Variational Methods in Materials Science and Image Processing

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Challenges: Minimize energies involving . . .

- bulk and interfacial energies
- vector valued fields
- higher order derivatives
- discontinuities of underlying fields

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Why Do We Care?

- Imaging
- Quantum Dots
- Foams
- Micromagnetic Materials
- Thin Structures
- etc.

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Outline

- black and white – the Mumford-Shah model;
- Rudin-Osher-Fatemi(ROF) model: staircasing;
- second-order models;
- denoising;
- colors – the RGB model;
- reconstructible images – uniformly sparse region.

"sharp interface" model

Mumford-Shah model

$$E(u) = \int_\Omega \left(|\nabla u|^p + |u-f|^2\right) dx + \int_{S(u)} \gamma(\nu) d\mathcal{H}^{N-1}$$

$|u-f|^2$ ... fidelity term
$p \geq 1$, $p = 1$ ... **TV model**

$u \in BV$ (bounded variation)
$Du = \nabla u \, \mathcal{L}^N \lfloor \Omega + [u] \otimes \nu \, \mathcal{H}^{N-1} \lfloor S(u) + C(u)$

De Giorgi, Ambrosio, Bertozzi, Carriero, Chambolle, Chan, Esedoglu, Leaci, P. L. Lions, Luminita, Y. Meyer, Morel, Osher, et. al.

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The Rudin-Osher-Fatemi Model

$$\mathrm{ROF}_{\lambda,f}(u) := |u'|(]a,b[) + \lambda \int_a^b (u-f)^2\,dx \qquad u \in BV(]a,b[)$$

Lemma [Exact minimizers for $ROF_{\lambda,f}$].

$f : [a,b] \to [0,1]$ nondecreasing,
$f_+(a) = 0$ and $f_-(b) = 1$,
The unique minimizer of $ROF_{\lambda,f}$ is

$$u(x) := \begin{cases} c_1 & \text{if } a \le x \le f^{-1}(c_1)\,, \\ f(x) & \text{if } f^{-1}(c_1) < x \le f^{-1}(c_2)\,, \\ c_2 & \text{if } f^{-1}(c_2) < x \le b \end{cases}$$

$f^{-1}(c) := \inf\{x \in [a,b] :\ f(x) \ge c\}$, $0 < c_1 < c_2 < 1$ s.t.
$2\lambda \int_a^{f^{-1}(c_1)} (c_1 - f(x))\,dx = 1$, $2\lambda \int_{f^{-1}(c_2)}^b (f(x) - c_2)\,dx = 1$.

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The Rudin-Osher-Fatemi Model: staircasing

T. Chan, A. Marquina and P. Mulet, SIAM J. Sci. Comput. **22** (2000), 503–516

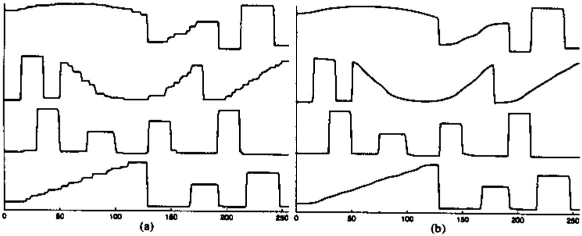

FIG. 8.2. (a) *Results of TV restoration;* (b) *results of our model.*

The Rudin-Osher-Fatemi Model: staircasing

Staircasing: "ramps" (i.e. affine regions) in the original image yield staircase-like structures in the reconstructed image.
Original edges are preserved BUT artificial/spurious ones are created . . . *"staircasing effect"*

The Rudin-Osher-Fatemi Model: staircasing. An example.

Other examples of staircasing also by Caselles, Chambolle and Novaga

$f(x) := x, \quad x \in [0,1]$ ... original 1D image
add "noise"

$$h_n(x) := \frac{i}{n} - x \qquad \text{if } \frac{i-1}{n} \le x < \frac{i}{n}, \; i = 1, \ldots, n$$

resulting degraded 1D image

$$f_n(x) := \frac{i}{n} \qquad \text{if } \frac{i-1}{n} \le x < \frac{i}{n}, \; i = 1, \ldots, n$$

Rmk: even though $h_n \to 0$ uniformly, the reconstructed image u_n preserves the staircase structure of f_n.

Theorem.

$\lambda > 4$, u_n ... unique minimizer of $\mathrm{ROF}_{\lambda, f_n}$ in $BV(]0,1[)$. For n sufficiently large there exist $0 < a_n < b_n < 1$,
$a_n \to \frac{1}{\sqrt{\lambda}}, \quad b_n \to 1 - \frac{1}{\sqrt{\lambda}}$,
$u_n = f_n$ on $[a_n, b_n]$, u_n is constant on $[0, a_n)$ and $(b_n, 1]$.

Second Order Models: The Blake-Zisserman Model

Leaci and Tomarelli, et.al.

$$E(u) = \int_\Omega W(\nabla u, \nabla^2 u)\, dx + |u - f|^2 dx + \int_{S(\nabla u)} \gamma(\nu) dH^{N-1}$$

Also, Geman and Reynolds, Chambolle and Lions, Blomgren, Chan and Mulet, Kinderman, Osher and Jones, etc.

Chan *et.al.* Model

With G. Dal Maso, G. Leoni, M. Morini

$$\mathcal{F}_p(u) = \int_\Omega \left(|\nabla u| + |u - f|^2\right)\, dx + \int_\Omega \psi(|\nabla u|)|\nabla^2 u|^p\, dx$$

$p \geq 1, \quad \psi \sim 0$ at ∞

$$\int_\infty^\infty (\psi(t))^{1/p}\, dt < +\infty, \qquad \inf_{t\in K} \psi(t) > 0$$

for every compact $K \subset \mathbb{R}$

All 1D!

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$p \in [1, +\infty)$

$$\mathcal{F}_p(u) := \int_a^b |u'|\,dx + \int_a^b \psi(|u'|)|u''|^p\,dx$$

E.g.

$$\psi(t) := \frac{1}{(1+t^2)^{\frac{1}{2}(3p-1)}}$$

the functional becomes

$$\int_a^b |u'|\,dx + \int_{\mathrm{Graph}\,u} |k|^p\,d\mathcal{H}^1$$

k ... curvature of the graph of u

in many computer vision and graphics applications, such as corner preserving geometry, denoising and segmentation with depth

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a few results. . .

- framework: minimization problem is well posed;
- compactness;
- integral representation of the relaxed functional:

$$\overline{\mathcal{F}_p}(u) := \inf \left\{ \liminf_{k \to +\infty} \mathcal{F}_p(u_k) : \ u_k \to u \text{ in } L^1(]a,b[) \right\}$$

- higher order regularization eliminates staircasing effect
  $f_k := f + h_k$, f smooth, $h_k \overset{*}{\rightharpoonup} 0$
  Is u_k smooth for $k >> 1$?
  Yes: $||u_k - u||_{W^{1,p}} \to 0$ if $p = 1$, $||u_k - u||_{C^1} \to 0$ if $p > 1$

Note: piecewise constant functions are approximable by sequences with bounded energy **only for** $p = 1$!

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Denoising

With R. Choksi and B. Zwicknagl

Given: Measured signal, disturbed by noise

$$f = f_0 + n, \qquad n - \text{noise}$$

Want: Reconstruction of clean f_0

Tool: Regularized approximation

$$\text{Minimize} \quad J(u) := ||u||_{\mathcal{H}}^k + \lambda ||u - f||_{\mathcal{W}}^m, \quad ; k, m \in \mathbb{N}$$

Questions: "Good" choice of

- fidelity measure $||\cdot||_{\mathcal{W}}$
- regularization measure $||\cdot||_{\mathcal{H}}$
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Properties of a "Good" Model

$$J(u) := ||u||_{\mathcal{H}}^{k} + \lambda ||u - f||_{\mathcal{W}}^{m}$$

- consistency: "simple" clean signals f should be recovered exactly

$$J(f) \leq J(u) \quad \text{for all} \quad u$$

- for a sequence of noise $h_n \rightharpoonup 0$, minimizers of the disturbed functionals

$$J_n(u) := ||u||_{\mathcal{H}}^{k} + \lambda ||u - f - h_n||_{\mathcal{W}}^{m} \qquad k, m \in \mathbb{N}$$

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Exact Reconstruction - Consistency

Question: For which f can we reconstruct f exactly?

For all $u \neq f$

$$J(f) \leq J(u) \Leftrightarrow ||f||_{\mathcal{H}}^k \leq ||u||_{\mathcal{H}}^k + \lambda ||u - f||_{\mathcal{W}}^m$$

Hence exact reconstruction if and only if

$$\lambda \geq \sup_{u \neq f} \frac{||f||_{\mathcal{H}}^k - ||u||_{\mathcal{H}}^n}{\lambda ||u - f||_{\mathcal{W}}^m}$$

So ... when is

$$\sup_{u \neq f} \frac{||f||_{\mathcal{H}}^k - ||u||_{\mathcal{H}}^k}{\lambda ||u - f||_{\mathcal{W}}^m} < +\infty ?$$

Bad News if the Fidelity Term Occurs With Power $m > 1$!

If $m > 1$, $||f||^k_{\mathcal{H}} \neq 0$ then

$$\sup_{u \neq f} \frac{||f||^k_{\mathcal{H}} - ||u||^k_{\mathcal{H}}}{\lambda ||u - f||^m_{\mathcal{W}}} = +\infty$$

Choose $u_\varepsilon := (1-\varepsilon)f$. Then

$$\sup_{u \neq f} \frac{||f||^k_{\mathcal{H}} - ||u||^k_{\mathcal{H}}}{\lambda ||u - f||^m_{\mathcal{W}}} \geq \sup_{0<\varepsilon<1} \frac{(1-(1-\varepsilon)^k)||f||^k_{\mathcal{H}}}{\varepsilon^m ||f||^m_{\mathcal{W}}}$$

$$= \sup_{0<\varepsilon<1} \frac{||f||^k_{\mathcal{H}}}{||f||^m_{\mathcal{W}}} \sum_{j=1}^{k} (-1)^{j+1} \binom{k}{j} e^{j-m} = \infty$$

Classical ROF: $J(u) = |u|_{BV} + \lambda ||u - f||^2_{L^2(\Omega)}$

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Weakly Vanishing Noise

Assume $h_n \rightharpoonup 0$ weakly in $\mathcal{W}$.
Disturbed functionals

$$J_n(u) := ||u||_{\mathcal{H}}^k + \lambda ||u - f - h_n||_{\mathcal{W}}^m$$

Question: What happens in the limit?

- convergence of minimizers to minimizers?
- convergence of the energies?

Γ-convergence

Assume that

- $\mathcal{H}$ is compactly embedded in $\mathcal{W}$
- *Brezis-Lieb Type Condition*: For all $f \in \mathcal{W}$

$$||f||_{\mathcal{W}}^{k} = \lim_{n\to\infty} (||f - h_n||_{\mathcal{W}}^{m} - ||h_n||_{\mathcal{W}}^{m})$$

Recall:

$$J_n(u) := ||u||_{\mathcal{H}}^{k} + \lambda ||u - f - h_n||_{\mathcal{W}}^{m}$$

Theorem.

J_n Γ-converge to

$$\tilde{J}(u) := ||u||_{\mathcal{H}}^{k} + \lambda ||u - f||_{\mathcal{W}}^{m} + \lambda \lim_{n\to\infty} ||h_n||_{\mathcal{W}}^{m}$$

with respect to the weak-* topology in $\mathcal{H}$.

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Examples: The Brezis-Lieb Condition Holds

- $\mathcal{W}$ is a Hilbert space, $m = 2$

if $h_n \rightharpoonup 0$ in $\mathcal{W}$ then

$$||f - h_n||^2_{\mathcal{W}} - ||h_n||^2_{\mathcal{W}} = ||f||^2_{\mathcal{W}} + ||h_n||^2_{\mathcal{W}} - 2(f, h_n)_{\mathcal{W}} - ||h_n||^2_{\mathcal{W}} \to ||f||^2_{\mathcal{W}}$$

E.g., $h_n \rightharpoonup 0$ in $L^2(\Omega)$

$$J_n(u) := ||u||_{W^{1,2}(\Omega)} + \lambda ||u - f - h_n||^2_{L^2(\Omega)}$$

Then J_n Γ-converge to

$$\tilde{J}(u) := ||u||_{W^{1,2}(\Omega)} + \lambda ||u - f||^2_{L^2(\Omega)} + \lambda \lim_{n\to\infty} ||h_n||^2_{L^2(\Omega)}$$

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Concentrations: The Brezis-Lieb Condition Holds

- Can handle concentrations

Let $h_n \rightharpoonup 0$ in $L^p(\Omega)$ and pointwise a.e. to 0

Brezis-Lieb Lemma

$0 < p < \infty$, $u_n \to u$ a.e., $\sup_n ||u_n||_{L^p} < \infty$
Then

$$\lim_n \left(||u_n||^p_{L^p(\Omega)} - ||u_n - u||^p_{L^p(\Omega)} \right) = ||u||^p_{L^p(\Omega)}$$

E.g.

$$h_n(x) := \begin{cases} n - n^2 x & 0 \le x \le 1/n \\ 0 & 1/n < x \le 1 \end{cases}$$

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Vector-Valued: Inpainting/Recolorization

With G. Leoni, F. Maggi, M. Morini

Restoration of color images by vector-valued BV functions

Recovery is obtained from few, sparse *complete* samples and from a significantly *incomplete* information

inpainting; recovery of damaged frescos

Figure: A fresco by Mantegna damaged during Second World War.

RGB model: $\mathbf{u_0} : R \to \mathbb{R}^3$ color image, $\mathbf{u_0} = (u_0^1, u_0^2, u_0^3)$ channels

$\mathcal{L} : \mathbb{R}^3 \to \mathbb{R}$ $\quad \mathcal{L}(\mathbf{y}) = L(\mathbf{e} \cdot \mathbf{y})$ projection on gray levels

L increasing function, $\mathbf{e} \in S^2$

$\mathcal{L}(\mathbf{u_0}) : R \to \mathbb{R}$ gray level associated with $\mathbf{u_0}$.

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RGB model: $\mathbf{u_0} : R \to \mathbb{R}^3$ color image, $\mathbf{u_0} = (u_0^1, u_0^2, u_0^3)$ channels

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$D \subset R \subset \mathbb{R}^2$ . . . *inpainting region*

RGB

observed (u_0, v_0)

u_0 . . . *correct* information on $R \setminus D$

v_0 . . . *distorted information* . . . only gray level is known on D;

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Goal

to produce a new color image that extends colors of the fragments to the gray region, constrained to match the known gray level

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The variational approach by Fornasier-March

Problem: Reconstruct $\mathbf{u_0}$ from the knowledge of $\mathcal{L}(\mathbf{u_0})$ in the damaged region D and of $\mathbf{u_0}$ on $R \setminus D$.

- Fornasier (2006) proposes to solve:

$$\min_{\mathbf{u} \in BV(R;\mathbb{R}^3)} |D\mathbf{u}|(R) + \lambda_1 \int_D |\mathcal{L}(\mathbf{u}) - \mathcal{L}(\mathbf{u_0})|^2 \, dx + \lambda_2 \int_{R \setminus D} |\mathbf{u} - \mathbf{u_0}|^2 \, dx$$

$\lambda_1, \lambda_2 > 0$ are fidelity parameters.

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a couple of questions. . .

- "optimal design" : what is the "best" D? How much color do we need to provide? And where?
- are we creating spurious edges?

For a "cartoon" u in SBV, i.e.

$$Du = \nabla u \mathcal{L}^2 \lfloor R + (u^+ - u^-) \otimes \nu \mathcal{H}^1 \lfloor S(u)$$

its edges are in . . . spt $D_s u = S(u)$

$$\mathrm{spt} D_s u_i \subset \mathrm{spt} D_s(\mathcal{L}(u_0))?$$

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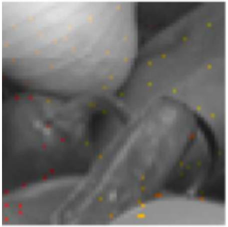

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Two reconstructions by Fornasier-March

Our analysis

How faithful is the reconstruction in the infinite fidelity limit ?

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- Sending λ_1 and $\lambda_2 \to \infty$ in

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How faithful is the reconstruction in the infinite fidelity limit?
the problem becomes

$$\min_{\mathbf{u} \in BV(R;\mathbb{R}^3)} |D\mathbf{u}|(R) \tag{P}$$

subject to $\mathbf{u} = \mathbf{u_0}$ on $R \setminus D$ and $L(\mathbf{u} \cdot \mathbf{e}) = L(\mathbf{u_0} \cdot \mathbf{e})$ in D.

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Definition

$\mathbf{u_0}$ is reconstructible over D if it is the unique minimizer of (P).

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$\lambda_1 = \lambda_2 = \infty$

$$(P)\,\inf\left\{|Du|(R) : u \in BV(R;\mathbb{R}^3), Lu = Lu_0 \quad \text{in } D, u = u_0 \quad \text{on } R \setminus D\right\}$$

Theorem

$u_0 \in BV(R;\mathbb{R}^3)$ and D open Lipschitz domain. Then (P) has a minimizer.

isoperimetric inequality $\rightarrow$ boundedness in BV

admissible images

Find conditions on the damaged region D *which render* $\mathbf{u_0}$ *reconstructible*

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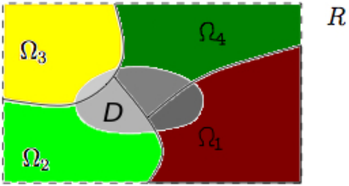

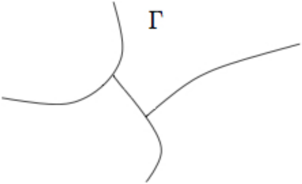

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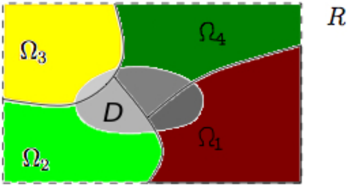

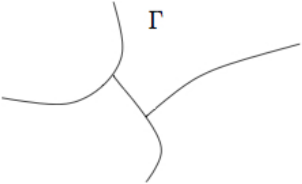

$$R = \Gamma \cup \bigcup_{k=1}^{N} \Omega_k\,, \quad \mathbf{u_0} = \sum_{k=1}^{N} \xi_k 1_{\Omega_k}\,,$$

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subject to $\mathbf{u} = \mathbf{u_0}$ in $R \setminus D$ and $\mathbf{u} \cdot \mathbf{e} = \mathbf{u_0} \cdot \mathbf{e}$ in D.

- Strenghthened notion of reconstructibility:

Definition

$\mathbf{u_0}$ is stably reconstructible over D if there exists $\varepsilon > 0$ such that all $\mathbf{u}$ of the form

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reconstructible images

when is an admissible image u_0 **reconstructible** over a damaged region S?

Answer: NO when a pair of neighboring colors ξ_h and ξ_k in u_0 share the same gray level, i.e., if $\mathcal{H}^1(\partial\Omega_k \cap \partial\Omega_h) > 0$ and $L\xi_h = L\xi_k$

Answer: YES if an algebraic condition involving the values of the colors and the angles of the corners possibly present in Γ is satisfied . . . quantitative validation of the model's accuracy

Minimal requirement: must be reconstructible over $S = \Gamma(\delta)$ for some $\delta > 0$, where

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u_0 **does not have** neighboring colors with the same gray level

$$z_k(x) := P\left(\frac{\xi_k - \xi_h}{|\xi_k - \xi_h|}\right) \qquad \text{if } x \in \partial\Omega_k \cap \partial\Omega_h \cap R\,,\, h \neq k\,,$$

where P is the orthogonal projection on $\langle e \rangle^{\perp}$

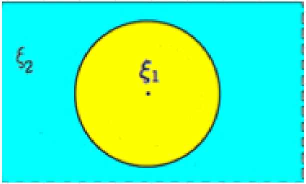
$$P(\xi) := \xi - (\xi \cdot e)e$$

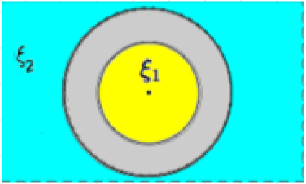
u_0 does not have neighboring colors with the same gray level IFF

$$\sup_{1 \leq K \leq N} ||z_k||_{L^\infty} < 1$$

A simple counterexample when $\|z_k\|_\infty < 1$ is not satisfied

- Original image $\mathbf{u_0}$:





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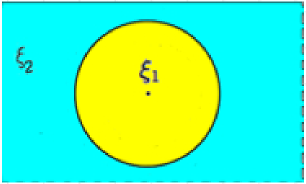
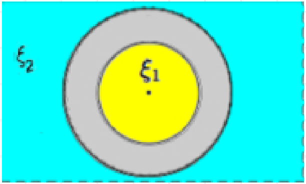
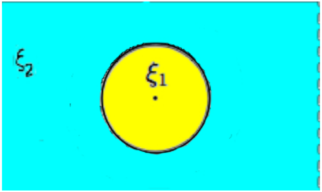




- Resulting image $\mathbf{u}$:



Adjoint colors have the same gray levels: may create spurious edges

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A simple analytical counterexample

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Adjoint colors have the same gray levels: may create spurious edges

A simple analytical counterexample

- Original image $\mathbf{u_0}$:

- Resulting image $\mathbf{u}$:

A spurious contour appears!

Minimality conditions

Theorem (Necessary and sufficient minimality conditions)

$D \subset R$ Lipschitz, $\mathcal{H}^1(\partial D \cap \Gamma) = 0$. Then the following two conditions are equivalent:

(i) *u_0 is stably reconstructible over D;*

(ii) *there exists a tensor field $M : D \to \langle e \rangle^{\perp} \otimes \mathbb{R}^2$ such that $\operatorname{div} M = 0$ in D*

$$\|M\|_{\infty} < 1 \quad \text{and} \quad M[\nu_{\Omega_k}] = -z_k \quad \text{on } D \cap \partial\Omega_k \,.$$

The tensor field M is called a calibration for $\mathbf{u_0}$ in D.

Minimality conditions

Theorem (Necessary and sufficient minimality conditions)

$D \subset R$ Lipschitz, $\mathcal{H}^1(\partial D \cap \Gamma) = 0$. Then the following two conditions are equivalent:

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1-Laplacian ...

Reformulate the minimization problem (P) as

$$\inf \left\{ F(u,D) : \; u \in BV(D;\mathbb{R}^3)\,,\; u\cdot e = u_0 \cdot e \;\mathcal{L}^2\text{-a.e. in } D \right\}\,,$$

where

$$F(u,D) := |Du|(D) + \sum_{k=1}^{N} \int_{\partial D \cap \Omega_k} |u - \xi_k| \, d\mathcal{H}^1 \,.$$

Euler-Lagrange equation: formally given by the 1-Laplacian Neumann problem

$$\begin{cases} \operatorname{div} \frac{Du}{|Du|} \parallel \mathbf{e} & \text{in } D\,, \\ P\left(\frac{Du}{|Du|}[\nu_D]\right) = -z & \text{on } \partial D\,,\; z := P\left(\frac{u-\xi_k}{|u-\xi_k|}\right) \end{cases}$$

Since this equation is in general not well-defined, $\frac{Du}{|Du|}$ is replaced by the calibration M

Hence, the conditions on M can be considered as a weak formulation of the Euler-Lagrange equations of F.

Necessary and sufficient minimality conditions

- Writing $M = (M^{(1)}, M^{(2)})$, locally there exists a Lipschitz function $f = (f^{(1)}, f^{(2)})$ such that $\|\nabla f\|_\infty < 1$,

$$[M^{(i)}]^\perp = -\nabla f^i \quad \text{and} \quad \partial_{\tau_{\Omega_k}} f = M[\nu_{\Omega_k}] = -z_k \quad \text{on } D \cap \partial\Omega_k \, .$$

- Hence, the construction of the calibration can be often reduced to a Lipschitz extension problem

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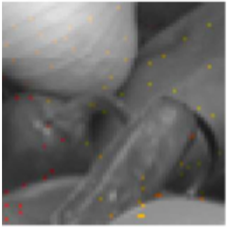
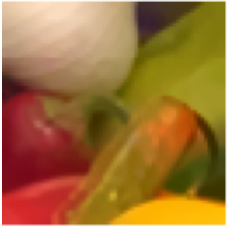
When is $\mathbf{u_0}$ stably reconstructible over D?

- Recall the reconstruction





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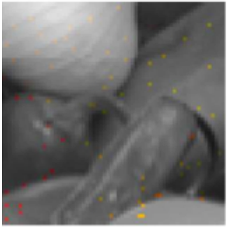

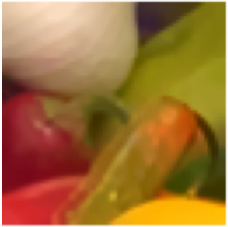

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ε-uniformly distributed undamaged regions

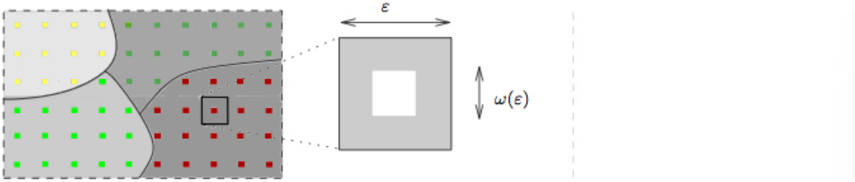
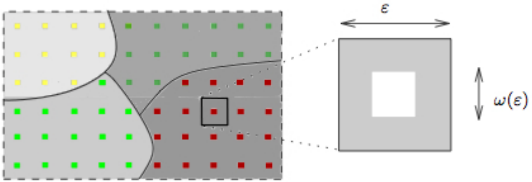


Figure: An ε-uniformly distributed undamaged region.

ε-uniformly distributed undamaged regions



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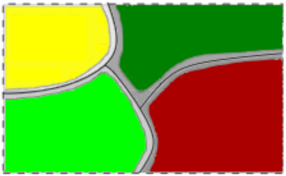
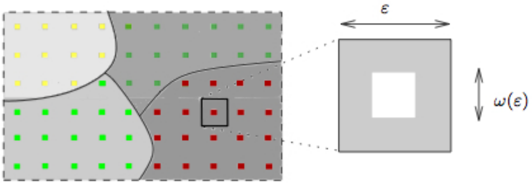


Figure: The damaged region contains a δ-neighborhood $\Gamma(\delta)$ of Γ.

ε-uniformly distributed undamaged regions



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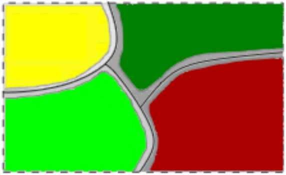


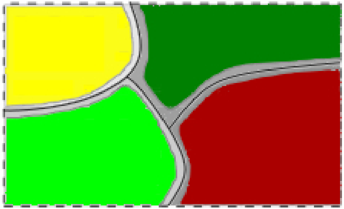
Figure: The damaged region contains a δ-neighborhood $\Gamma(\delta)$ of Γ.

It is natural to assume that $\mathbf{u_0}$ is stably reconstructible over $\Gamma(\delta)$ for some $\delta > 0$.

Can treat more general non-periodic geometries, e.g. $Q(x, \omega(\varepsilon))$ is replaced by a closed connected set with diameter of order $\omega(\varepsilon)$

A natural assumption

- $\mathbf{u_0}$ is stably reconstructible over $\Gamma(\delta)$ for some $\delta > 0$.



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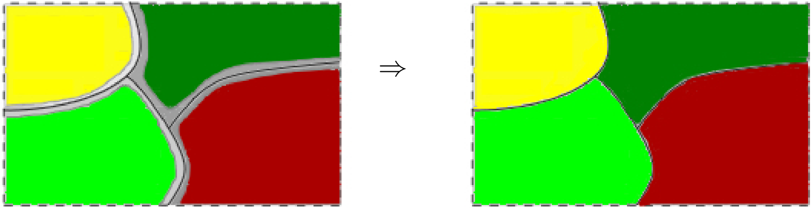


uniformly sparse region: an asymptotic result

The TV model provides asymptotically exact reconstruction on generic color images . . . No info on gray levels!!!

Theorem

$u_0 \in BV(R;\mathbb{R}^3) \cap L^\infty(R;\mathbb{R}^3)$

$$D_\varepsilon \subset R \cap \left(\bigcup_{x \in \varepsilon\mathbb{Z}^2} \overline{Q(x,\varepsilon)} \setminus \overline{Q(x,\omega(\varepsilon))} \right) ,$$

Let u_ε be minimizer of

$$\inf \{ |Du|(R) : u = u_0 \text{ on } R \setminus D_\varepsilon \}$$

Then

$$u_\varepsilon \to u_0 \qquad \text{in } L^1$$

Admissible ε-uniformly distributed undamaged regions

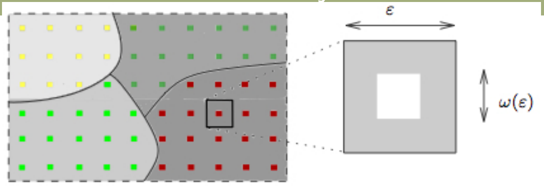
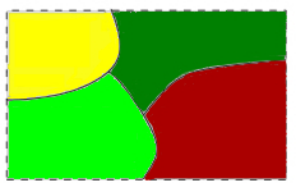


Figure: Denote by D_ε the damaged region



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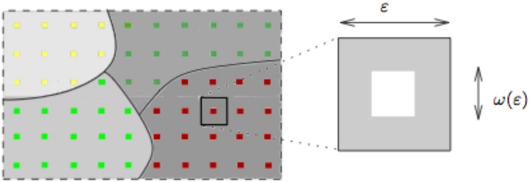

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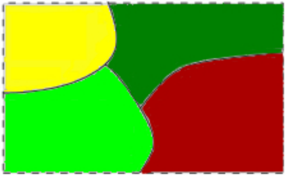

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Theorem

Let $\mathbf{u_0}$ be stably reconstructible over $\Gamma(\delta)$ for some $\delta > 0$. Assume that

$$\lim_{\varepsilon \to 0^+} \frac{\omega(\varepsilon)}{\varepsilon} = 0 \,, \qquad \lim_{\varepsilon \to 0^+} \frac{\omega(\varepsilon)}{\varepsilon^2} = \infty \,.$$

Then, there exists $\varepsilon_0 > 0$ such that $\mathbf{u_0}$ is stably reconstructible over D_ε for all $\varepsilon \leq \varepsilon_0$.

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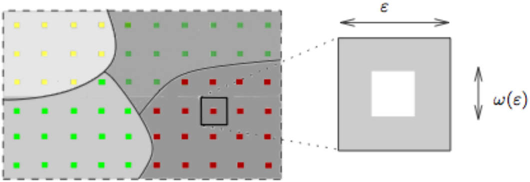

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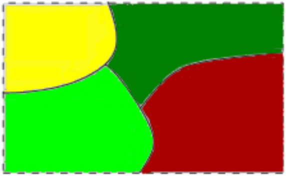

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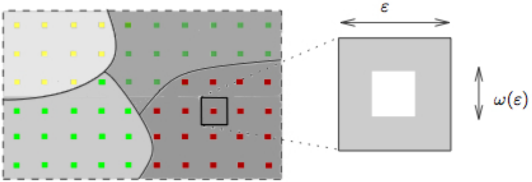

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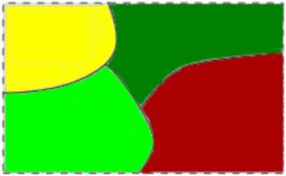

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uniformly sparse region: scaling ε^2 from below for $\omega(\varepsilon)$ is sharp

if $\omega(\varepsilon) \leq c\varepsilon^2$ cannot expect exact reconstruction.

Counterexample with

$$\omega(\varepsilon) \leq c\varepsilon^2$$

for c small enough

$u_0 = \chi_\Omega \xi_0$, $R := (0,3) \times (0,3)$, $\Omega := (1,2) \times (1,2)$.

Outline

- wetting and zero contact angle;
- surface diffusion in epitaxially strained solids;
- shapes of islands;
- steps and terraces in epitaxially strained islands.

The Context

With N. Fusco, G. Leoni, M. Morini

Strained epitaxial films on a relatively thick substrate

plane linear elasticity (In-GaAs/GaAs or SiGe/Si)

- free surface of film is *flat* until reaching a critical thikness
- *lattice misfits* between substrate and film induce *strains* in the film
- Complete relaxation to bulk equilibrium $\Rightarrow$ crystalline structure would be discontinuous at the interface
- Strain $\Rightarrow$ flat layer of film morphologically unstable or metastable after a critical value of the thickness is reached (competition between surface and bulk energies)

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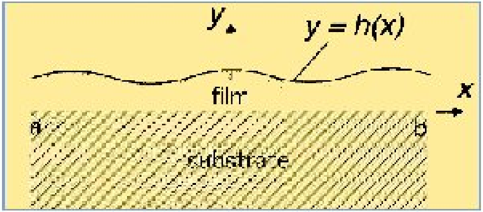
islands

To release some of the elastic energy due to the strain: atoms on the free surface rearrange and morphologies such as formation of island (*quatum dots*) of pyramidal shapes are energetically more economical

quantum dots: the profile . . .



some potential applications

optical and optoelectric devices (quantum dot laser), information storage, . . .

electronic properties depend on the *regularity* of the dots, *size*, *spacing*, etc.

some questions

- explain how isolated islands are separated by a *wetting layer*
- validate the *zero contact angle* between wetting layer and the island

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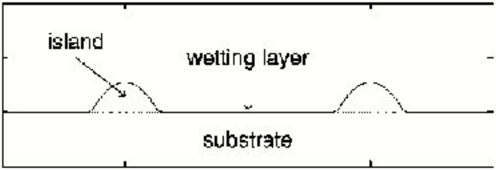
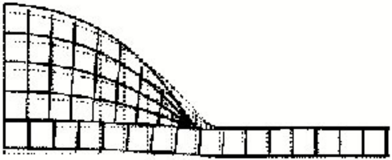
wetting layer and zero contact angle, islands



Islands and wetting layers



Lattice mismatch at an island-substrate interface.

Sharp Interface Model

Brian Spencer, Bonnetier and Chambolle, Chambolle and Larsen; Caflish, W. E, Otto, Voorhees, et. al.

$$\Omega_h := \{\mathbf{x} = (x, y) : \; a < x < b, \; y < h(x)\}$$

$h : [a, b] \to [0, \infty)$ ... graph of h is the *profile of the film*

$y = 0 \ldots$ film/substrate interface

mismatch strain (at which minimum energy is attained)

$$\mathbf{E}_0(y) = \begin{cases} e_0 \mathbf{i} \otimes \mathbf{i} & \text{if } y \geq 0, \\ 0 & \text{if } y < 0, \end{cases}$$

more on the model

$e_0 > 0$
$\mathbf{i}$ the unit vector along the x direction

elastic energy per unit area: $W\left(\mathbf{E} - \mathbf{E}_0\left(y\right)\right)$

$$W\left(\mathbf{E}\right) := \frac{1}{2}\mathbf{E} \cdot C\left[\mathbf{E}\right], \quad E(u) := \frac{1}{2}(\nabla u + (\nabla u)^T)$$

C ... positive definite fourth-order tensor

film and the substrate have similar material properties, share the same homogeneous elasticity tensor C

sharp interface model

$$\varphi_0(y) := \begin{cases} \gamma_{\text{film}} & \text{if } y > 0, \\ \gamma_{\text{sub}} & \text{if } y = 0. \end{cases}$$

Total energy of the system:

$$F(\mathbf{u}, \Omega_h) := \int_{\Omega_h} W(\mathbf{E}(\mathbf{u})(\mathbf{x}) - \mathbf{E}_0(y))\, d\mathbf{x} + \int_{\Gamma_h} \varphi_0(y)\, d\mathcal{H}^1(\mathbf{x}),$$

$\Gamma_h := \partial\Omega_h \cap ((a, b) \times \mathbb{R})$ … *free surface of the film*

hard to implement . . .

Sharp interface model is difficult to be implemented numerically. Instead: *boundary-layer model*; discontinuous transition is regularized over a thin transition region of width δ ("smearing parameter").

$$\mathbf{E}_\delta(y) := \frac{1}{2} e_0 \left(1 + f\left(\frac{y}{\delta}\right)\right) \mathbf{i} \otimes \mathbf{i}, \quad y \in \mathbb{R},$$

$$\varphi_\delta(y) := \gamma_{\mathsf{sub}} + (\gamma_{\mathsf{film}} - \gamma_{\mathsf{sub}}) f\left(\frac{y}{\delta}\right), \quad y \geq 0,$$

$$f(0) = 0, \quad \lim_{y \to -\infty} f(y) = -1, \quad \lim_{y \to \infty} f(y) = 1.$$

regularized energy

Regularized total energy of the system

$$F_\delta(\mathbf{u}, \Omega_h) := \int_{\Omega_h} W(\mathbf{E}(\mathbf{u})(\mathbf{x}) - \mathbf{E}_\delta(y))\, d\mathbf{x} + \int_{\Gamma_h} \varphi_\delta(y)\, d\mathcal{H}^1(\mathbf{x})$$

$$\text{Two regimes}: \begin{cases} \gamma_{\mathsf{film}} \geq \gamma_{\mathsf{sub}} \\ \gamma_{\mathsf{film}} < \gamma_{\mathsf{sub}} \end{cases}$$

wetting, etc.

asymptotics as $\delta \to 0^+$

- $\gamma_{\mathrm{film}} < \gamma_{\mathrm{sub}}$
  relaxed surface energy density is no longer discontinuous: it is constantly equal to γ_{film}... WETTING!
- more favorable to cover the substrate with an infinitesimal layer of film atoms (and pay surface energy with density γ_{film}) rather than to leave any part of the substrate exposed (and pay surface energy with density γ_{sub})
- wetting regime: regularity of local minimizers $(\mathbf{u}, \Omega)$ of the limiting functional F_∞ under a volume constraint.

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- wetting regime: regularity of local minimizers $(\mathbf{u}, \Omega)$ of the limiting functional F_∞ under a volume constraint.

cusps and vertical cuts

The profile *h* of the film for a locally minimizing configuration is regular except for at most a finite number of *cusps* and *vertical cuts* which correspond to vertical cracks in the film.

[Spencer and Meiron]: steady state solutions exhibit cusp singularities, time-dependent evolution of small disturbances of the flat interface result in the formation of deep grooved cusps (also [Chiu and Gao]); experimental validation of sharp cusplike features in $SI_{0.6}$ $Ge_{0.4}$

zero contact-angle condition between the wetting layer and islands

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regularization ...

- conclude that the graph of h is a Lipschitz continuous curve away from a finite number of singular points (cusps, vertical cuts).

- ... and more: Lipschitz continuity of h +blow up argument+classical results on corner domains for solutions of **Lamé systems** of $h \Rightarrow$ decay estimate for the gradient of the displacement $\mathbf{u}$ near the boundary $\Rightarrow C^{1,\alpha}$ regularity of h and $\nabla\mathbf{u}$; bootstrap.

this takes us to linearly isotropic materials

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Linearly isotropic elastic materials

$$W(\mathbf{E}) = \frac{1}{2}\lambda\left[\mathrm{tr}(\mathbf{E})\right]^2 + \mu\,\mathrm{tr}\left(\mathbf{E}^2\right)$$

λ and μ are the (constant) Lamé moduli

$$\mu > 0\,, \quad \mu + \lambda > 0\,.$$

Euler-Lagrange system of equations associated to W

$$\mu\Delta\mathbf{u} + (\lambda+\mu)\,\nabla(\mathrm{div}\,\mathbf{u}) = \mathbf{0} \quad \text{in } \Omega.$$

Regularity of Γ: No corners

$$\Gamma_{\text{sing}} := \Gamma_{\text{cusps}} \cup \{(x, h(x)) : h(x) < h^-(x)\}$$

Already know that $\Gamma_{\rm sing}$ is finite.

Theorem

$(\mathbf{u}, \Omega) \in X$ ... δ-local minimizer for the functional F_∞.
Then $\Gamma \setminus \Gamma_{\text{sing}}$ is of class $C^{1,\sigma}$ for all $0 < \sigma < \frac{1}{2}$.

As an immediate corollary, get the zero contact-angle condition

Corollary

$(\mathbf{u}, \Omega) \in X$ ... local minimizer for the functional F_∞.
If $\mathbf{z}_0 = (x_0, 0) \in \Gamma \setminus \Gamma_{\text{sing}}$ then $h'(x_0) = 0$.

next . . .

- 3D case!
- surface diffusion in epitaxially strained solids ($2D$)
- shapes of islands

surface diffusion in epitaxially strained solids

With N. Fusco, G. Leoni, M. Morini

Einstein-Nernst volume preserving evolution law:

$$V = C\Delta_\Gamma \mu$$

V . . . normal velocity of evolving interface

Δ_Γ . . . tangential Laplacian

μ . . . chemical potential, first variation of the free-energy functional

$$\int_{\Omega_h} W(\mathbf{E}(\mathbf{u}))\, \mathbf{dx} + \int_{\mathbf{\Gamma_h}} \varphi(\theta) \mathbf{d}\mathcal{H}^{\mathbf{1}}$$

ill-posed . . . so add a perturbation

Get (with $C = 1$)

$$V = ((\varphi_{\theta\theta} + \varphi)k + W(\mathbf{E}(\mathbf{u})))_{\sigma\sigma}$$

k . . . curvature of Γ_h
$(\cdot)_\sigma$ . . . tangential derivative
$u(\cdot, t)$ . . . elastic equilibrium in $\Omega_{h(\cdot,t)}$ under periodic b. c.

$$V = \left((\varphi_{\theta\theta} + \varphi)k + W(\mathbf{E}(\mathbf{u})) - \varepsilon\left(\mathbf{k}_{\sigma\sigma} + \frac{1}{2}\mathbf{k}^3\right)\right)_{\sigma\sigma}$$

H^{-1}- gradient flow for (Cahn and Taylor)

$$\int_{\Omega_h} W(\mathbf{E}(\mathbf{u}))\,\mathbf{dx} + \int_{\Gamma_h}\left(\varphi(\theta) + \frac{\varepsilon}{2}\mathbf{k}^2\right)\mathbf{d}\mathcal{H}^1$$

De Giorgi's minimizing movements: short time existence, uniqueness, regularity

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shapes of islands

With A. Pratelli and B. Zwicknagl

We proved that the shape of the island evolves with the size:

small islands always have the half-pyramid shape, and as the volume increases the island evolves through a sequence of shapes that include more facets with increasing steepness – half pyramid, pyramid, half dome, dome, half barn, barn

This validates what was experimentally and numerically obtained in the physics and materials science literature

More in progress! . . .

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