Some recent developments on the longtime behaviour of discretized Allen-Cahn equations

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11th European-Maghrebian Workshop, Hammamet, Sept. 3-7, 2018

The Allen-Cahn equation

$$u_t - \Delta u + f'(u) = 0, \qquad \text{in } \Omega \times (0, +\infty),$$

with $f'(u) = u^3 - u$ and Dirichlet or no-flux boundary condition
Ω is a bounded domain of $\mathbf{R}^N$, $1 \leq N \leq 3$.
The AC equation is L^2 **gradient flow** for the functional

$$\mathcal{E}(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 + f(u)dx,$$

where $f(u) = (u^2 - 1)^2/4$. In particular,

$$\frac{d\mathcal{E}(u(t))}{dt} = -\int_\Omega |u_t(t)|^2 dx \leq 0.$$

Convergence to a single equilibrium was proved by **Simon'83** using a generalization of the Lojasiewicz inequality (+ Lasalle's invariance principle and regularizing property)

The modified Allen-Cahn equation

$$\beta u_{tt} + u_t - \Delta u + f'(u) = 0, \qquad \text{in } \Omega \times (0, +\infty),$$

with $\beta > 0$, $f'(u) = u^3 - u$ and no-flux or Dirichlet boundary condition.
Ω is a bounded domain of $\mathbf{R}^N$, $1 \leq N \leq 3$.
On multiplying scalarly by u_t, we see that

$$\frac{d\mathcal{E}(u(t))}{dt} = -\int_\Omega |u_t(t)|^2 dx \leq 0,$$

where

$$\mathcal{E}(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 + f(u) + \frac{\beta}{2}|u_t|^2 dx.$$

Jendoubi'98 proved convergence to an equilibrium by generalizing Simon's approach.

Convergence to a single equilibrium for such PDEs is well-understood (gradient-like structure, precompactness of trajectories, Lojasiewicz-Simon inequality).

Contributors: Haraux, Chill, Jendoubi, Bolte;
Huang, Takac, Grasselli, Schimperna, Gatti, Miranville, Rougirel, Wu, Zhang, Abels, Wilke, ...

see the **review book of [Haraux & Jendoubi'15]**.

Question: what happens for a time and/or space discretization of the PDE ?

We focus on the **time discretization** (in finite or infinite dimension).

The Cahn-Hilliard equation

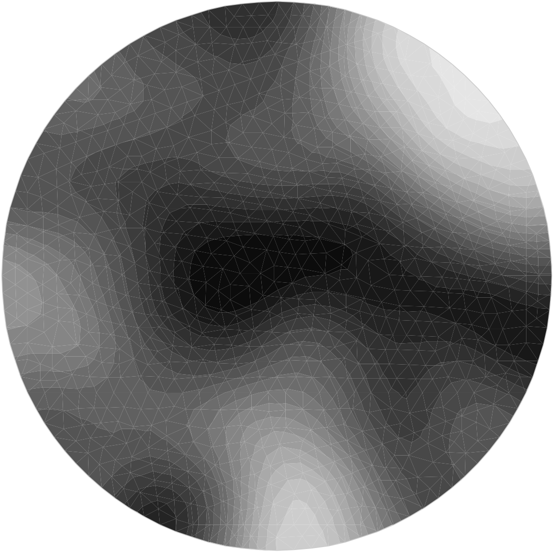
$$u_t = -\alpha \Delta^2 u + \Delta f'(u), \qquad \text{in } \Omega \times (0, +\infty),$$

with $f'(u) = u^3 - u$ and Neumann boundary condition

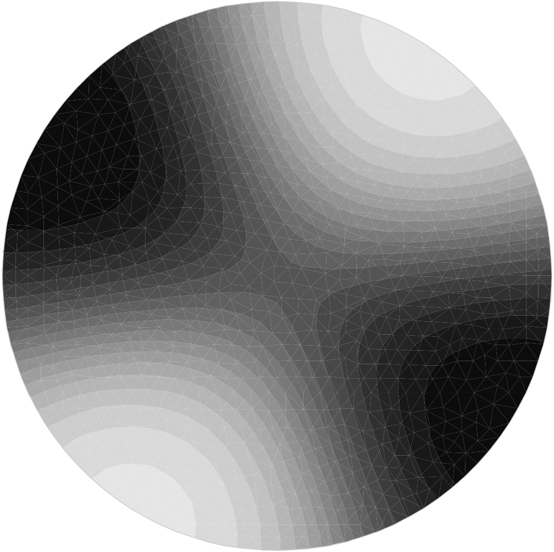
- Simulation on the "unit disc" for $\alpha = 0.05$
- P1-P1 finite elements (splitting method for the bilaplacian)
- Backward Euler
- $\Delta t = 0.015$ and 600 iterations.

(FreeFem++ software)
Rk: H^{-1} gradient flow for the functional

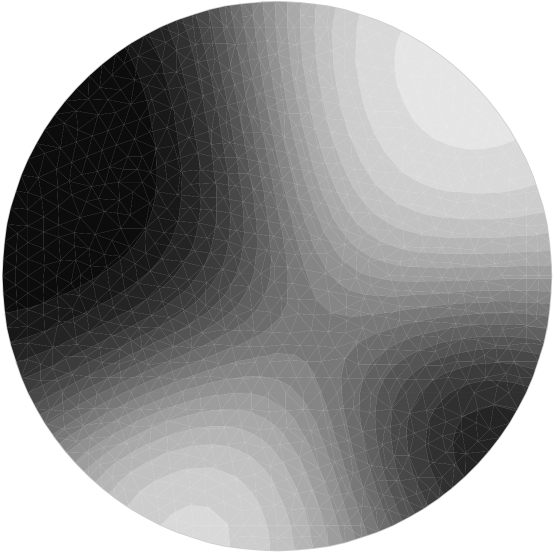
$$\mathcal{E}(u) = \int_\Omega \frac{\alpha}{2} |\nabla u|^2 + f(u) dx.$$



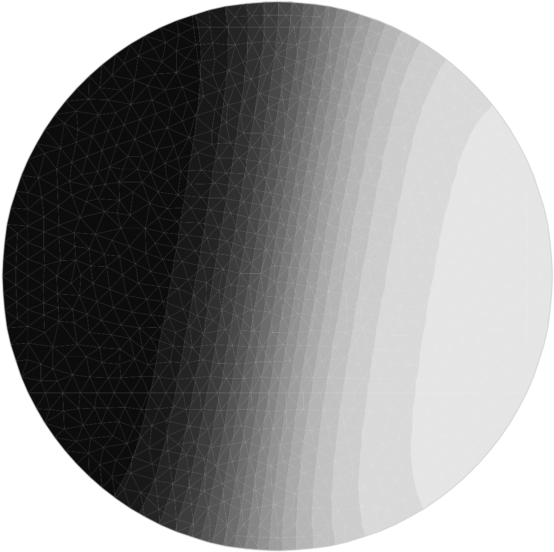
Initial state



Iteration $n = 100$



Iteration $n = 400$



A steady state for the Cahn-Hilliard equation

Phase-field crystal equation

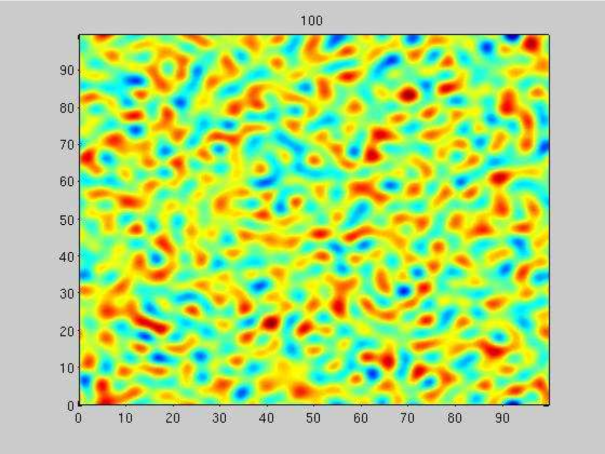
$$u_t = \Delta(u + 2\Delta u + \Delta^2 u + f'(u)) \text{ in } \Omega \times \mathbf{R}_+,$$

with periodic boundary conditions and $f'(u) = u^3 + ru$ $(r < 0)$.

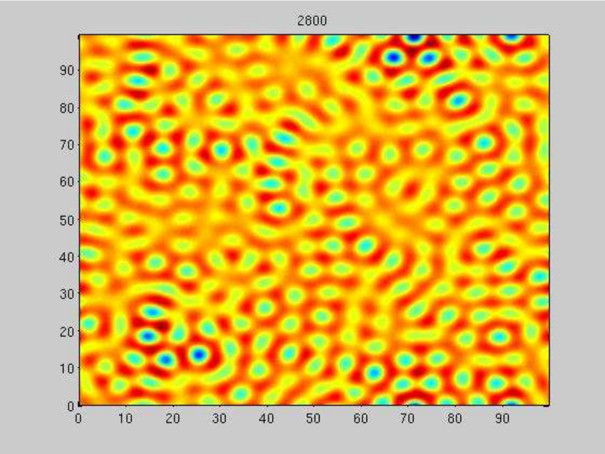
- Finite difference (FFT) in space : 256×256 grid
- linearly implicit Euler scheme in time: $\delta t = 0.01$
- $r = -0.9$, $\int_\Omega u_0 = 0.54|\Omega|$, 15000 iterations
- Matlab software

Rk: H^{-1} gradient flow for the Swift-Hohenberg functional

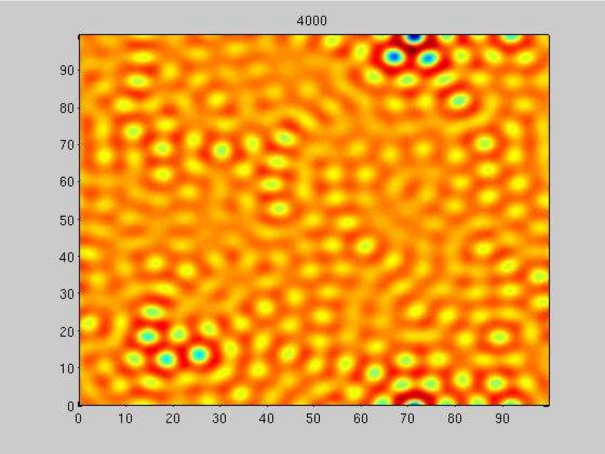
$$\mathcal{E}(u) = \int_\Omega \frac{1}{2}\left(u^2 - 2|\nabla u|^2 + |\Delta u|^2\right) + f(u)dx.$$



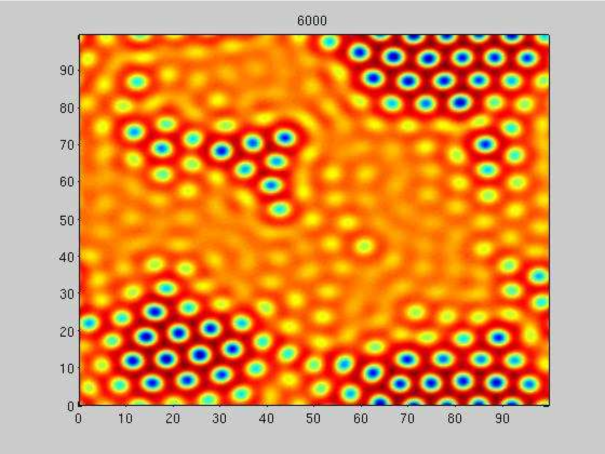
PFC, iteration $n = 100$



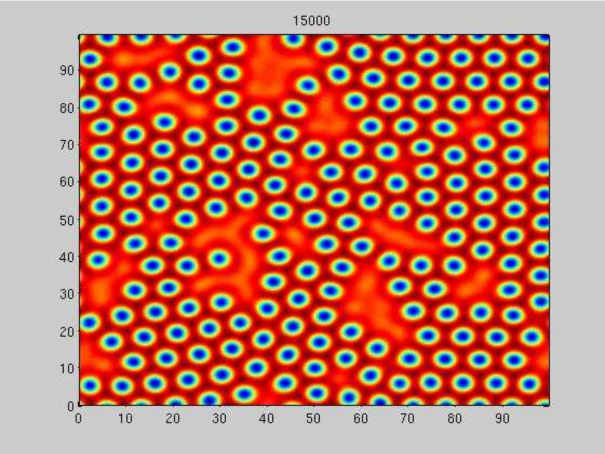
PFC, iteration $n = 2800$



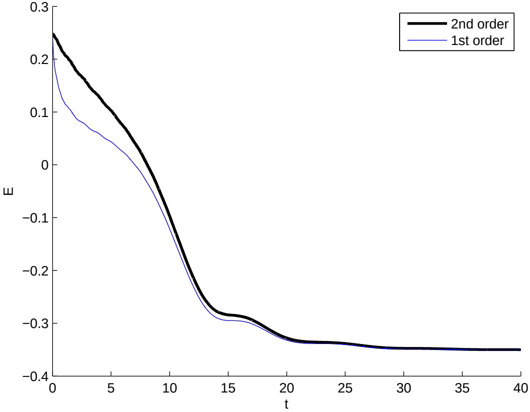
PFC, iteration $n = 4000$



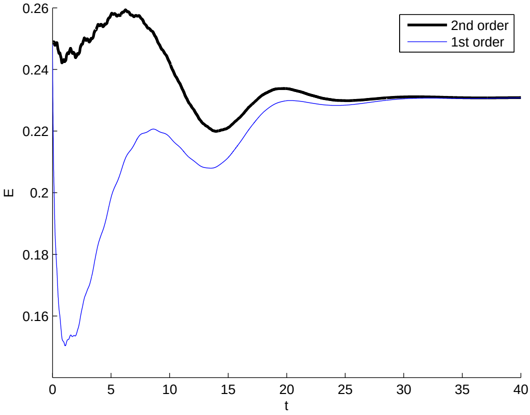
PFC, iteration $n = 6000$



PFC, iteration $n = 15000$



Pseudo-energy for the MPFC, $\langle u_t(0) \rangle = 0$



Pseudo-energy for the MPFC, $\langle u_t(0) \rangle \neq 0$

A general convergence result

Theorem (Absil, Mahony & Andrews'05)

Let $\Phi : \mathbf{R}^d \to \mathbf{R}$ be real analytic and $U \in C^1(\mathbf{R}_+, \mathbf{R}^d)$. Assume that there exists $\delta > 0$ and $\tau \geq 0$ such that for all $t > \tau$,

$$-\frac{d\Phi(U(t))}{dt} = -\nabla\Phi(U(t)) \cdot U'(t) \geq \delta \|\nabla\Phi(U(t))\| \, \|U'(t)\|,$$

*(**angle condition**), and*

$$\frac{d\Phi(U(t))}{dt} = 0 \Rightarrow U'(t) = 0.$$

*(**weak decrease condition**).*
Then either $\|U(t)\| \to +\infty$ or there exists $U^\star \in \mathbf{R}^d$ such that $U(t) \to U^\star$.

- NB : no reference to the dynamical system (but in general U satisfies an ODE and Φ is a Lyapunov function associated to the ODE) : an optimization approach
- 4 assumptions : analycity, angle condition, weak decrease condition, and $\|U(t)\| \not\to +\infty$ (compactness)

See also **Barta-Chill-Fasangova'10**

Example 1 : gradient-flow

Consider the **gradient flow**

$$U'(t) = -\nabla F(U(t)) \quad t \geq 0, \tag{1}$$

where $U = (u_1, \ldots, u_d)^t$, $F \in C^{1,1}_{loc}(\mathbf{R}^d, \mathbf{R})$.
We choose $\Phi = F$ and we have

$$-\frac{d\Phi(U(t))}{dt} = -\nabla F(U(t)) \cdot U'(t) = \|U'(t)\|^2 = \|\nabla F(U(t))\| \, \|U'(t)\|$$

so that the **angle condition** is satisfied (with $\delta = 1$), and the **weak decrease condition** also.
Thus : if F is real analytic and if U is bounded, then $U(t) \to U^\star$ as $t \to +\infty$, where $\nabla F(U^\star) = 0$. (**Lojasiewicz'65**)

Example 2 : Second-order gradient-like system

$$U''(t) + U'(t) + \nabla F(U(t)) = 0, \quad t \geq 0, \tag{2}$$

where $F \in C^2(\mathbf{R}^d, \mathbf{R})$.
The energy estimate is obtained on multiplying (2) by $U'(t)$:

$$\|U'(t)\|^2 + \frac{d}{dt}\left(\frac{1}{2}\|U'(t)\|^2 + F(U(t))\right) = 0, \quad \forall t \geq 0.$$

Strong Lyapunov functional, obtained for $\varepsilon > 0$ small (and for U bounded):

$$\Phi(U, V) = \frac{1}{2}\|V\|^2 + F(U) + \varepsilon\langle \nabla F(U), V\rangle.$$

We write (2) as a first order system

$$\begin{cases} U' = V, \\ V' = -V - \nabla F(U) \end{cases} \tag{3}$$

Since

$$\Phi(U, V) = \frac{1}{2}\|V\|^2 + F(U) + \varepsilon\langle \nabla F(U), V\rangle,$$

we have

$$\nabla\Phi(U, V) = \begin{cases} \partial_U \Phi(U, V) = \nabla F(U) + \varepsilon\nabla^2 F(U) V \\ \partial_V \Phi(U, V) = V + \varepsilon\nabla F(U) \end{cases}$$

Assume that U is bounded. Then V is also bounded, by the energy estimate. By computation, for $\varepsilon > 0$ small enough,

$$-\nabla\Phi(U,V)\cdot(U',V') \geq c_1\left(\|V\|^2 + \|\nabla F(U)\|^2\right)$$

Moreover,

$$\|\nabla\Phi(U,V)\| \leq c_2\left(\|V\|^2 + \|\nabla F(U)\|^2\right)^{1/2},$$

$$(\|U'\|^2 + \|V'\|^2)^{1/2} \leq c_3\left(\|V\|^2 + \|\nabla F(U)\|^2\right)^{1/2},$$

so that the **angle condition** is satisfied (with $\delta = c_1/(c_2 c_3)$), and the **weak decrease condition** as well. Thus, if F is real analytic on $\mathbf{R}^d$, then $(U(t),V(t)) \to (U^\star,0)$ as $t \to +\infty$, where $\nabla F(U^\star) = 0$. (**Haraux & Jendoubi'98**).

Counter-example

The convergence result of **Absil, Mahony and Andrews'05** can fail if $\Phi \in C^\infty(\mathbf{R}^d)$ when $d \geq 2$. "first" counterexample in **Palis and De Melo'82**.

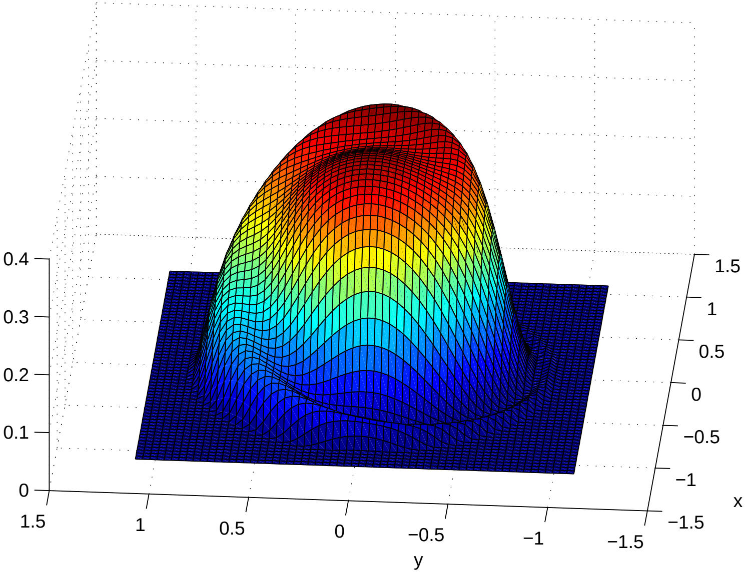
The following counter-example is given in **Absil, Mahony and Andrews'05** ("mexican hat function"):

$$F(r,\theta) = e^{-1/(1-r^2)}\left[1 - \frac{4r^4}{4r^4 + (1-r^2)^4}\sin(\theta - \frac{1}{1-r^2})\right],$$

if $r < 1$ and $F(r,\theta) = 0$ otherwise. We have $F \in C^\infty$, $F(r,\theta) > 0$ for $r < 1$ so every point on the circle $r = 1$ is a global minimizer. We can check that the curve defined by

$$\theta = 1/(1-r^2)$$

is a trajectory of the gradient flow $U'(t) = -\nabla F(U(t))$.



“Mexican hat” function

Definition

We say that $\Phi \in C^1(\mathbf{R}^d, \mathbf{R})$ *satisfies the* **Łojasiewicz inequality** *near some point* $U^\star \in \mathbf{R}^d$ *if there exist* $\theta \in (0, 1/2]$, $\sigma > 0$ *and* $\gamma > 0$ *s.t. for all* $V \in \mathbf{R}^d$,

$$\|V - U^\star\| < \sigma \Rightarrow |\Phi(V) - \Phi(U^\star)|^{1-\theta} \leq \gamma \|\nabla\Phi(V)\|. \quad (4)$$

θ is called a **Lojasiewciz exponent** of $U^\star$. If Φ is analytic near $U^\star$, then Φ satisfies the Lojasiewicz inequality near $U^\star$ (**Lojasiewicz'65**).

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Example: for $d = 1$ and $p \geq 2$, $x \mapsto |x|^p$ satisfies (4) at $x = 0$ with $\theta = 1/p$. (NB : also true for $1 < p \leq 2$!).

In the "generic case" where $\nabla^2\Phi(U)$ invertible, $\theta = 1/2$.

Counter-example: for $d = 1$, the C^∞ function $x \mapsto \exp(-1/x^2)$ satisfies (4) at $x = 0$ only for $\theta = 0$ (too weak).

A general convergence result (proof)

Theorem (Absil, Mahony & Andrews'05)

Let $\Phi : \mathbf{R}^d \to \mathbf{R}$ be real analytic and $U \in C^1(\mathbf{R}_+, \mathbf{R}^d)$. Assume that there exists $\delta > 0$ and $\tau \geq 0$ such that for all $t > \tau$,

$$-\frac{d\Phi(U(t))}{dt} = -\nabla\Phi(U(t)) \cdot U'(t) \geq \delta \|\nabla\Phi(U(t))\| \, \|U'(t)\|,$$

*(**angle condition**), and*

$$\frac{d\Phi(U(t))}{dt} = 0 \Rightarrow U'(t) = 0.$$

*(**weak decrease condition**).*
Then either $\|U(t)\| \to +\infty$ or there exists $U^\star \in \mathbf{R}^d$ such that $U(t) \to U^\star$.

A proof (convergence)

$$
\begin{aligned}
-[\Phi(U(t))^\theta]' &= -\theta U'(t)\cdot\nabla\Phi(U(t))\Phi(U(t))^{\theta-1} \\
\text{a.c.} \quad &\geq \theta\delta\|U'(t)\|\|\nabla\Phi(U(t))\|\Phi(U(t))^{\theta-1} \\
\text{Loja.} \quad &\geq \theta\delta\gamma^{-1}\|U'(t)\|,
\end{aligned}
$$

so $$\Phi(U(t_n))^\theta - \Phi(U(t))^\theta \geq \theta\delta\gamma^{-1}\int_{t_n}^{t}\|U'(s)\|ds.$$

A proof (convergence)

Let $t_n \to +\infty$ s.t. $U(t_n) \to U^\star$. $\Phi(U(t))$ is nonincreasing and so has a limit $\Phi^\star = \Phi(U^\star) = 0$. We may assume $\Phi(U(t)) > 0$ (by the w.d.c.). Choose n large enough so that $\|U(t_n) - U^\star\| < \sigma/2$ and $\theta^{-1}\delta^{-1}\gamma\Phi(U(t_n))^\theta < \sigma/2$, and define

$$t^+ = \sup\{t \geq t_n \mid \|U(s) - U^\star\| < \sigma \quad \forall s \in [t_n, t)\}.$$

For $t \in [t_n, t^+)$, we have

$$\begin{array}{rcl} -[\Phi(U(t))^\theta]' & = & -\theta U'(t) \cdot \nabla\Phi(U(t))\Phi(U(t))^{\theta-1} \\ \text{a.c.} & \geq & \theta\delta\|U'(t)\|\|\nabla\Phi(U(t))\|\Phi(U(t))^{\theta-1} \\ \text{Loja.} & \geq & \theta\delta\gamma^{-1}\|U'(t)\|, \end{array}$$

$$\text{so} \quad \Phi(U(t_n))^\theta - \Phi(U(t))^\theta \geq \theta\delta\gamma^{-1}\int_{t_n}^{t} \|U'(s)\| ds.$$

Thus $\|U(t) - U(t_n)\| < \sigma/2$, $\forall t \in [t_n, t^+)$ and so $t^+ = +\infty$, otherwise $\|U(t^+) - U^\star\| = \sigma$ and

$$\|U(t^+) - U^\star\| \leq \|U(t^+) - U(t_n)\| + \|U(t_n) - U^\star\| < \sigma,$$

a contradiction. QED.

A first result (discrete and explicit)

Theorem (Absil, Mahony and Andrews'05)

Let $\Phi : \mathbf{R}^d \to \mathbf{R}$ be real analytic and $(U^n)_n$ in $\mathbf{R}^d$ such that

$$\Phi(U^n) - \Phi(U^{n+1}) \geq \delta \|\nabla\Phi(U^n)\| \, \|U^{n+1} - U^n\|$$

*for all n, for some $\delta > 0$ (**angle condition**), and*

$$\Phi(U^{n+1}) = \Phi(U^n) \Rightarrow U^{n+1} = U^n$$

*(**descent condition**).*
Then either $U^n \to +\infty$ or there exists $U^\star \in \mathbf{R}^d$ such that $U^n \to U^\star$.

In **Alaa & P.'13**, we generalized the previous result in order to handle more general situations:

- Replace "real analytic" by "Lojasiewicz inequality" :
- Include implicit schemes or linearly implicit schemes
- Consider Schemes with variable stepsize
- Multi-step schemes

See also **Attouch & Bolte'09**, **Merlet & P.'10**, **Grasselli & P.'12**.

Assumptions: two descent conditions

Definition (Alaa and P.'13)

Let $(\tau_n)_n$ be a bounded sequence of positive real numbers and let $(U^n)_{n\in\mathbf{N}}$ be a sequence in $\mathbf{R}^d$. We say that $(U^n)_n$ satisfies assumptions (5) and (6) for the function $\Phi \in C^1(\mathbf{R}^d,\mathbf{R})$ if there exist two constants $c_s > 0$ and $\delta > 0$ such that

$$\Phi(U^n) - \Phi(U^{n+1}) \geq \frac{c_s}{\tau_n}\|U^{n+1} - U^n\|^2, \quad \forall\ n \geq 0. \tag{5}$$

and

$$\Phi(U^n) - \Phi(U^{n+1}) \geq \tau_n\delta\|\nabla\Phi(U^{n+1})\|^2, \quad \forall\ n \geq 0. \tag{6}$$

NB: (5) and (6) imply the **implicit angle condition**:

$$\Phi(U^n)-\Phi(U^{n+1}) \geq (c_s\delta)^{1/2}\left\|\nabla\Phi(U^{n+1})\right\|\left\|U^{n+1} - U^n\right\| \quad \forall n \geq 0,$$

Theorem (Convergence result - Alaa and P.'13)

Let $(\tau_n)_n$ be a bounded sequence of positive real numbers, and let $(U^n)_n$ be a sequence in $\mathbf{R}^d$ which has at least one accumulation point $U^\star$. Assume that $(U^n)_n$ satisfies assumptions (5) and (6) for the function $\Phi \in C^1(\mathbf{R}^d, \mathbf{R})$ and that Φ satisfies the Łojasiewicz inequality near $U^\star$. Then the whole sequence $(U^n)_n$ converges to $U^\star$.

See also **Attouch, Bolte & Svaiter'13**, **de Carvalho Bento, da Cruz Neto, Soubeyran & de Sousa Junior'16**

Theorem (Convergence rates - Alaa and P.'13)

Let assumptions of the previous Theorem be satisfied, and let θ denote a Łojasiewicz exponent of Φ near $U^\star$. Then the following estimates hold:

1. *if $\theta = 1/2$, there exist $C > 0$, $\alpha > 0$ and $\bar{n} \in \mathbf{N}^\star$ such that*

$$\|U^n - U^\star\| \leq C \exp\left(-\alpha \sum_{k=0}^{n-1} \tau_k\right) \quad \forall n \geq \bar{n}; \tag{7}$$

2. *if $\theta \in (0, 1/2)$, there exist $C > 0$ and $\bar{n} \in \mathbf{N}^\star$ such that*

$$\|U^n - U^\star\| \leq C \left(\sum_{k=0}^{n-1} \tau_k\right)^{-\theta/(1-2\theta)} \quad \forall n \geq \bar{n}. \tag{8}$$

Let $\{(\tau_n^\tau)_n \ : \tau > 0\}$ denote a family of bounded sequences of positive real numbers. The family is indexed by $\tau = \sup\{\tau_n^\tau \ : n \geq 0\}$. (for a constant stepsize $\tau_n^\tau = \tau$ for all n).

Theorem (Stability as $\tau \to 0$ - Alaa and P.'13)

Let $(U_\tau^n)_{n\geq 0}$ denote a family of sequences in $\mathbf{R}^d$ indexed by $\tau \in (0, \tau^\star]$ with $0 < \tau^\star < +\infty$. Assume that there exist a function $\Phi \in C^1(\mathbf{R}^d, \mathbf{R})$ and two positive constants c_s, δ independent of τ such that assumptions (5) and (6) hold for every sequence $(U_\tau^n)_n$, i.e.

$$\begin{aligned} \Phi(U_\tau^n) - \Phi(U_\tau^{n+1}) &\geq \frac{c_s}{\tau_n} \|U_\tau^{n+1} - U_\tau^n\|^2, \quad \forall\ n \geq 0, \\ \Phi(U_\tau^n) - \Phi(U_\tau^{n+1}) &\geq \tau_n \delta \|\nabla\Phi(U_\tau^{n+1})\|^2, \quad \forall\ n \geq 0. \end{aligned}$$

If $\bar{U}$ is a local minimizer of Φ, and if Φ satisfies the Łojasiewicz inequality near $\bar{U}$, then for all $\epsilon > 0$, there exists $\rho > 0$ such that for all $\tau \in (0, \tau^\star]$, if $\left\| U_\tau^0 - \bar{U} \right\| < \rho$, the sequence $(U_\tau^n)_n$ converges and satisfies $\left\| U_\tau^n - \bar{U} \right\| \leq \epsilon$ for all $n \geq 0$.

Discretizations of the gradient flow

$$U' + AU + \nabla F(U) = 0 \quad t \geq 0, \tag{9}$$

where A is a symmetric positive semi-definite matrix of size d, and $F \in C^1(\mathbf{R}^d, \mathbf{R})$. Equation (9) is a gradient-flow for the energy

$$E(V) = \frac{1}{2}\langle AV, V\rangle + F(V) \quad V \in \mathbf{R}^d, \tag{10}$$

For implicit schemes, we assume that ∇F satisfies a one-sided Lipschitz condition

$$\langle \nabla F(U) - \nabla F(V), U - V\rangle \geq -c_F\|U - V\|^2 \quad \forall U, V \in \mathbf{R}^d, \tag{11}$$

for some (optimal) constant $c_F \geq 0$.
For explicit or linearly implicit schemes, we assume that ∇F is Lipschitz continuous, i.e.

$$\|\nabla F(U) - \nabla F(V)\| \leq L_F\|U - V\| \quad \forall U, V \in \mathbf{R}^d, \tag{12}$$

for some (optimal) constant $L_F \geq 0$.

We consider the following time discretizations of (9) with variable time step:

- Implicit Euler scheme (IE)

$$\frac{U^{n+1}-U^n}{\tau_n}+AU^{n+1}+\nabla F(U^{n+1})=0 \quad n\geq 0; \qquad (13)$$

- Linearly implicit Euler scheme (LIE)

$$\frac{U^{n+1}-U^n}{\tau_n}+AU^{n+1}+\nabla F(U^{n})=0 \quad n\geq 0; \qquad (14)$$

- Explicit Euler scheme (EE)

$$\frac{U^{n+1}-U^n}{\tau_n}+AU^{n}+\nabla F(U^{n})=0 \quad n\geq 0; \qquad (15)$$

- Stabilized first order linearly implicit scheme (S1LI)

$$(\frac{1}{\tau_n} + S)(U^{n+1} - U^n) + AU^{n+1} + \nabla F(U^n) = 0 \quad n \geq 0, \ (16)$$

where $S \geq 0$ denotes a constant which will be specified later on;

- Stabilized first order implicit scheme (S1I)

$$(\frac{1}{\tau_n} + S)(U^{n+1} - U^n) + AU^{n+1} + \nabla F(U^{n+1}) = 0 \quad n \geq 0, \ (17)$$

where $S \geq 0$ is a constant which will be specified later on.

scheme	∇F	$\tau^\star$	S
IE (13)	(11)	$\tau^\star < 2/c_F$	/
LIE (14)	(12)	$\tau^\star < 2/L_F$	/
EE (15)	(12)	$\tau^\star < 2/(\lambda_d + L_F)$	/
S1LI (16)	(12)	$\tau^\star < \infty$	$S \geq L_F/2$
S1I (17)	(11)	$\tau^\star < \infty$	$S \geq c_F/2$

Table : Assumptions

For every scheme, we choose $\Phi = E$ (the stability result near a local minimizer also applies)

scheme	c_s	δ
IE (13)	$c_s = 1 - c_F\tau^\star/2$	$\delta = c_s$
LIE (14)	$c_s = 1 - L_F\tau^\star/2$	$\delta = c_s/(1 + L_F\tau^\star)^2$
EE (15)	$c_s = 1 - (\lambda_d + L_F)\tau^\star/2$	$\delta = c_s/(1 + (\lambda_d + L_F)\tau^\star)^2$
S1LI (16)	$c_s = 1$	$\delta = 1/(1 + (S + L_F)\tau^\star)^2$
S1I (17)	$c_s = 1$	$\delta = 1/(1 + c_F\tau^\star)^2$

Table : Conclusions

Example of a two-step scheme

We consider a second order linearly implicit scheme with fixed stepsize (S2LI): for all $n \geq 0$,

$$\frac{1}{2\tau}(3U^{n+1} - 4U^n + U^{n-1}) + AU^{n+1} + 2\nabla F(U^n) - \nabla F(U^{n-1}) = 0. \tag{18}$$

For the Lyapunov functional, we use a first order approximation of the energy E.

NB : other (stable) multistep (BDF) schemes can be considered in the same way, up to order 5, cf. **Stuart-Humphries'96**, **Bouchriti-Pierre-Alaa submitted**

Discretizations of the modified gradient flow

$$\beta U'' + U' + AU + \nabla F(U) = 0, \quad t \geq 0, \tag{19}$$

where $U \in C^2(\mathbf{R}_+, \mathbf{R}^d)$ is the unknown, $\beta > 0$, A is a symmetric positive semi-definite matrix of size d, and $F \in C^2(\mathbf{R}^d, \mathbf{R})$.
Equation (19) is equivalent to the first-order system:

$$\begin{cases} U' = V \\ \beta V' = -V - AU - \nabla F(U). \end{cases} \tag{20}$$

- Implicit Euler (IE): for $n \geq 0$,

$$\begin{cases} (U^{n+1} - U^n)/\tau_n = V^{n+1} \\ \beta(V^{n+1} - V^n)/\tau_n = -V^{n+1} - AU^{n+1} - \nabla F(U^{n+1}). \end{cases} \tag{21}$$

If the stepsize is constant, i.e. $\tau_n = \tau$ for all n, then by eliminating V^n, (21) is equivalent to the two-step scheme

$$\beta \frac{U^{n+1} - 2U^n + U^{n-1}}{\tau^2} + \frac{U^{n+1} - U^n}{\tau} + AU^{n+1} + \nabla F(U^{n+1}) = 0.$$

Moreover, if $\beta/\tau = 1/2$, the latter is (curiously) equivalent to a second order implicit discretization of the gradient flow;

- A linearly implicit first order scheme (LI)

$$\begin{cases}(U^{n+1}-U^n)/\tau_n = V^{n+1} \\ \beta(V^{n+1}-V^n)/\tau_n = -V^{n+1} - AU^{n+1} - \nabla F(U^n)\end{cases} \tag{22}$$

If $\tau_n = \tau$ for all n, this scheme is equivalent to

$$\beta\frac{U^{n+1}-2U^n+U^{n-1}}{\tau^2} + \frac{U^{n+1}-U^n}{\tau} + AU^{n+1} + \nabla F(U^n) = 0;$$

- A stabilized first order linearly implicit scheme (S1LI):

$$\begin{cases}(U^{n+1}-U^n)/\tau_n = V^{n+1} \\ \beta(V^{n+1}-V^n)/\tau_n = -V^{n+1} - S(U^{n+1}-U^n) - AU^{n+1} - \nabla F(U^n\end{cases} \tag{23}$$

If $\tau_n = \tau$ for all n, this scheme is equivalent to

$$\beta\frac{U^{n+1}-2U^n+U^{n-1}}{\tau^2} + (\frac{1}{\tau}+S)(U^{n+1}-U^n) + AU^{n+1} + \nabla F(U^n) = 0,$$

Theorem (Alaa and P.'13)

Assume that F satisfies (12), that $\tau^\star < 1/\max\{L_F/2 - S, 0\}$ (with $S \geq 0$), and let $(U^n, V^n)_n$ be a sequence in $\mathbf{R}^d \times \mathbf{R}^d$ which complies with the S1LI scheme (23). If $(U^n)_n$ is bounded and if E satisfies the Łojasiewicz inequality near an accumulation point $U^\star$ of $(U^n)_n$, then

$$\lim_{n\to+\infty} (U^n, V^n) = (U^\star, V^\star),$$

for some $V^\star \in \mathbf{R}^d$. Moreover, the convergence rates of Theorem 3.4 are valid for any Łojasiewicz exponent of E near $U^\star$.

A similar result for the IE scheme (see also **Grasselli and P.'12**). See also **Grasselli & P.'16** for a second order discretization of the MPFC.

Example 1: Galerkin approximation with analytic nonlinearity

We consider a Galerkin approximation of the nonlinear damped wave equation

$$\beta u_{tt} + u_t - \Delta u + f'(u) = 0 \quad x \in \Omega,\ t > 0, \tag{24}$$

where $\beta \geq 0$, $f : \mathbf{R} \to \mathbf{R}$ is real analytic, and Ω is a bounded open subset of $\mathbf{R}^N$ ($N \in \mathbf{N}^\star$).

For the Galerkin approximation of (24), we assume that

$$V^h \text{ is a finite dimensional subspace of } H^1(\Omega) \cap L^\infty(\Omega), \tag{25}$$

(FE or spectral discretization) The space discrete variational formulation of (24) reads : find $u^h : [0, +\infty) \to \mathbf{R}$ such that

$$\beta(u^h_{tt}, \varphi^h) + (u^h_t, \varphi^h) + (\nabla u^h, \nabla \varphi^h) + (f'(u^h), \varphi^h) = 0 \ \forall \varphi^h \in V^h, \tag{26}$$

where $(\cdot,\cdot)$ denotes the $L^2(\Omega)$-scalar product.

Choosing an orthonormal basis of V^h, (26) is equivalent to its matrix version:

$$\beta U'' + U' + AU + \nabla F(U) = 0 \quad t \geq 0, \tag{27}$$

Allen-Cahn equation. We assume that $\beta = 0$ (parabolic case) and

$$f(s) = \sum_{k=0}^{2p} a_k s^k \quad \forall s \in \mathbf{R} \quad (a_{2p} > 0),$$

for some $p \in \mathbf{N}^\star$. Then f is analytic, coercive and satisfies the one-sided Lipschitz condition for some constant $c_f \geq 0$. We can apply the convergence results for all the implicit schemes.
sine-Gordon equation. We assume that $\beta > 0$, that

$$f'(s) = a \sin s \quad \forall s \in \mathbf{R} \quad (a > 0),$$

and that $V^h \subset H_0^1(\Omega)$. The convergence results apply for the 3 schemes considered.

FE with numerical integration and truncated potential

We assume that V^h is a P^k or Q^k FE space.
We use a numerical integration $(\cdot,\cdot)_h$ with some basic properties.
The space discretization reads: find $u^h : [0,+\infty) \to \mathbf{R}$ such that

$$\beta(u^h_{tt},\varphi^h)_h+(u^h_t,\varphi^h)_h+(\nabla u^h,\nabla\varphi^h)_h+(f'(u^h),\varphi^h)_h = 0\,\forall\varphi^h \in V^h. \tag{28}$$

Its matrix version is again

$$\beta U'' + U' + AU + \nabla F(U) = 0 \quad t \geq 0, \tag{29}$$

The function f is the truncated potential

$$f(s) = \begin{cases} (s^2-1)^2/4 & \text{if } |s| \leq M, \\ (3M^2-1)s^2/2 - 2M^3|s| + (3M^4+1)/4 & \text{if } |s| > M. \end{cases}$$

Then f' is Lipschitz continuous on $\mathbf{R}$, and we can show that $E(V) = \langle AV, V\rangle/2 + F(V)$ is **subanalytic**. In particular, by **Bolte, Daniilidis & Lewis'06**, E satisfies the Lojasiewicz inequality near every $U \in \mathbf{R}^d$.
Thus, we have convergence to equilibrium for every scheme considered ($\beta = 0$ and $\beta > 0$).

Convergence to equilibrium in infinite dimension

$$\mathcal{E}(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 + f(u)dx, \qquad \text{with } f(u) = (u^2-1)^2/4.$$

Ω a bounded domain or $\mathbf{R}^N$, $1 \le N \le 3$.

Theorem (A Lojasiewicz-Simon inequality)

Let $u^\star \in H_0^1(\Omega)$. There exist $\theta \in (0,1/2)$ and $\sigma > 0$ s.t. $\forall u \in H_0^1(\Omega)$,

$$\|u-u^\star\|_{H_0^1(\Omega)} < \sigma \Rightarrow |\mathcal{E}(u)-\mathcal{E}(u^\star)|^{1-\theta} \le \|-\Delta u + f'(u)\|_{H^{-1}(\Omega)}.$$

The backward Euler scheme with fixed time step $\tau > 0$ for AC reads: let $u^0 \in H_0^1(\Omega)$ and for $n = 0, 1, \dots$ let $u^{n+1} \in H_0^1(\Omega)$ solve

$$\frac{u^{n+1}-u^n}{\tau} - \Delta u^{n+1} + f'(u^{n+1}) = 0.$$

Convergence to equilibrium in infinite dimension

issues: Lojasiewicz-Simon inequality, choice of norms, pre-compactness of trajectories

- *A descent method (discretized nonlocal CH):* **Gajewski & Griepentrog'06**
- *1st order time semi-discrete for AC:* **[Merlet & P.'10], [Bolte, Daniilidis, Ley, Mazet'10]**
- *2nd order time semi-discrete for CH (BDF2):* **[Antonietti, Merlet, P. & Verani]'16**
- *BDF3, 4 and 5 for AC:* **[Bouchriti, P., Alaa submitted]**
- *1st order time semi-discrete for MAC:* **[P. & Rogeon'16]**

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- *1st order time semi-discrete for MAC:* **[P. & Rogeon'16]**
- BDF6 for AC: **open case** (gradient-flow structure ?)
- 2nd order time semi-discrete for MAC: **open case** (pre-compactness of trajectories ?)
- Semi-implicit schemes: **open case** (Lojasiewicz-Simon inequality ?)

Global dynamics: a 1d example

$$u_t - \nu \Delta u + u^3 - u = 0, \quad x \in [0,1], \ t \geq 0, \ (\nu > 0)$$

$$u(0,t) = u(1,t) = -1, \ t \geq 0.$$

Due to the gradient flow structure and the boundary condition, the global attractor is $\mathcal{A} = \{-1\}$.
The problem has many metastable "almost stationary" equilibria which live up to a time $t^\star \approx e^{\nu^{-1/2}}$.

Allen-Cahn animation for $\nu = 0.0016$

Thank you !