional attractors :

Conservation of the total mass ($< u >$) : we restrict ourselves to

$$\Phi_m = \{(u, \psi) \in \Phi, \ < u >= m\}, \ m \in (-1, 1)$$

Theorem : For every $m \in (-1, 1)$, the semigroup $S(t)$ acting on Φ_m possesses the finite-dimensional global attractor $\mathcal{A}_m$ (in $H^{-1}(\Omega) \times L^2(\Gamma)$) which is bounded in $\mathcal{C}^\alpha(\Omega) \times \mathcal{C}^\alpha(\Gamma)$, $0 < \alpha < \frac{1}{4}$.

Global attractor : unique compact set of Φ_m which is invariant ($S(t)\mathcal{A}_m = \mathcal{A}_m, \ t \geq 0$) and attracts all bounded sets of initial data

Existence of the global attractor : follows from classical results

Finite-dimensionality : construction of an exponential attractor

Exponential attractor : compact and positively invariant ($S(t)\mathcal{M}_m \subset \mathcal{M}_m,\ t \geq 0$) set which contains the global attractor and has finite fractal dimension

We need some (asymptotically) compact smoothing property on the difference of 2 solutions

We have

$$\|u_1(t) - u_2(t)\|^2_{\Phi^{\mathrm{w}}} \leq ce^{-\beta t}\|u_1(0) - u_2(0)\|^2_{\Phi^{\mathrm{w}}} + c' \int_0^t \|\theta(u_1(s) - u_2(s))\|^2_{L^2(\Omega)} ds$$

$\beta > 0$, θ : smooth cut-off function

$\Phi^{\mathrm{w}} = H^{-1}(\Omega) \times L^2(\Gamma)$

$\rightarrow$ The semigroup is a contraction, up to $\|\theta(u_1 - u_2)\|_{L^2(0,t;L^2(\Omega))}$

Compactness : We work on spaces of trajectories and use the compactness of

$$L^2(0,t;H^1(\Omega)) \cap H^1(0,t;H^{-3}(\Omega)) \subset L^2(0,t;L^2(\Omega))$$

We have

$$\|\frac{\partial}{\partial t}[\theta(u_1 - u_2)]\|^2_{L^2(0,t;H^{-3}(\Omega))} + \|\theta(u_1 - u_2)\|^2_{L^2(0,t;H^1(\Omega))} \leq ce^{c't}\|u_1(0) - u_2(0)\|^2_{H^{-1}(\Omega)\cap L^2(\Gamma)}$$

$u_1(0), u_2(0) \in B_{H^{-1}(\Omega)\cap L^2(\Gamma)}(u_0, \epsilon)$, $\epsilon > 0$ small