Winter School
Mathematical Models for Wetting
Analysis and Simulation

Veilbronn, February 13-17, 2012

Quasistatic evolution and Contact angle hysteresis in capillarity

Giovanni Alberti

based on a joint work with Antonio DeSimone
(ARMA 202 (2011), pp. 295-348)

Aim of these lectures:

Introduce a model used to explain contact angle hysteresis in capillarity

Prove some existence result related to this model

The first two lectures will be actually devoted to background material.

Proofs will be sometimes omitted or replaced by formal arguments, and sometimes sketched in more details.

Plan

1. Introduction to quasistatic evolution
   a.k.a. rate-independent evolutionary systems
   Reference: Mielke's lecture notes

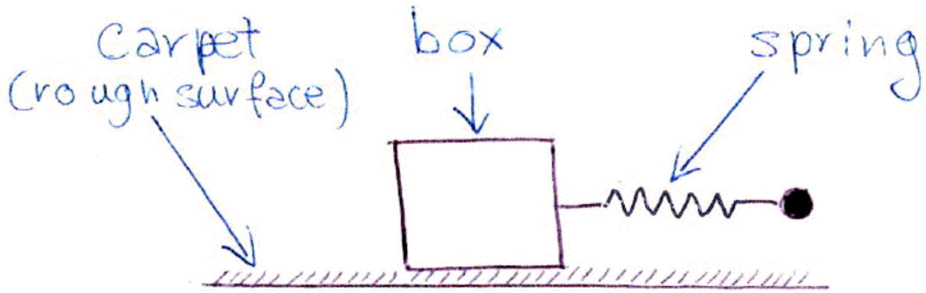
2. The classical model of capillarity

3. Quasistatic evolution of drops and contact angle hysteresis
   Reference: Sections 1 & 2 of my paper with De Simone

4. Rigorous existence results
   Reference: Section 3 of my paper plus Evans-Gariepy book for the theory of finite perimeter sets.

1. Introduction to quasistatic evolution

1.1. Basic example



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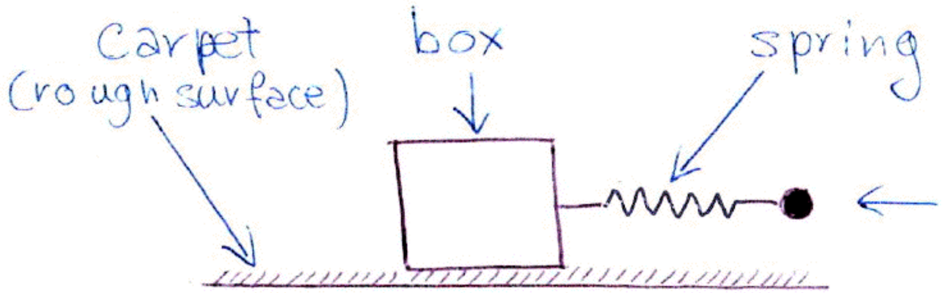
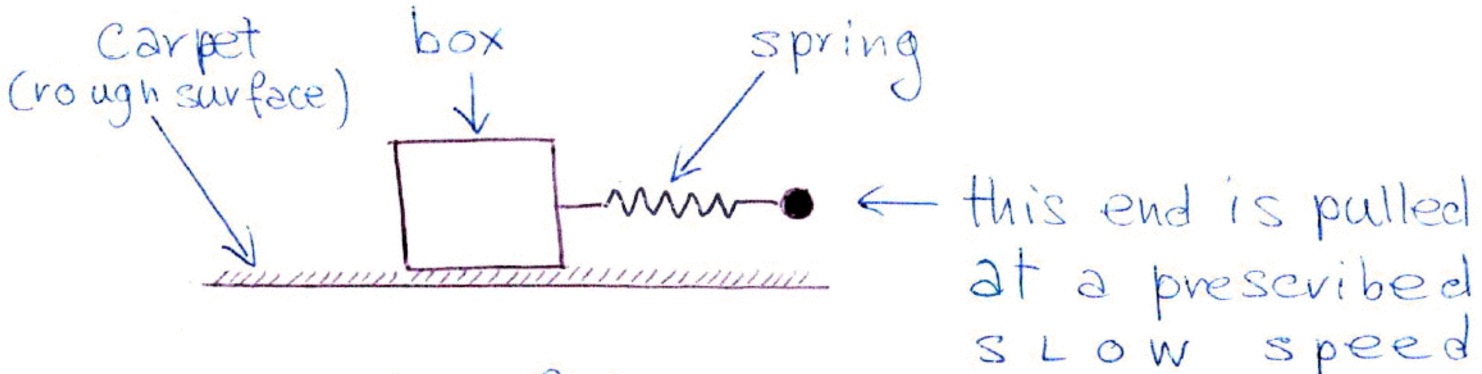


this end is pulled at a prescribed slow speed

1. Introduction to quasistatic evolution

1.1. Basic example



$x = x(t)$ center of the box

Forces acting on the box:

f_e: due to the spring,

f_a: dry friction, due to the carpet.

Here $x \in \mathbb{R}$ or $\mathbb{R}^2$, but in what follow we can think $x \in \mathbb{R}^d$, representing a point mass.

More generally, we assume that the mass is subject to a force f_e which depends on <u>time</u> and <u>position</u> and is conservative.

That is,

$$f_e = -\partial_x \underset{\substack{\uparrow \\ \text{potential energy}}}{\mathcal{E}}(t,x)$$

What about f_a? The simplest assumption is

- $f_a = -k\frac{v}{|v|}$ if $v \neq 0$,

- $f_a = -f_e$ and $|f_a| \leq k$ if $v = 0$.

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unit ball

That is, $-f_a \in A(v)$ where $A(v) := \begin{cases} kB & \text{if } v = 0 \\ \left\{ k \frac{v}{|v|} \right\} & \text{if } v \neq 0 \end{cases}$

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Note that $A(v) = \underline{\partial R(v)}$ where $R(v) := k|v|$

Subdifferential of the
Dissipation Rate R at v

The equation of dynamics is then

$$\underbrace{m}_{\text{mass}} \ddot{x} = f_a + f_e$$

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$$m\ddot{x} = f_a + f_e$$

mass

the assumption of quasistatic evolution is that $m\ddot{x}$ can be neglected (!)

$$0 = f_a + f_e \qquad (1)$$

(this is a balance equation)

We are then considering some limit regime (obtained by sending m to 0 or considering longer and longer time scales).

And indeed the body moves even if the total force is 0!

<u>NOTE</u> You may not like that $m \to 0$ without f_a vanishing, but this is easily fixed....

1.2. Differential formulation
(of solution of quasi-static evolution)

In view of previous remarks we can rewrite the balance eq. $0 = f_e + f_a$ as

$$0 \in \underset{\substack{\| \\ -f_e}}{\partial_x \mathcal{E}(t,x)} + \underset{\substack{\cup\!\!\!\shortmid \\ -f_a}}{\partial \mathcal{R}(\dot{x})} . \qquad \text{(DF)}$$

1.3. Energetic formulation

Define the <u>dissipation potential</u>

$$\mathcal{D}(x, x') := R\,|x - x'|$$

Then (DF) is equivalent to the following conditions:

Stability: $\forall t$, $x(t)$ is a critical point of

$$x \longmapsto \mathcal{E}(t, x) + \mathcal{D}(x, x(t)) \qquad \text{(St)}$$

Energy-Dissipation balance: $\forall\, t_0 < t_1$

$$\mathcal{E}(t_1, x(t_1)) - \mathcal{E}(t_0, x(t_0)) = \int_{t_0}^{t_1} \partial_t \mathcal{E}(t, x(t))\,dt - \int_{t_0}^{t_1} R(\dot{x}(t))\,dt \qquad \text{(EDb)}$$

The reason (EDb) is called Energy-Dissipation balance is

$$\int_{t_0}^{t_1} \partial_t \mathcal{E}(t, x(t))\,dt = \text{work of external forces}$$

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Indeed the work done by f_a in $[t_0, t_1]$ is

$$-\int_{t_0}^{t_1} f_a\,dx = \int_{t_0}^{t_1} \underbrace{\partial\mathcal{R}(\dot{x})\cdot\dot{x}}_{= k\frac{\dot{x}}{|\dot{x}|}\cdot\dot{x}}\,dt = \int_{t_0}^{t_1} \underbrace{\mathcal{R}(\dot{x})}_{= k|\dot{x}|}\,dt$$

$$k\frac{\dot{x}}{|\dot{x}|}\cdot\dot{x} = k\,|\dot{x}|$$

1.4. "Equivalence" of differential and energetic formulation

(St) + (EDb) $\Rightarrow$ (DF)

Assume everything as smooth as needed!

If x satisfies (St) then

$$0 \in \partial_x \mathcal{E}(t, x(t)) + \underbrace{\partial_{x'} \mathcal{D}(x(t), \dot{x}(t))}_{= \kappa \bar{B}}$$

that is

$$|-\partial_x \mathcal{E}(t, x(t))| \leq \kappa \qquad (2)$$

Take (EDb) with t insted of t_1 and differentiate w.r.t. t:

$$\frac{d}{dt}\Big(\mathcal{E}(t,x(t))\Big) = \partial_t \mathcal{E}(t,x(t)) - \mathcal{R}(\dot{x}(t))$$

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$$\parallel$$

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$$-\partial_x \mathcal{E}(t,x(t)) \cdot \dot{x}(t) = K\,|\dot{x}(t)| \qquad (3)$$

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Writing $\omega := -\partial_x \mathcal{E}(t, x(t))$, (2) and (3) become

$$|\omega| \leq k \quad \text{and} \quad w \cdot \dot{x}(t) = k\,|\dot{x}(t)|$$

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$$|\omega| \le k \quad \text{and} \quad w \cdot \dot{x}(t) = k\,|\dot{x}(t)|$$

hence $w = k\dfrac{\dot{x}(t)}{|\dot{x}(t)|} \iff -\partial_x \mathcal{E}(t,x) = \mathcal{R}(\dot{x}) \iff$ (DF)

(DF) $\Longrightarrow$ (St) + (EDb)

Indeed

$$\underbrace{0 \in \partial_x \mathcal{E}(t,x) + \partial R(\dot{x})}_{\text{(DF)}} \Longrightarrow \underbrace{0 \in \partial_x \mathcal{E}(t,x) + \partial_{x'} \mathcal{D}(x,x)}_{\text{(St)}}$$

because $\partial R(v) = \left\{ k \frac{v}{|v|} \right\} \subset kB = \partial_{x'} \mathcal{D}(x,x) \quad \forall v, x.$

Moreover

$$\mathcal{E}(t_1, x(t_1)) - \mathcal{E}(t_0, x(t_0)) = \int_{t_0}^{t_1} \frac{d}{dt}\left(\mathcal{E}(t, x(t))\right) dt$$

$$= \int_{t_0}^{t_1} \partial_t \mathcal{E}(t, x(t))\, dt + \int_{t_0}^{t_1} \partial_x \mathcal{E}(t, x(t)) \cdot \dot{x}(t)\, dt$$

because of (DF) $\longrightarrow$ $\parallel$

$$-\int_{t_0}^{t_1} \partial \mathcal{R}(\dot{x}(t)) \cdot \dot{x}(t)\, dt$$

$$\parallel$$

$$-\int_{t_0}^{t_1} k \frac{\dot{x}}{|\dot{x}|} \cdot \dot{x}\, dt$$

$$\parallel$$

$$-\int_{t_0}^{t_1} k |\dot{x}|\, dt$$

$$\parallel$$

$$-\int_{t_0}^{t_1} \mathcal{R}(\dot{x}(t))\, dt$$

1.5. Weak formulation

The problem with the differential formulation (DF) is that requires x to be somewhat smooth. But solutions of our problems are expected to be discontinuous!

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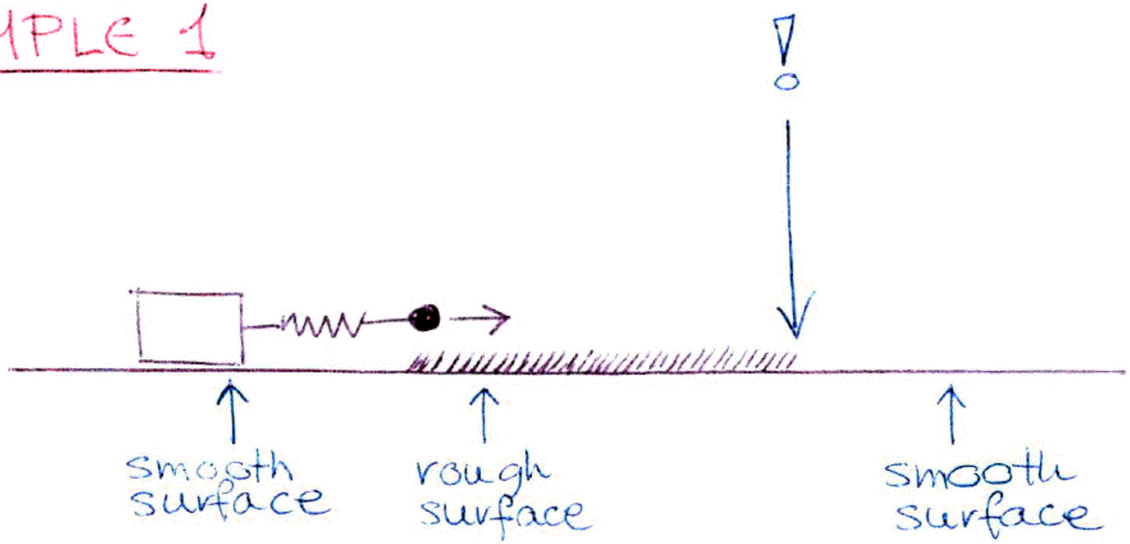
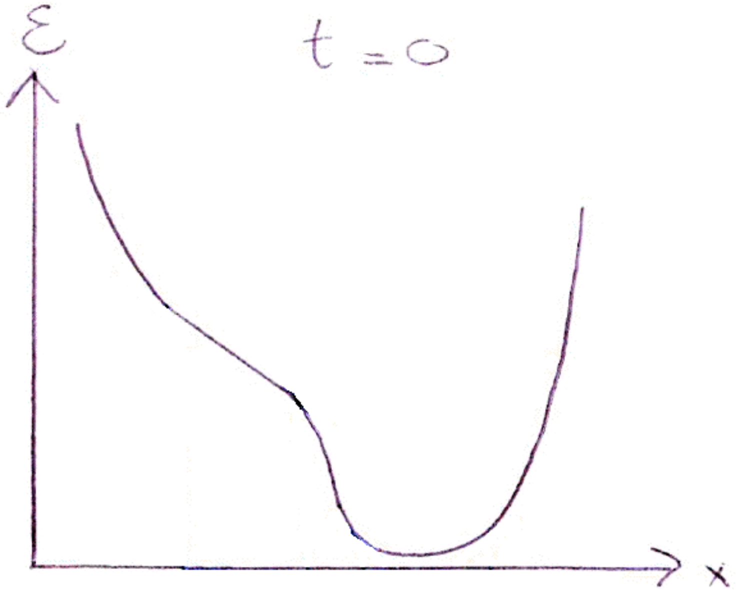


EXAMPLE 2 (assume $k=1$)



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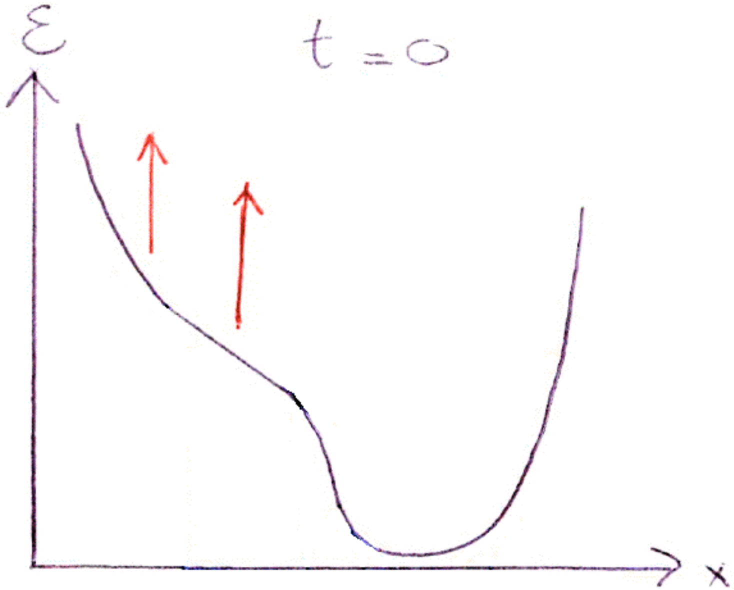

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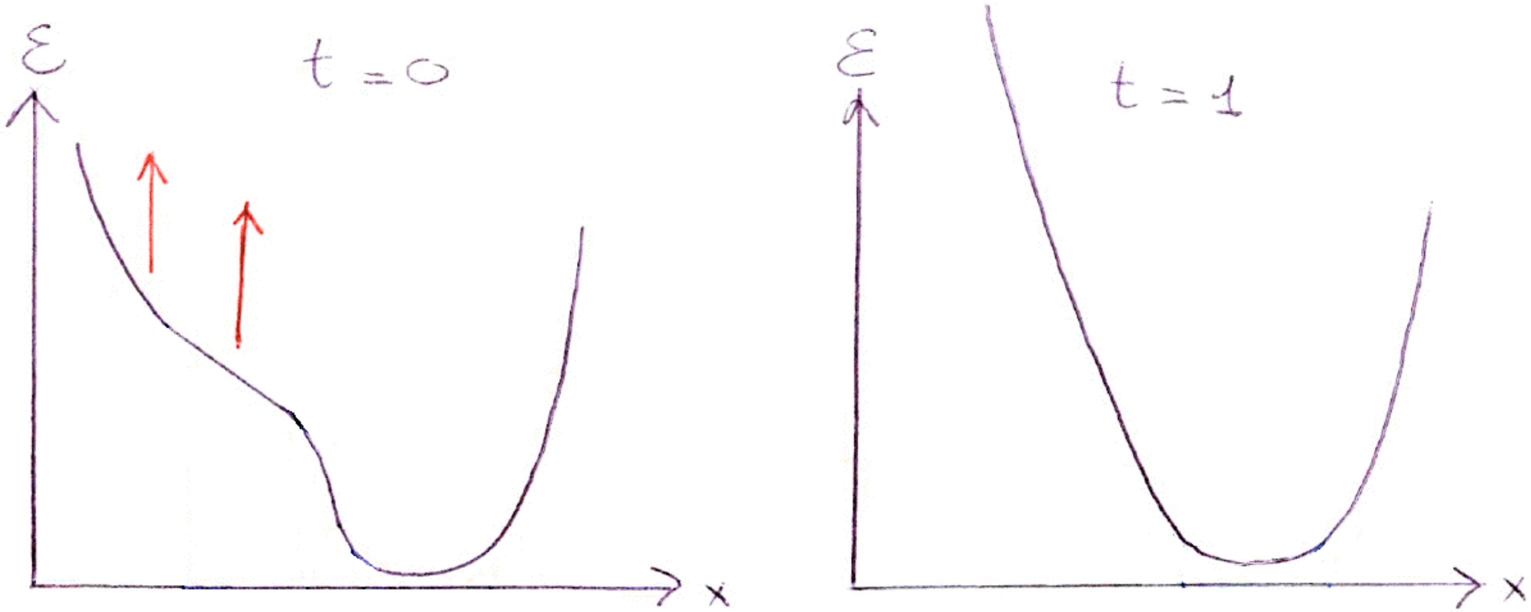

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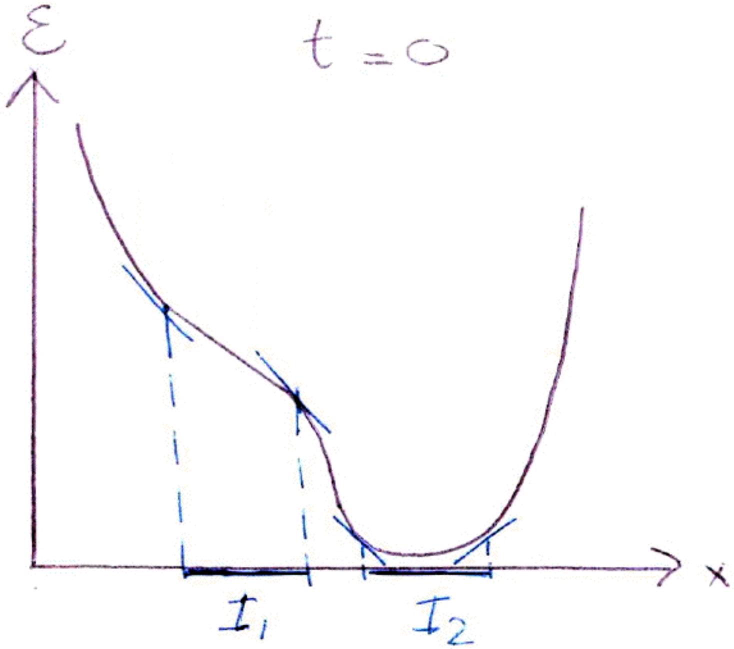
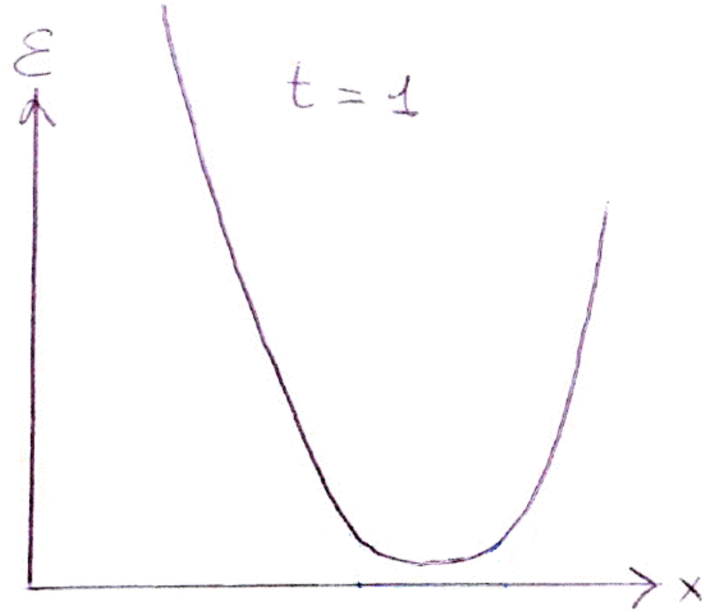


Intervals of stable points



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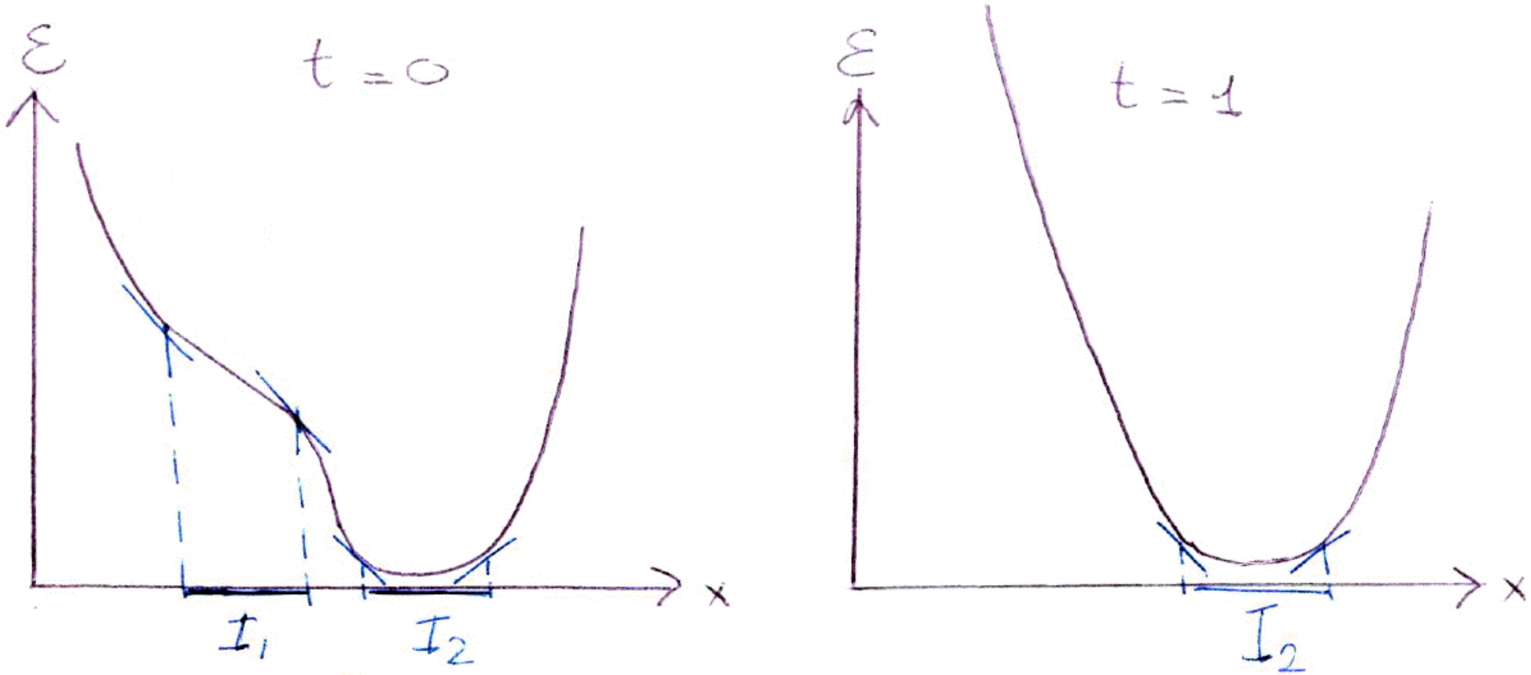

Intervals of stable points

I_1 disappear after some time

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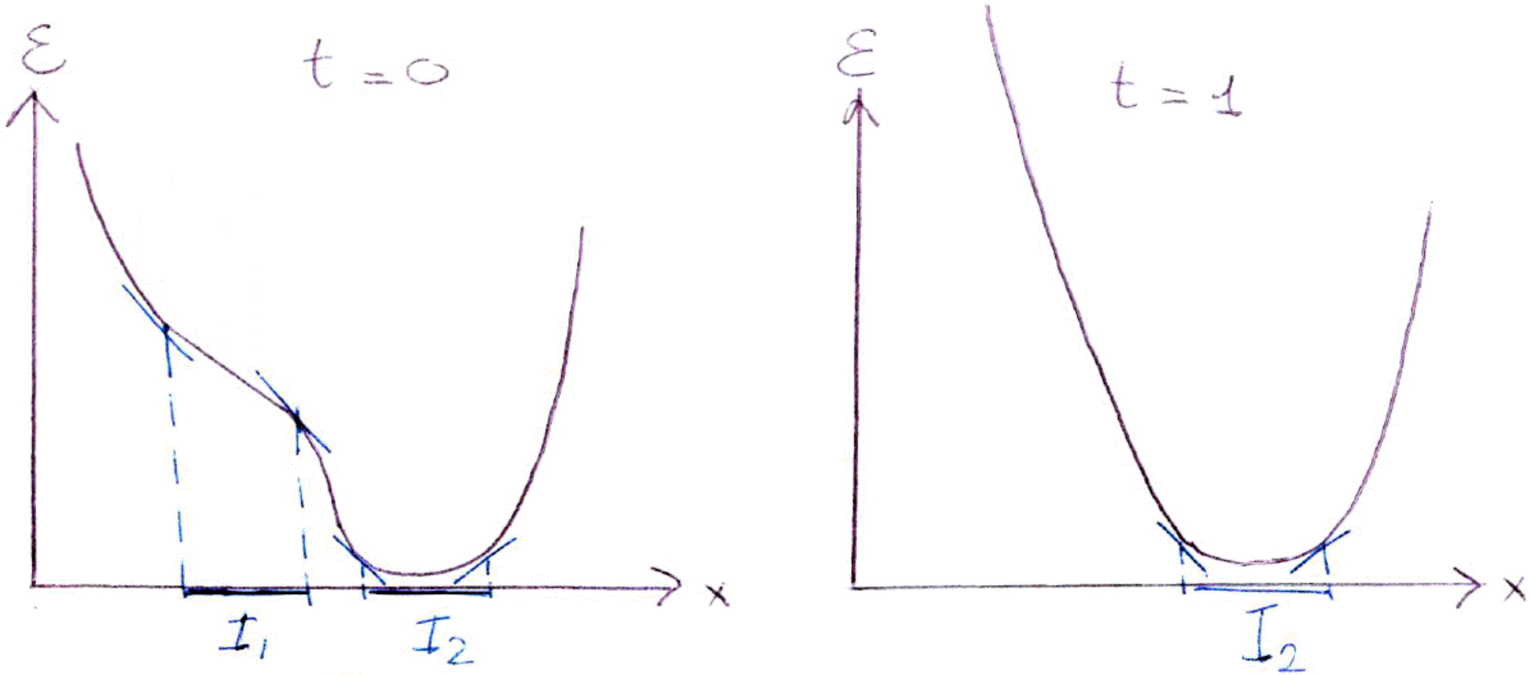

Intervals of stable points

I_1 disappear after some time

If $x(0) \in I_1$, at some moment x will jump to I_2.

We need a weak formulation that allows for discontinuous solutions.

This is obtained by suitably modifying the <u>energetic formulation</u>.

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But

$$\int_{t_0}^{t_1} R(\dot{x}(t))\,dt = k \cdot \int_{t_0}^{t_1} |\dot{x}(t)|\,dt = k \cdot \overbrace{\mathrm{Length}(x, [t_0, t_1])}^{\mathrm{Var}(x, [t_0, t_1])}$$

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$$= K \cdot \sup_{\dots} \sum_i |x(s_i) - x(s_{i-1})|$$

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So we replace (St) and (EDb) by

Global Stability : $\forall t$,

$$\left.\begin{array}{l} x(t) \text{ minimizes } x \longmapsto \mathcal{E}(t,x) + \mathcal{D}(x, x(t)) \\ \left[\, x(t) \in \operatorname{argmin} \left\{ \mathcal{E}(t,x) + \mathcal{D}(x,x(t)) \right\} \right] \end{array}\right\} \text{(GS)}$$

Energy-Dissipation balance : $\forall\, t_0 < t_1$

$$\left.\mathcal{E}(t_1, x(t_1)) - \mathcal{E}(t_0, x(t_0)) = \int_{t_0}^{t_1} \partial_t \mathcal{E}(t, x(t))\, dt - \mathrm{Diss}(x, [t_0, t_1])\right\} \text{(EDb)}$$

1.6. Existence result

Under suitable assumptions on $\mathcal{E}$,

[for <u>example</u>: $\mathcal{E}(t,x) \to +\infty$ as $|x| \to +\infty$ unif. in t
and $|\partial_t \mathcal{E}|$ bounded ...]

For every x_0 which is stable at time $t=0$ exists $x : [0,T] \to \mathbb{R}^d$ with bounded variation (that is, $\mathrm{Var}(x,[0,T]) < +\infty$) s.t.

- $x(0) = x_0$;
- $x(t)$ is globally stable $\forall t \in [0,T]$;
- x satisfies the Energy-Dissipation balance.

1.7. Proof by time discretization

<u>Euristic</u> Consider the equation (DF):

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replace $\dot{x}(t)$ with $\frac{x(t)-x(t-\delta)}{\delta}$, and use that $\partial \mathcal{R}$ is 0-homogeneous

$$0 \in \partial_x \mathcal{E}(t,x) + \partial \mathcal{R}\big(x(t)-x(t-\delta)\big)$$

$$\Updownarrow$$

$x(t)$ is a critical point of $x \mapsto \mathcal{E}(t,x) + \mathcal{D}\big(x, x(t-\delta)\big)$

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$$0 \in \partial_x \mathcal{E}(t,x) + \partial R\big(x(t) - x(t-\delta)\big)$$

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$$x(t) \text{ is a critical point of } x \mapsto \mathcal{E}(t,x) + D\big(x, x(t-\delta)\big)$$

Based on this, we propose the following:

Construction of discretized solutions.

Fix $\delta > 0$.

Let $x^\delta(0) := x_0$.

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For every $t \in [0,T]$ let $t_\delta := \sup\{n\delta \text{ s.t. } n\delta \leq t\}$ and set

$$x^\delta(t) := x^\delta(t_\delta).$$

Convergence to energetic solution

Then, after extracting a suitable subsequence, as $\delta \to 0$, $x^\delta(t)$ converge to some $x(t)$ for every t, and $x(t)$ is an energetic solution with initial condition x_0.

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[These bounds will be proved at the very end.]

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Plus Helly's theorem

Let (x^δ) be a sequence of maps from $[0,T]$ to $\mathbb{R}^d$ such that (i) and (ii) hold.

Then, possibly passing to a subsequence, $x_\delta(t)$ converge to some $x(t)$ for every $t \in [0,T]$.

Moreover $Var(x, [0,T]) \leq \liminf_{\delta \to 0} Var(x^\delta, [0,T])$

Second Step (Proof of global stability)

$\forall t, \ \forall x \in \mathbb{R}^d$

$$\mathcal{E}(t_\delta, x^\delta(t)) + \mathcal{D}(x^\delta(t), x^\delta(t_\delta - \delta))$$
$$\leq \mathcal{E}(t_\delta, x) + \mathcal{D}(x, x^\delta(t_\delta - \delta))$$

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and passing to the limit as $\delta \to 0$

$$\mathcal{E}(t, x(t)) + \mathcal{D}(x(t), y) \quad \text{accumulation point of } x^\delta(t_\delta - \delta)$$
$$\leq \mathcal{E}(t, x) + \mathcal{D}(x, y)$$

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accumulation point of $x^\delta(t_\delta - \delta)$

$$\leq \mathcal{E}(t, x) + \mathcal{D}(x, y)$$

and by the triangle inequality

$$\mathcal{E}(t, x(t)) \leq \mathcal{E}(t, x) + \mathcal{D}(x, x(t)) .$$

Third Step (proof of $\geq$ in (EDb)).

This inequality follows from global stability.

Fix $T_0 < T_1$.

Choose t_i s.t. $T_0 = t_0 < t_1 < \cdots < t_n = T_1$.

Let $x_i := x(t_i)$. Then

$$\mathcal{E}(t_i, x_i) \leq \mathcal{E}(t_i, x_{i+1}) + \mathcal{D}(x_i, x_{i+1})$$

$$\Downarrow$$

$$\mathcal{E}(t_i, x_{i+1}) - \mathcal{E}(t_i, x_i) \geq -\mathcal{D}(x_i, x_{i+1})$$

$$\Downarrow$$

$$\mathcal{E}(t_{i+1}, x_{i+1}) - \mathcal{E}(t_i, x_i) \geq \int_{t_i}^{t_{i+1}} \partial_t \mathcal{E}(t, x_{i+1})\,dt - \mathcal{D}(x_{i+1}, x_i)$$

And summing over all i we get

$$\mathcal{E}(T_1, x(T_1)) - \mathcal{E}(T_0, x(T_0)) \geqslant$$

$$\geqslant \int_{T_0}^{T_1} \partial_t \mathcal{E}(t, \tilde{x}(t))\, dt - \sum_i \mathcal{D}(x_i, x_{i+1})$$

$$\geqslant \int_{T_0}^{T_1} \partial_t \mathcal{E}(t, \tilde{x}(t))\, dt - \mathrm{Diss}(x, [T_0, T_1])$$

And summing over all i we get

$$\mathcal{E}(T_1, x(T_1)) - \mathcal{E}(T_0, x(T_0)) \geq$$

$$\geq \int_{T_0}^{T_1} \partial_t \mathcal{E}(t, \tilde{x}(t))\, dt - \sum_i \mathcal{D}(x_i, x_{i+1})$$

$$\geq \underbrace{\int_{T_0}^{T_1} \partial_t \mathcal{E}(t, \tilde{x}(t))\, dt}_{} - \mathrm{Diss}(x, [T_0, T_1])$$

this can be taken close to

$$\int_{t_0}^{T_1} \partial_t \mathcal{E}(t, x(t))\, dt$$

by suitable choice of t_i....

Fourth Step (Proof of $\leq$ in (EDb)).

Set $t_n := n\delta$, $x^\delta_n := x^\delta(t_n)$.

By definition of x^δ_n

$$\mathcal{E}(t_n, x^\delta_n) + \mathcal{D}(x^\delta_n, x^\delta_{n-1}) \leq \mathcal{E}(t_n, x^\delta_{n-1})$$

$$\Downarrow$$

$$\mathcal{E}(t_n, x^\delta_n) - \mathcal{E}(t_n, x^\delta_{n-1}) \leq -\mathcal{D}(x^\delta_n, x^\delta_{n-1})$$

$$\Downarrow$$

$$\mathcal{E}(t_n, x^\delta_n) - \mathcal{E}(t_{n-1}, x^\delta_{n-1})$$

$$\leq \int_{t_{n-1}}^{t_n} \partial_t \mathcal{E}(t, \underset{\substack{\parallel \\ x^\delta(t)}}{x^\delta_{n-1}})\, dt - \mathcal{D}(x^\delta_n, x^\delta_{n-1})$$

summing over all n

$$\mathcal{E}(T, x^\delta(T)) - \mathcal{E}(0, x^\delta(0))$$

$$\leq \int_0^T \partial_t \mathcal{E}(t, x^\delta(t))\,dt - \sum_n \mathcal{D}(x_n^\delta, x_{n-1}^\delta)$$

$$= \int_0^T \partial_t \mathcal{E}(t, x^\delta(t))\,dt - \mathcal{D}iss(x^\delta, [0,T])$$

passing to the limit as $\delta \to 0$

$$\mathcal{E}(T, x(T)) - \mathcal{E}(0, x(0))$$

$$\leq \int_0^T \partial_t \mathcal{E}(t, x(t))\,dt - \mathcal{D}iss(x, [0,T])$$

Final details: bound on energy

We have seen that

$$\mathcal{E}(t_n, x_n^\delta) + \mathcal{D}(x_n^\delta, x_{n-1}^\delta) \le \mathcal{E}(t_n, x_{n-1}^\delta).$$

Hence

$$\begin{aligned}\mathcal{E}(t_n, x_n^\delta) &\le \mathcal{E}(t_n, x_{n-1}^\delta)\\ &= \mathcal{E}(t_{n-1}, x_{n-1}^\delta) + \int_{t_{n-1}}^{t_n} \partial_t \mathcal{E}(t, x_{n-1}^\delta)\,dt\\ &\le \mathcal{E}(t_{n-1}, x_{n-1}^\delta) + m\,(t_n - t_{n-1})\end{aligned}$$

$\|\partial_t \mathcal{E}\|_\infty$

Hence, by iteration

$$\mathcal{E}(t_n, x_n^\delta) \le \mathcal{E}(0, x_0) + m t_n$$

and in fact also a bit more

$$\mathcal{E}(t, x^\delta(t)) \le \mathcal{E}(0, x_0) + mt.$$

Final details: bound on $|x^\delta(t)|$

Since $\mathcal{E}(t,x) \to +\infty$ uniformly in t as $|x| \to \infty$, the bound on energy proved before implies that $|x^\delta(t)|$ is uniformly bounded in t and δ.

(This was needed in the proof of compactness.)

Final details: bound on variations

At some moment we proved that

$$\mathcal{E}(T, x^\delta(T)) - \mathcal{E}(0, x^\delta(0))$$
$$\leq \int_0^T \partial_t \mathcal{E}(t, x^\delta(t))\, dt - \mathcal{D}iss\,(x^\delta, [0,T]).$$

Hence

$$\mu \operatorname{Var}(x^\delta, [0,T]) = \mathcal{D}iss\,(x^\delta, [0,T])$$
$$\leq \int_0^T \partial_t \mathcal{E} \cdots + \mathcal{E}(0, x^\delta(0)) - \mathcal{E}(T, x^\delta(T))$$
$$\leq mT + \mathcal{E}(0, x_0)$$

$\| \partial_t \mathcal{E} \|_\infty$

So $\operatorname{Var}(x^\delta, [0,T])$ are uniformly bounded in δ.

(This was needed in the proof of compactness)