

EQUILIBRIUM CONFIGURATIONS FOR EPITAXIALLY STRAINED CRYSTALLINE FILMS AND MATERIAL VOIDS

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work in collaboration with M. Friedrich (University of Münster)

CMAF, École Polytechnique

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CNA Seminar

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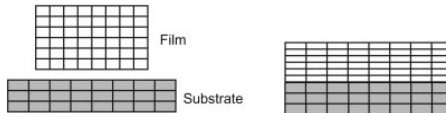
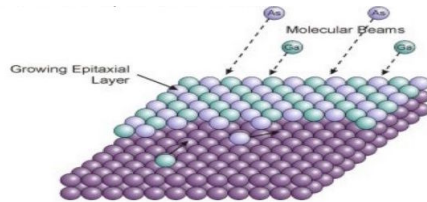
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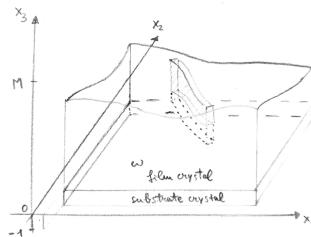
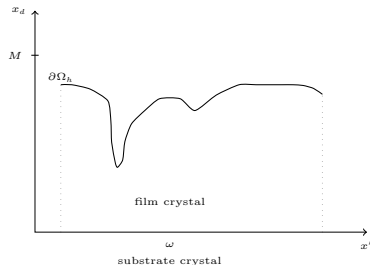
Here: minimization and approximation for static energies in any space dimension, in the context of linearized elasticity. Available results either in 2d for 1d 'discontinuity curves' with a bounded number of connected components or in simplified settings for elastic energy.

Epitaxially strained crystalline films



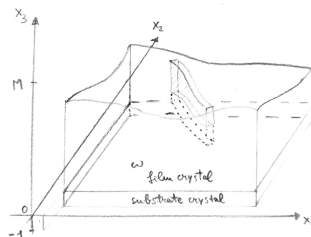
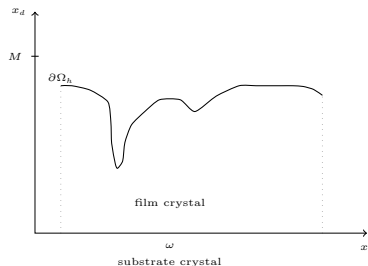
Etero-epitaxy: different lattice parameters between substrate and film crystals

Epitaxially strained crystalline films



Competition between elastic bulk energy and surface tension energy

Epitaxially strained crystalline films



Competition between elastic bulk energy and surface tension energy

Bonnetier-Chambolle '02:

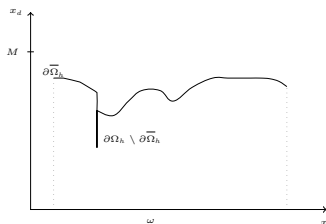
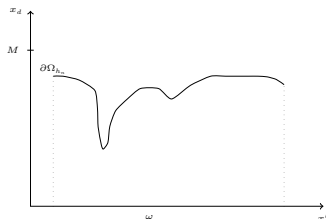
$$G(u, h) = \int_{\Omega_h^+} \mathbb{C} e(u) : e(u) dx + \int_{\omega} \sqrt{1 + |\nabla h(x_1, x_2)|^2} d(x_1, x_2).$$

where $e(u) = \frac{1}{2}(\nabla u + (\nabla u)^T)$ and

$$h \in C^1(\omega; [0, M]), \|h\|_1 = m, \omega \subset \mathbb{R}^2, \Omega_h^+ := \{x \in \omega \times \mathbb{R} : 0 < x_3 < h(x_1, x_2)\},$$

$$u|_{\Omega_h^+} \in H^1(\Omega_h^+), u = 0 \text{ in } (\omega \times (0, M+1)) \setminus \Omega_h^+, u = u_0 \text{ in } \omega \times (0, 1)$$

Equilibrium configurations for epitaxially stained crystalline films in 2D



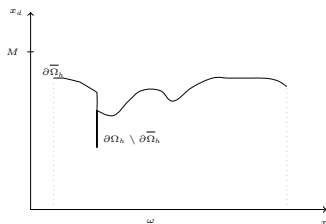
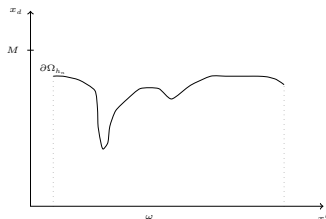
In **2D** (so x_1 instead of (x_1, x_2) in G): for $\Omega = \omega \times (-1, M + 1)$

$$\Omega \setminus \Omega_{h_n} \xrightarrow{\mathcal{H}} \Omega \setminus \Omega_h \quad \text{for some } h: \omega \rightarrow \mathbb{R}^+ \text{ lsc}$$

$$\partial\Omega_{h_n} \xrightarrow{\mathcal{H}} K \supset \partial\Omega_h = \partial\bar{\Omega}_h \cup (\partial\Omega_h \setminus \partial\bar{\Omega}_h)$$

Gołab Theorem (since $\partial\Omega_{h_n}$ **connected in 1d**): $\mathcal{H}^1(K) \leq \liminf_n \mathcal{H}^1(\partial\Omega_{h_n})$

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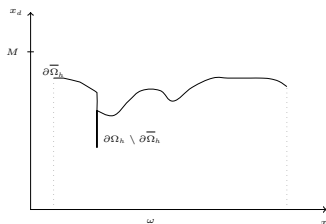
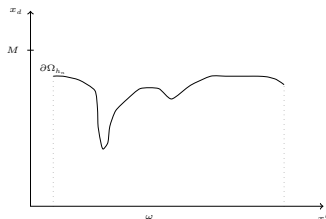
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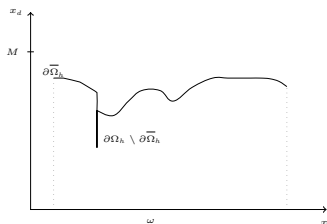
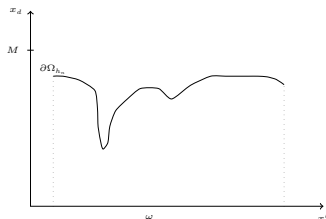
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Korn Inequality in any $A \subset \Omega_h$ Lipschitz $\implies u_n \rightharpoonup u$ in $H_{\text{loc}}^1(\Omega_h; \mathbb{R}^2)$ and

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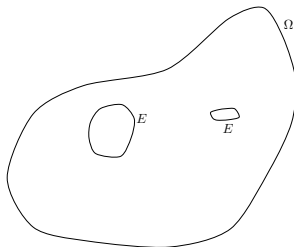
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Therefore **COMPACTNESS** for (u_n, h_n) with $G(u_n, h_n) \leq M$ and

$$\tilde{G}(u, h) := \int_{\Omega_h^+} \mathbb{C} e(u) : e(u) \, dx + \mathcal{H}^1(\partial\bar{\Omega}_h) + 2\mathcal{H}^1(\partial\Omega_h \setminus \partial\bar{\Omega}_h) \leq \liminf_n G(u_n, h_n)$$



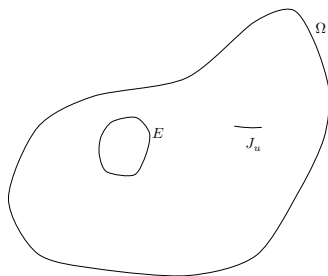
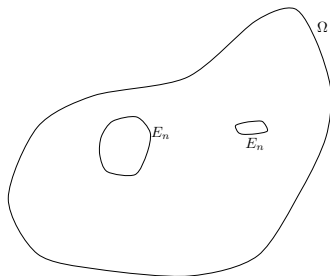
Braides-Chambolle-Solci '07:

$$F(u, E) = \int_{\Omega \setminus E} \mathbb{C} e(u) : e(u) \, dx + \int_{\Omega \cap \partial E} \varphi(\nu_E) \, d\mathcal{H}^{d-1}.$$

where φ is a norm and represents a possibly anisotropic density.

Minimization under Dirichlet b.c. on $\partial_D \Omega \subset \partial \Omega$ and a volume constraint on E .

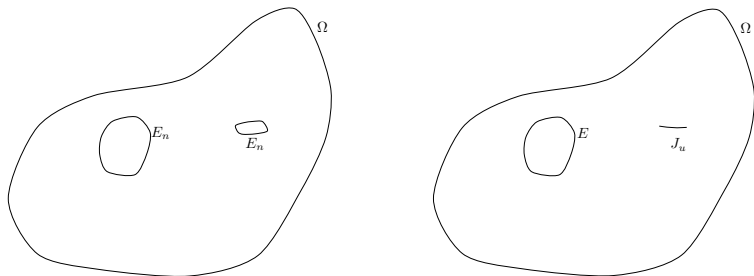
Equilibrium configurations for material voids



In 2D: assuming an **equibounded number of connected components** for voids, one may still use **Gołab Theorem** to say

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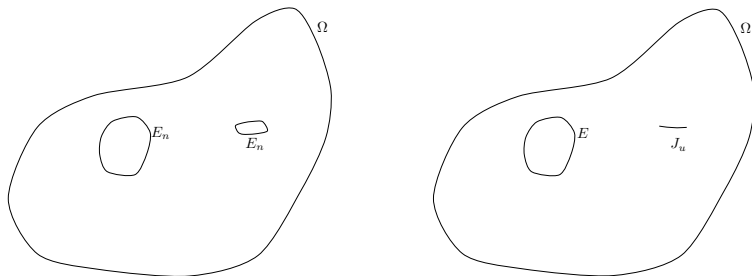


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The situation may be reproduced for connected surfaces (like graphs) in **3D**

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- Ambrosio, Novaga, Paolini / Fonseca, Pratelli, Zwicknagl / Dal Maso, Fonseca, Leoni / Caroccia, Cristoferi: **related energies**

We look for the biggest lower semicontinuous functionals \overline{F} and \overline{G} with $\overline{F} \leq F$ and $\overline{G} \leq G$, wrt convergence in measure for \mathbf{u} and in L^1 for χ_E or h .

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To prove that

- if $u_n \rightarrow u$ a.e. in Ω , $\chi_{E_n} \rightarrow \chi_E$ in $L^1(\Omega)$ then

$$\overline{F}(u, E) \leq \liminf_{n \rightarrow \infty} F(u_n, E_n);$$

- for all (u, E) with $\overline{F}(u, E) < +\infty$, there are $(u_n, E_n) \rightarrow (u, E)$ with

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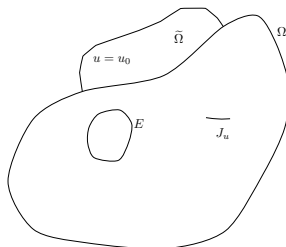
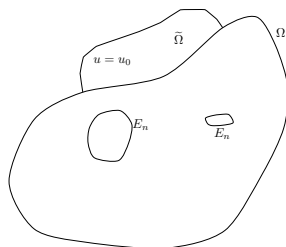
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Bon-Cha '02: $d = 2$ for G ; Cha-Sol '07: any d but ∇u in place of $e(u)$ for G ;
Bra-Cha-Sol '07: any d but ∇u in place of $e(u)$ for F .

Form of \overline{F} and minimization



Theorem (C.-Friedrich)

$$F_{\text{Dir}}(\mathbf{u}, \mathbf{E}) = \int_{\Omega \setminus \mathbf{E}} \mathbb{C} e(\mathbf{u}) : e(\mathbf{u}) \, dx + \int_{(\Omega \cup \partial_D \Omega) \cap \partial \mathbf{E}} \varphi(\nu_{\mathbf{E}}) \, d\mathcal{H}^{d-1}$$

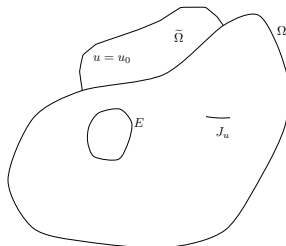
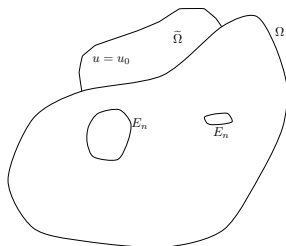
if \mathbf{E} Lipschitz, $|\mathbf{E}| = m \in (0, |\Omega|)$, $\mathbf{u}|_{\Omega \setminus \overline{\mathbf{E}}} \in H^1(\Omega \setminus \mathbf{E}; \mathbb{R}^d)$, $\mathbf{u}|_{\mathbf{E}} = 0$, $\mathbf{u}|_{\tilde{\Omega} \setminus \Omega} = u_0$

relaxes into

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if $|\mathbf{E}| = m$, $\mathcal{H}^{d-1}(\partial^* \mathbf{E}) < +\infty$, $\mathbf{u} = \mathbf{u} \chi_{E_0}$, for $\mathbf{u}' := u_0$ on $\tilde{\Omega} \setminus \Omega$.

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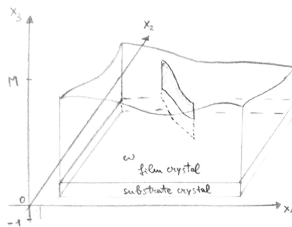
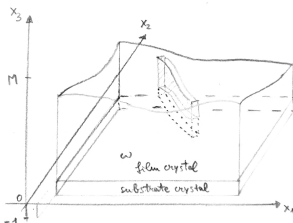
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$$\overline{F}_{\text{Dir}}(\mathbf{u}, \mathbf{E}) = \int_{\Omega \setminus \mathbf{E}} \mathbb{C} e(\mathbf{u}) : e(\mathbf{u}) \, dx + \int_{(\Omega \cup \partial_D \Omega) \cap \partial^* \mathbf{E}} \varphi(\nu_{\mathbf{E}}) \, d\mathcal{H}^{d-1} + \int_{J_{\mathbf{u}'} \cap (\Omega \cup \partial_D \Omega) \setminus \mathbf{E}^1} 2\varphi(\nu_{\mathbf{u}}) \, d\mathcal{H}^{d-1}$$

if $|\mathbf{E}| = m$, $\mathcal{H}^{d-1}(\partial^* \mathbf{E}) < +\infty$, $\mathbf{u} = \mathbf{u} \chi_{E_0}$, for $\mathbf{u}' := u_0$ on $\tilde{\Omega} \setminus \Omega$.

Moreover, $\overline{F}_{\text{Dir}}$ admits minimizers

Form of \overline{G} and compactness



$$\Omega = \omega \times (-1, M+1)$$

Theorem (C.-Friedrich)

$$G(u, h) = \int_{\Omega_h^+} \mathbb{C} e(u) : e(u) dx + \int_{\omega} \sqrt{1 + |\nabla h(x')|^2} dx'$$

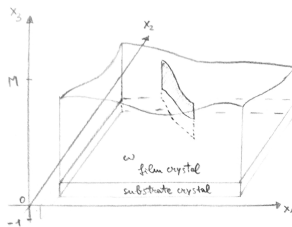
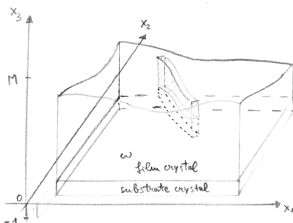
$$h \in C_m^1(\omega; [0, M]), u|_{\Omega_h^+} \in H^1(\Omega_h^+), u=0 \text{ in } (\omega \times \mathbb{R}^+) \setminus \Omega_h^+, u=u_0 \text{ in } \omega \times (0, 1)$$

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$$\overline{G}(u, h) = \int_{\Omega_h^+} \mathbb{C} e(u) : e(u) dx + \mathcal{H}^{d-1}(\partial^* \Omega_h \cap \Omega) + 2\mathcal{H}^{d-1}(J'_u \cap \Omega_h^1)$$

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Moreover, any (u_n, h_n) with $\overline{G}(u_n, h_n) < M$ has a converging subsequence

The functional framework

E set of finite perimeter ($\chi_E \in BV(\Omega)$)

$$E^s = \{x \in \mathbb{R}^d: \lim_{\varrho \rightarrow 0} \frac{|E \cap B_\varrho(x)|}{|B_\varrho(x)|} = s\}$$

$$\partial^* E = \mathbb{R}^d \setminus (E^0 \cup E^1) \text{ essential boundary}$$

$$\overline{F}(u, E), \overline{G}(u, h) \sim \int_{\Omega} \mathbb{C}e(u) : e(u) \, dx + \mathcal{H}^{d-1}(J_u) =: \text{Gr}(u)$$

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- Control of $e(u) \rightsquigarrow$

$$BD(\Omega) := \{u \in L^1(\Omega; \mathbb{R}^d) : Eu \in \mathcal{M}_b(\Omega; \mathbb{M}_{sym}^{d \times d})\} = \{u : \sup_{|\varphi| \leq 1} \int_{\Omega} u \cdot E\varphi < \infty\}$$

$$u \in BD(\Omega) \implies Eu = e(u)\mathcal{L}^d + (u^+ - u^-) \odot \nu_u \mathcal{H}^{d-1} \llcorner J_u + E^c u$$

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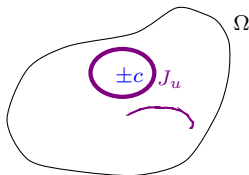
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- But no L^1 control of $u \rightsquigarrow GSBD(\Omega)$ Dal Maso '12

($u \in GSBV$ if truncations in SBV , now they destroy control on Eu)



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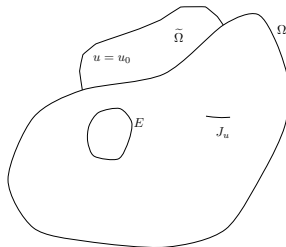
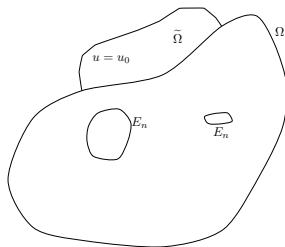
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J_u still $(d-1)$ -countably rectifiable and for \mathcal{L}^d -a.e. x , $e(u)(x)$ s.t.

$$\text{ap lim}_{y \rightarrow x} \frac{(u(y) - u(x) - e(u)(x)(y - x)) \cdot (y - x)}{|y - x|^2} = 0,$$



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Proven similarly to Ambrosio-Tortorelli approximation for Griffith with Dirichlet b.c. in Chambolle-C. '19

- lim inf by slicing argument (separately for bulk and surface part)
- lim sup by an adaptation of density of Chambolle-C. '19 + BraChaSol'07

Density in $GSBD$ (Chambolle-C. '19)

$\forall \mathbf{u}$ t.q. $\text{Gr}_{\text{Dir}}(\mathbf{u}) < \infty \quad \exists \mathbf{u}_k$ t.q. $J_{\mathbf{u}_k}$ of class C^1 , $\mathbf{u}_k \in C^\infty(\Omega \setminus J_{\mathbf{u}_k})$, and

$$\mathbf{u}_k \longrightarrow \mathbf{u} \text{ a.e.}, \quad \text{Gr}_{\text{Dir}}(\mathbf{u}_k) \longrightarrow \text{Gr}_{\text{Dir}}(\mathbf{u})$$

Compactness (Chambolle-C.)

Let $u_n \in GSBD^2(\Omega)$ with

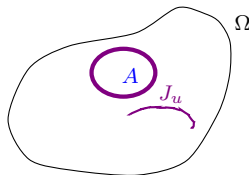
$$\int_{\Omega} |e(u_n)|^2 dx + \mathcal{H}^{d-1}(J_{u_n}) < M.$$

Then, up to a subsequence, for $A := \{x : |u_n(x)| \rightarrow \infty\}$, there is $u \in GSBD^2(\Omega)$, $u = 0$ in A s.t.

$$u_n \rightarrow u \quad \text{a.e. in } \Omega \setminus A,$$

$$e(u_n) \rightharpoonup e(u) \quad \text{in } L^2(\Omega \setminus A; \mathbb{M}_{sym}^{d \times d}),$$

$$\mathcal{H}^{d-1}(J_u \cup \partial^* A) \leq \liminf_{n \rightarrow \infty} \mathcal{H}^{d-1}(J_{u_n}).$$



Much more difficult both in \liminf and in \limsup , due to constraints on the jump set

To prove the verticality we use a variant of the

σ^2 -convergence (Dal Maso-Francfort-Toader '05, Giacomini-Ponsiglione '06)

$\Gamma_n \subset U$, $\sup_n \mathcal{H}^{d-1}(\Gamma_n) < \infty$. Then $\Gamma_n \xrightarrow{\sigma^2} \Gamma$ iff

- (i) $\left((v_n)_n \subset SBV^2(U), J_{v_n} \subset \Gamma_n, v_n \rightarrow v \right) \implies J_v \subset \Gamma$
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We introduce an analogous notion of sets convergence for the “Griffith energy space” $GSBD^2$ in place of SBV^2 , that we call σ_{sym}^2 -convergence.

New technical point: consider also a limit set G_∞ with finite perimeter and $\partial^* G_\infty \subset \Gamma$, inside which we do not control anything

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σ_{sym}^2 -convergence (C.-Friedrich)

$\Gamma_n \subset U$, $\sup_n \mathcal{H}^{d-1}(\Gamma_n) < \infty$, $U \subset U'$, $|U' \setminus U| > 0$. Then $\Gamma_n \xrightarrow{\sigma_{\text{sym}}^2} (\Gamma, G_\infty)$ with

$$\partial^* G_\infty \cap U' \subset \Gamma, \quad \Gamma \cap (G_\infty)^1 = \emptyset \quad \text{iff}$$

- (i) $\left((v_n)_n \subset GSBD^2(U'), J_{v_n} \subset \Gamma_n, v_n = 0 \text{ in } U' \setminus U, v_n \rightarrow v \right) \implies (J_v \setminus \Gamma) \subset (G_\infty)^1$
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Compactness for σ_{sym}^2 -convergence

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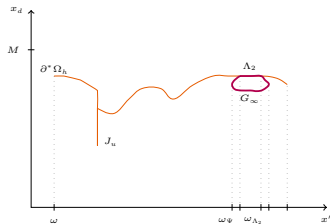
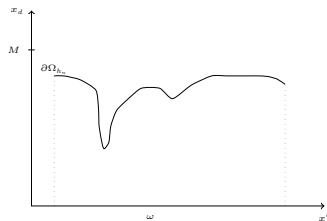
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Compactness (C.-Friedrich)

Every $(\Gamma_n)_n$ with $\sup_n \mathcal{H}^{d-1}(\Gamma_n) < \infty$, σ_{sym}^2 converges, up to a subsequence, to (Γ, G_∞) with

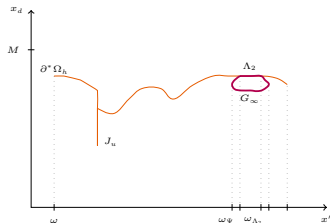
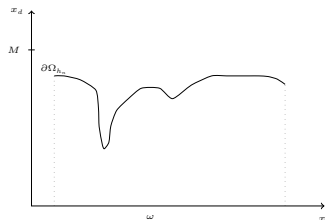
$$\mathcal{H}^{d-1}(\Gamma) \leq \liminf_{n \rightarrow \infty} \mathcal{H}^{d-1}(\Gamma_n).$$

Lower limit and compactness for G



1st step: $\partial\Omega_{h_n} \xrightarrow{\sigma_{\text{sym}}^2} (\Gamma, \emptyset)$

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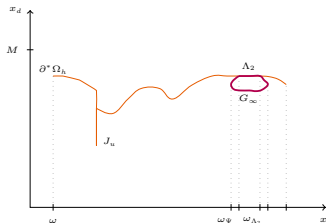
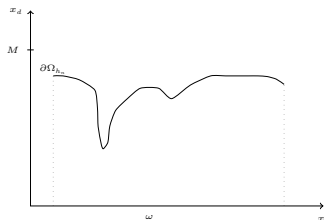


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1 **Area Formula:** $\int_{\omega} \#(\Lambda_y^{e_d}) d\mathcal{H}^{d-1}(y) = \int_{\Lambda} |\nu_{\Lambda} \cdot e_d| d\mathcal{H}^{d-1} =: I_V(\Lambda)$

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- 2 $I_V(\Gamma) = I_V(J_v) \leq \liminf_n I_V(J_{v_n}) \leq \liminf_n I_V(\Gamma_n) = \mathcal{H}^{d-1}(\omega)$
for $(v_n)_n$, v as in (ii) σ_{sym}^2
- 3 $v_n = \psi \chi_{\Omega_{h_n}} \rightarrow \psi \chi_{\Omega_h}$ in (i) $\sigma_{\text{sym}}^2 \implies \Gamma \supset (\partial^* G_{\infty} \cap U') \cup (\partial^* \Omega_h \cap U' \cap (G_{\infty})^0)$
- 4 $I_V(\Gamma) \geq 2\mathcal{H}^{d-1}(\omega_{\Psi}) + \mathcal{H}^{d-1}(\omega) - \mathcal{H}^{d-1}(\omega_{\Lambda_2}) \geq \mathcal{H}^{d-1}(\omega) + \mathcal{H}^{d-1}(\omega_{\psi})$

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3rd step: For $(v_n)_n$, v as in (ii) σ_{sym}^2 , we apply lsc for voids (surface part) to $E_n = \Omega \setminus \Omega_{h_n}$, $E = \Omega \setminus \Omega_h$, $v_n \chi_{\Omega \setminus E_n}$, $v \chi_{\Omega \setminus E}$. Then

$$\mathcal{H}^{d-1}(\partial^* \Omega_h \cap \Omega) + 2\mathcal{H}^{d-1}(\Sigma) \leq \liminf_{n \rightarrow \infty} \mathcal{H}^{d-1}(\partial \Omega_{h_n})$$

2nd step: $\Sigma := \Gamma \cap \Omega_h^1$ is vertical in Ω_h^1 , i.e. $(\Sigma + te_d) \cap \Omega_h^1 \subset \Sigma$

For $(v_n)_n$, v as in (ii) σ_{sym}^2 , also

$$v'_n(x) := v_n(x', x_d - t)\chi_{\Omega_{h_n}}(x) \rightarrow v'(x) := v(x', x_d - t)\chi_{\Omega_h}(x)$$

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Final step: Lsc for volume part from that for voids +

(i) in σ_{sym}^2 for u_n , $u \implies J'_u \cap \Omega_h^1 := (J_u + \mathbb{R}e_d) \cap \Omega_h^1 \subset \Sigma$

Theorem (C.-Friedrich)

$$G(u, h) = \int_{\Omega_h^+} \mathbb{C} e(u) : e(u) \, dx + \int_{\omega} \sqrt{1 + |\nabla h(x')|^2} \, dx'$$

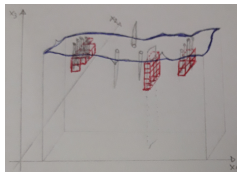
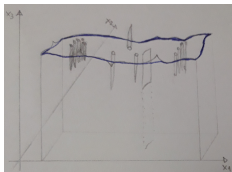
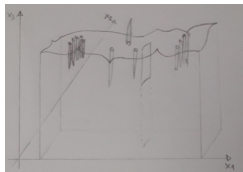
$$h \in C_m^1(\omega; [0, M]), \quad u|_{\Omega_h^+} \in H^1(\Omega_h^+), \quad u=0 \text{ in } (\omega \times \mathbb{R}^+) \setminus \Omega_h^+, \quad u=u_0 \text{ in } \omega \times (0, 1)$$

relaxes into

$$\overline{G}(u, h) = \int_{\Omega_h^+} \mathbb{C} e(u) : e(u) \, dx + \mathcal{H}^{d-1}(\partial^* \Omega_h \cap \Omega) + 2\mathcal{H}^{d-1}(J'_u \cap \Omega_h^1)$$

$$\text{if } u = u \chi_{\Omega_h}, \quad u = u_0 \text{ in } \omega \times (-1, 0), \quad h \in BV_m(\omega; [0, M]), \quad J'_u := J_u + \mathbb{R}^+ e_d,$$

Upper limit for G

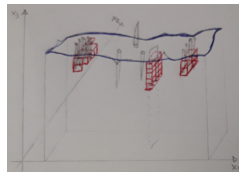
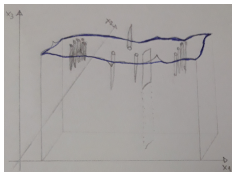
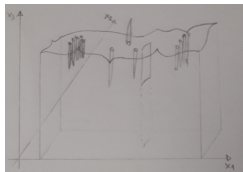


Step 1: smooth function g approximating h (in L^1 -norm) \rightarrow possible set with small diffuse measure in Ω_g

For **Step 2** clean up the jump set 'remaining below': careful use of 'quantitative' Poincaré-Korn inequality

$$\int_{Q_r} |u - a_r|^2 dx \leq C r \int_{Q_r} |e(u)|^2 dx,$$

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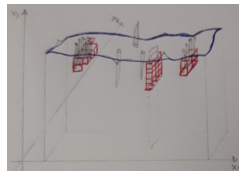
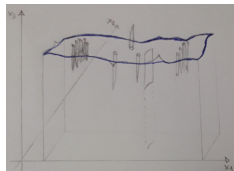
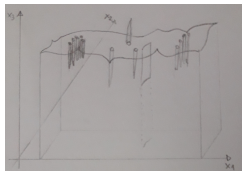


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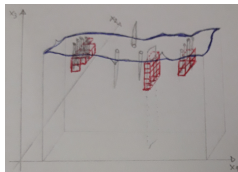
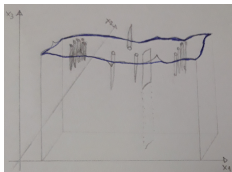
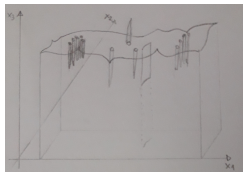
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Put 0 in cubes with 'large' jump set and with 'small' jump set and 'small' $|\Omega_h^1|$ for verticality

Generalized compactness (Chambolle-C.'20 Preprint)

Let $u_n \in GSBD^2(\Omega)$ with $\int_{\Omega} |e(u_n)|^2 dx + \mathcal{H}^{d-1}(J_{u_n}) < M$. Then there are $\mathcal{P} = (P_j)_j$ a Caccioppoli partition, $(a_n)_n$ with $a_n = \sum_{j \in \mathbb{N}} a_n^j \chi_{P_j}$ and

$$|a_n^j(x) - a_n^i(x)| \rightarrow +\infty \quad \text{for -a.e. } x \in \Omega, \text{ for all } i \neq j,$$

pw infinitesimal rigid motions, $u \in GSBD^2(\Omega)$ s.t. (up to a subsequence)

$$u_n - a_n \rightarrow u \quad \text{a.e. in } \Omega,$$

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- This permits to deal with non-homogeneous bulk energies.
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- First application of σ^2 -convergence: existence of quasi-static evolution for non convex elastic energies in brittle fracture
- Regularity issues in 3d: even prove that the graph of equilibria is closed is hard

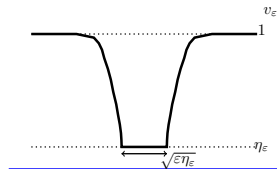
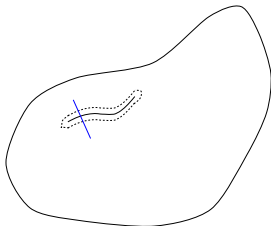
THANK YOU!

$$D_\varepsilon(\mathbf{u}, v) := \int_{\Omega} \left(v \mathbb{C} e(\mathbf{u}) : e(\mathbf{u}) + \frac{(1-v)^2}{4\varepsilon} + \varepsilon |\nabla v|^2 \right) dx \quad \text{in } H_{u_0}^1(\Omega; \mathbb{R}^d) \times V_{\eta_\varepsilon}^1$$

with $V_{\eta_\varepsilon}^1 = \{\eta_\varepsilon \leq v \leq 1, \text{tr } v = 1 \text{ on } \partial_D \Omega\}$, $H_{u_0}^1 = \{\mathbf{u} \in H^1 : \text{tr } \mathbf{u} = \text{tr } u_0 \text{ on } \partial_D \Omega\}$,

Γ -converge as $\varepsilon \rightarrow 0$ (with $\frac{\eta_\varepsilon}{\varepsilon} \rightarrow 0$) to

$$D(\mathbf{u}, 1) := \int_{\Omega} \mathbb{C} e(\mathbf{u}) : e(\mathbf{u}) dx + \mathcal{H}^{d-1}(J_{\mathbf{u}} \cup (\partial_D \Omega \cap \{\text{tr } \mathbf{u} \neq \text{tr } u_0\}))$$



Phase-field approximation for \overline{G}

$$W(0) = W(1) = 0, W > 0 \text{ in } (0, 1), \frac{1}{c_W} = \int_0^1 \sqrt{2W(s)} ds, \Omega = \omega \times (-1, M+1)$$

$$G_\varepsilon(u, v) := \int_\Omega \left((v^2 + \eta_\varepsilon) f(e(u)) + c_W \left(\frac{W(v)}{\varepsilon} + \frac{\varepsilon}{2} |\nabla v|^2 \right) \right) dx$$

$$u \in H^1(\Omega; \mathbb{R}^d), \quad u = u_0 \text{ in } \omega \times (-1, 0),$$

$$v \in H^1(\Omega; [0, 1]), \quad v = 1 \text{ in } \omega \times (-1, 0), \quad v = 0 \text{ in } \omega \times (M, M+1) \quad \partial_d v \leq 0 \text{ a.e. in } \Omega,$$

“ Γ -converge” (in the sense that $v_\varepsilon \rightarrow \chi_{\Omega_h}$) as $\varepsilon \rightarrow 0$ to

$$\overline{G}(u, h) = \int_{\Omega_h^+} \mathbb{C} e(u) : e(u) dx + \mathcal{H}^{d-1}(\partial^* \Omega_h \cap \Omega) + 2\mathcal{H}^{d-1}(J'_u \cap \Omega_h^1)$$

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