Mathematical elasticity – when calculus of variations meets mechanics

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based on a joint work with
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August 6, 2018

Elasticity

$\Omega \subset \mathbb{R}^3$ reference configuration

$y : \bar{\Omega} \to \mathbb{R}^3$ deformation

$F := \nabla y$ deformation gradient , $\det F > 0$

$T : \bar{\Omega} \to \mathbb{R}^{3\times 3}$ 1st Piola-Kirchhoff stress tensor

$f : \Gamma_1 \to \mathbb{R}^3$ density of surface forces

$T(x) := \hat{T}(x, \nabla y(x))$ constitutive law (Cauchy elasticity)

$\operatorname{div} T = 0$ equilibrium equations
$y = y_0$ on $\Gamma_0 \subset \partial\Omega$, f=Tn on $\Gamma_1 \subset \partial\Omega$ boundary conditions

Hyperelasticity

Assumption: 1st Piola-Kirchhoff stress tensor T has a potential:

$$T_{ij} := \frac{\partial W(\nabla y)}{\partial F_{ij}}$$

$W : \mathbb{R}^{3\times 3} \to \mathbb{R} \cup \{+\infty\}$ stored energy density
Work can be stored in elastic materials (no loss)

Hyperelasticity

$$J(y) := \int_\Omega W(\nabla y(x))\,\mathrm{d}x - \int_{\Gamma_1} f \cdot y\,\mathrm{d}S\ .$$

Minimizers of J formally satisfy equilibrium equations.

Properties of W

(i) $W : \mathbb{R}^{3\times 3}_{+} \to \mathbb{R}$ is continuous

(ii) $W(F) = W(RF)$ for all $R \in \mathrm{SO}(3)$ and all $F \in \mathbb{R}^{3\times 3}$

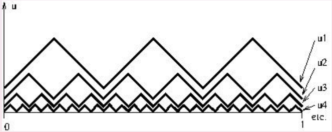
(iii) $W(F) \to +\infty$ if $\det F \to 0_+$

(iv) $W(F) = +\infty$ if $\det F \leq 0$ (This excludes convexity of W)

Nonconvexity could be fatal....(at least in 1D)

$$I(u) := \int_0^1 (1 - |u'|)^2 + u^2 \, \mathrm{d}x \ .$$

Consider $\{u_k\}$ a sequence of zig-zag functions driving I to its infimum.



$$u_k \to 0 \text{ in } L^2(0,1)$$

$$u_k' \to 0 \text{ weakly in } L^2(0,1)$$

$$0 = \inf I = \lim_{k\to\infty} I(u_k) < I(0) = 1$$

No weak lower semicontinuity and no minimizer because $I(u) > 0$.

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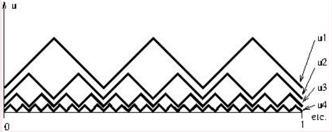

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Polyconvexity – Ball (1977), Morrey (1952)

J.M. Ball's notion of **polyconvexity** (1977)

$$W(F) = h(F, \mathrm{cof}\, F, \det F) \text{ if } \det F > 0$$

$$\mathrm{cof}\, F := (\det F) F^{-\top}$$

$h : \mathbb{R}^{19} \to \mathbb{R}$ is **convex**

Existence of solutions

(i) W polyconvex, $W(F) = +\infty$ if $\det F \leq 0$

(ii) $W(F) = W(RF)$ for all $R \in \mathrm{SO}(3)$ and all $F \in \mathbb{R}^{3\times 3}$

(iii) $W(F) \to +\infty$ if $\det F \to 0_+$

(iv) $C(|F|^p + |\mathrm{cof}\, F|^q + \det F^r) \leq W(F)$ for $p > 3$, $q \geq 3/2$, $r > 1$, $C > 0$

Minimizers of J exist in
$\emptyset \neq \mathcal{A} := \{W^{1,p}(\Omega; \mathbb{R}^3),\ y = y_0 \text{ on } \Gamma_0,\ \det \nabla y > 0\}$, if there is y such that $J(y) < +\infty$.

Polyconvexity

- It is relatively easy to construct polyconvex functions.
- Examples for various crystallographic structures (V. Ebbing).
- It allows us to ensure injectivity of deformations and orientation preservation.

Existence of solutions

The proof is based on convexity of h and special properties of determinants and cofactors, namely if $y_k \rightharpoonup y$ in $W^{1,p}$ for $p > 3$ then (Reshetnyak, 1968)

$$\det \nabla y_k \rightharpoonup \det \nabla y \text{ in } L^{p/3}$$

and

$$\mathrm{cof}\, \nabla y_k \rightharpoonup \mathrm{cof}\, \nabla y \text{ in } L^{p/2} \ .$$

Why is it so?

....because determinant is the divergence.

If $\varphi \in C_0^\infty(\Omega)$ the **strong** convergence of $y_k \to y$ and the **weak** convergence of partial derivatives of y_k allows us to write ($n = 2$):

$$\int_\Omega \varphi \det \nabla y_k \,\mathrm{d}x = \int_\Omega \frac{\partial}{\partial x_1}\left(y_k^1 \frac{\partial y_k^2}{\partial x_2}\right)\varphi + \frac{\partial}{\partial x_2}\left(-y_k^1 \frac{\partial y_k^2}{\partial x_1}\right)\varphi \,\mathrm{d}x$$
$$= -\int_\Omega \left(y_k^1 \frac{\partial y_k^2}{\partial x_2}\right)\frac{\partial \varphi}{\partial x_1} + \left(y_k^1 \frac{\partial y_k^2}{\partial x_1}\right)\frac{\partial \varphi}{\partial x_2}\,\mathrm{d}x$$
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Density of $C_0^\infty(\Omega)$ in $L^{p/(p-n)}(\Omega)$ finishes the argument.

We can replicate the above calculation for all other subdeterminants/minors of the gradient matrix.

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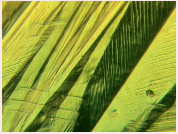
Beyond polyconvexity

In many applications polyconvexity is not suitable, e.g., in modeling of shape memory alloys, where W has a multiwell structure, e.g.

$$W(F) = \min_i W_i(F) ,$$

where

$$W_i(F) \text{ is minimized iff } F = RF_i, F_i \in \mathbb{R}^{3\times 3}_+ \text{ given, } R \text{ rotation}$$

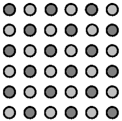


Courtesy of Institute of Physics, ASCR.

Shape memory alloys

Principle of shape memory:

◦ high temperature:
atomic grid with high symmetry (usually cubic):
the so-called austenite, higher heat capacity



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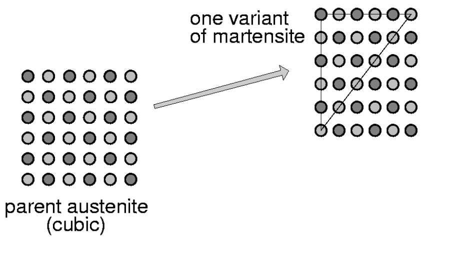

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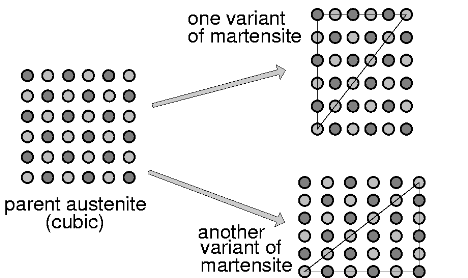

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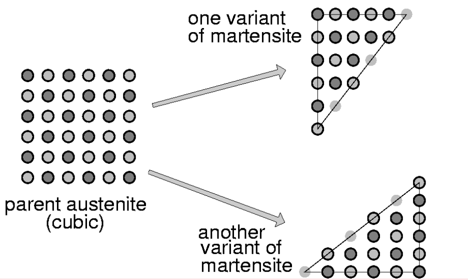

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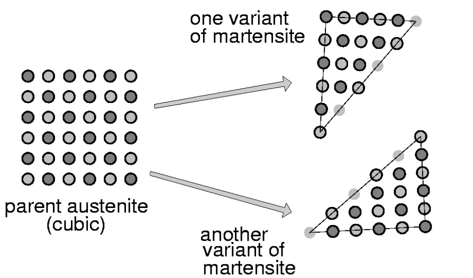

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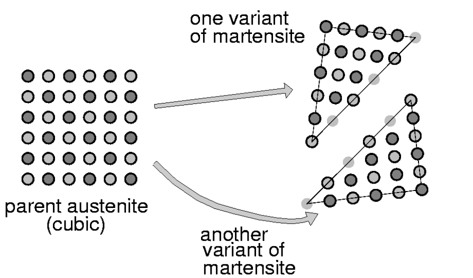

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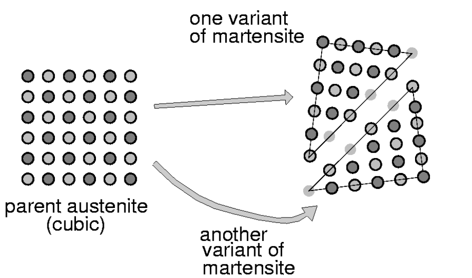

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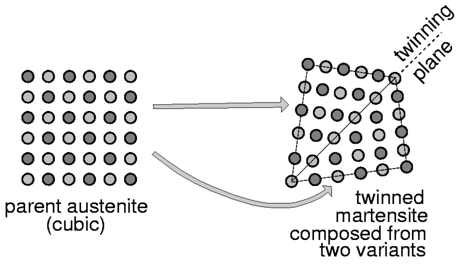

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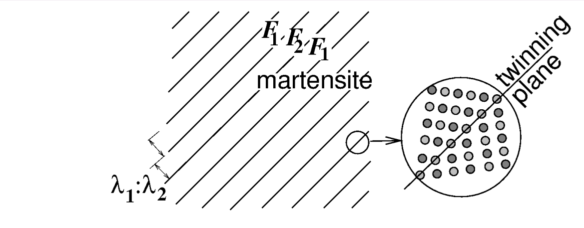

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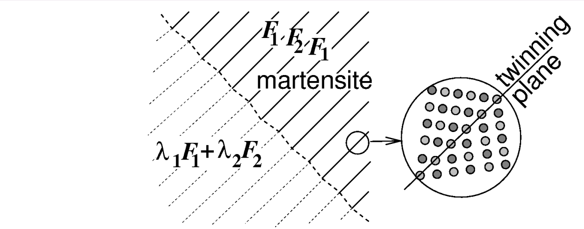

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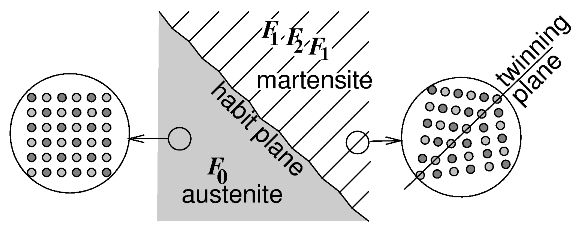

How about if W is not polyconvex?

If

$$c(-1+|F|^p) \le W(F) \le C(1+|F|^p)$$

and quasiconvex, i.e.,

$$W(F)|\Omega| \le \int_\Omega W(\nabla\varphi(x))\,dx$$

for all $\varphi \in W^{1,\infty}(\Omega;\mathbb{R}^3)$, $\varphi(x) = Fx$ on $\partial\Omega$ then J is wlsc on $W^{1,p}$, $(p > 1)$

The upper bound is not suitable for elasticity!

$$W = W_1 + W_2 \;,$$

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Quasiconvexity in elasticity

- quasiconvexity is necessary and sufficient but polynomial upper bounds on W allow for non-physical states
- frame-indifference implies $W(F) = \bar{W}(C)$, $C = F^\top F$, $\det C \geq 0$, i.e., we lose control over the sign of $\det F$
- relaxation of multi-well problems, i.e., finding the largest quasiconvex function below W (mostly impossible)
- $C = F^\top F = (QF)^\top (QF) = (RF)^\top (RF)$, $Q \in \mathrm{O}(3) \setminus \mathrm{SO}(3)$, $R \in \mathrm{SO}(3)$ existence of "dark orbits" QF which are not physical
- One of the problems in J.M. Ball's survey "Open problems in elasticity":
  Prove the existence of energy minimizers for elastostatics for quasiconvex stored-energy functions satisfying

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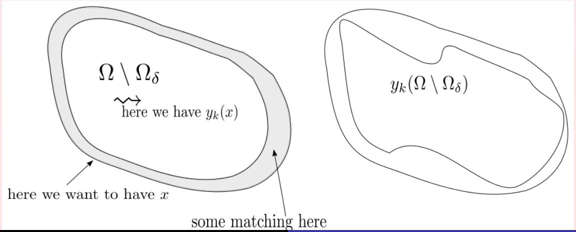
Why is it difficult?

To exploit quasiconvexity we need to manipulate boundary data of the sequence. If $y_k \rightharpoonup y$ in $W^{1,p}$, $y(x) = x$ and $y_k(x) = x$ for $x \in \partial\Omega$ then quasiconvexity immediately implies that

$$\liminf_{k\to\infty} \int_\Omega W(\nabla y_k)\,\mathrm{d}x \geq \int_\Omega W(\nabla y)\,\mathrm{d}x \ .$$

If $y_k(x) \neq x$ on $\partial\Omega$ but $y_k \rightharpoonup y$ we modify y_k to $w_k \in W^{1,p}$ such that $|y_k \neq w_k| + |\nabla y_k \neq \nabla w_k| \to 0$ and $w_k \rightharpoonup x$, $w_k(x) = x$ on $\partial\Omega$, and

$$\liminf_{k\to\infty} \int_\Omega W(\nabla y_k)\,\mathrm{d}x = \liminf_{k\to\infty} \int_\Omega W(\nabla w_k)\,\mathrm{d}x \geq \int_\Omega W(I)\,\mathrm{d}x \ .$$



Why is it difficult?

- The key ingredient in the proof of this proposition is the construction of some kind of cut-off
- Usually we take some smooth $\eta_\delta : \bar{\Omega} \to [0,1]$, $|\nabla \eta_\delta| < C/\delta$

$$\eta_\delta(x) := \begin{cases} 1 & \text{in } \Omega_\delta \\ 0 & \text{on } \partial\Omega \ . \end{cases}$$

- $$w_{k(\delta)\delta} = \eta_\delta y_k + (1-\eta_\delta)x$$
- But our constraint $\det > 0$ *is not convex*
  $\rightsquigarrow$ we may easily "fall out" from the set of deformations.

Constructing a cut-off under the $\det \neq 0$ constraint

- ... in some situations we can find remedy in *convex integration* and partial differential inclusions, solve $\nabla w_k(x) \in S$ if $x \in \Omega_\delta$, S contains invertible matrices only
- B.B., M.K., G. Pathó; 2012: $p = +\infty$ $S = \lambda O(n)$, $\lambda \neq 0$
- Rindler, Koumatos, Wiedemann; 2013: $p < n$, S contains matrices with positive determinant
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What else can we do ? Non-simple material regularization

The energy is regularized as

$$J(y) = \int_\Omega W(\nabla y) + \varepsilon |\nabla^2 y|^p \mathrm{d}x.$$

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The energy is regularized as

$$J(y) = \int_{\Omega} W(\nabla y) + \varepsilon |\nabla^2 y|^p \mathrm{d}x.$$

- the regularization is related to interfacial energies
- e.g. it penalizes fast spatial oscillations of the gradient
- this yields existence of minimizers since now the energy is convex in the highest gradient

[Ball, Crooks, 2011], [Ball, Mora-Corral, 2009]

What else can we do ? Non-simple material regularization

The energy is regularized as

$$J(y) = \int_\Omega W(\nabla y) + \varepsilon |\nabla^2 y|^p \mathrm{d}x.$$

Nevertheless, a clear physical justification of this particular form seems not to be clear...

Why is polyconvexity ok?

- It exploits weak continuity of $y \mapsto \det \nabla y$ and $y \mapsto \operatorname{cof} \nabla y$ from Sobolev to Lebesgue spaces, convexity, and the Hahn-Banach theorem/Mazur lemma
- No cut-off needed!
- We should try to exploit it more!

Gradient-polyconvexity

$$J(y) := \int_\Omega \hat{W}(\nabla y(x), \nabla \mathrm{cof}\, \nabla y(x), \nabla \det \nabla y(x))\, \mathrm{d}x - \ell(y),$$

$\hat{W}(F, \cdot, \cdot)$ is convex.
Additionally, we assume that for some $c > 0$, and $p, q, r, s \geq 1$ it holds that

$$\hat{W}(F, \Delta_1, \Delta_2) \geq \begin{cases} c\big(|F|^p + (\det F)^{-s} + |\Delta_1|^q + |\Delta_2|^r\big) & \text{if } \det F > 0, \\ \infty & \text{otherwise.} \end{cases}$$

Gradient-polyconvexity

How is this different to

$$J(y) = \int_\Omega W(\nabla y) + \varepsilon|\nabla^2 y|^p \mathrm{d}x?$$

Admissible deformations are in $W^{2,p}$!

Example

Take $\Omega = (0,1)^3$ and deformation $\big($for some $t \geq 1\big)$

$$y(x_1, x_2, x_3) := \left(x_1^2, x_2\, x_1^{t/(t+1)}, x_3\, x_1^2\right) ,$$

$$\text{so that } \nabla y(x_1, x_2, x_3) = \begin{pmatrix} 2x_1 & 0 & 0 \\ \frac{t}{t+1} x_2\, x_1^{-1/(t+1)} & x_1^{t/(t+1)} & 0 \\ 2\, x_1\, x_3 & 0 & x_1^2 \end{pmatrix} .$$

It follows that

$$0 < \det \nabla y \in W^{1,\infty}(\Omega) \quad \operatorname{cof} \nabla y \in W^{1,\infty}(\Omega; \mathbb{R}^{3\times 3})$$

But $\nabla^2 y \notin L^1(\Omega; \mathbb{R}^{3\times 3\times 3}) \rightsquigarrow y \notin W^{2,1}(\Omega; \mathbb{R}^3)$

On the other hand, $y \in W^{1,p}(\Omega; \mathbb{R}^3) \cap L^\infty(\Omega; \mathbb{R}^3)$ for every $1 \leq p < 1 + t$.

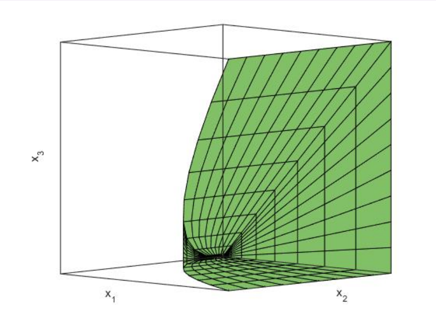

Figure: Deformed cube in the frame of the reference domain $(0,1)^3$ as in the example for $t = 100$. (Picture by J. Valdman)

St. Venant-Kirchhoff material

Let $\varphi : \mathbb{R}^{3\times 3} \to \mathbb{R}$ be a stored energy density of an anisotropic Saint Venant-Kirchhoff material, i.e.,

$$0 \leq \varphi(F) := \frac{1}{8}\mathcal{C}(F^\top F - \mathrm{Id}) : (F^\top F - \mathrm{Id}) \ ,$$

where $\mathcal{C}$ is the fourth-order and positive definite tensor of elastic constants.

Then

$$\hat{W}(G) := \begin{cases} \varphi(G) + \alpha(|\nabla \mathrm{cof}\, G|^q + |\nabla \det G|^r + (\det G)^{-s}) & \text{if } \det G > 0, \\ \infty & \text{otherwise} \end{cases}$$

is gradient polyconvex.

Existence of minimizers

Theorem (BB, MK, AS)

Let be W gradient polyconvex on Ω and $\hat{W}$ coercive as above. Let $p > 2$, $q \geq \frac{p}{p-1}$, $r > 1$, $s > 0$ and assume that for some given measurable function $y_0 : \Gamma_0 \to \mathbb{R}^3$ the following set

$$\begin{aligned}\mathcal{A} := \{ & y \in W^{1,p}(\Omega; \mathbb{R}^3) : \\ & \operatorname{cof} \nabla y \in W^{1,q}(\Omega; \mathbb{R}^{3\times 3}),\ \det \nabla y \in W^{1,r}(\Omega), \\ & (\det \nabla y)^{-s} \in L^1(\Omega),\ \det \nabla y > 0 \text{ a.e. in } \Omega,\ y = y_0 \text{ on } \Gamma_0\}\end{aligned}$$

is nonempty. If $\inf_{\mathcal{A}} J < \infty$ then the functional

$$J = \int_\Omega \hat{W}(\nabla y(x), \nabla \operatorname{cof} \nabla y(x), \nabla \det \nabla y(x))\, \mathrm{d}x$$

has a minimizer on $\mathcal{A}$.

Remarks

- We can also add dependence on $x, y(x)$ without major changes
- The non-emptiness of

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has to be assumed!

$$\Downarrow$$

An analogous situation also happens in classical polyconvexity

&

Actually, this is connected to the relaxation problem....

Sketch of proof I

- Take a minimizing sequence $\{y_k\}$ with $y_k \rightharpoonup y$ in $W^{1,p}(\Omega;\mathbb{R}^3)$
- Based on coercivity we have that

$$\operatorname{cof}\nabla y_k \rightharpoonup H \text{ in } W^{1,q}(\Omega;\mathbb{R}^{3\times 3}) \quad \text{and} \quad \det\nabla y_k \rightharpoonup \delta \text{ in } W^{1,r}(\Omega).$$

- Due to the coercivity $\int_\Omega \frac{1}{(\det\nabla y)^s}\mathrm{d}x$, $\det\nabla y > 0$.

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The weak limit is in $\mathcal{A}$.

Sketch of proof II

To pass to the limit in

$$\int_\Omega \hat{W}(\nabla y(x), \nabla \mathrm{cof}\, \nabla y(x), \nabla \det \nabla y(x))\,\mathrm{d}x$$
$$\leq \liminf_{k\to\infty} \int_\Omega \hat{W}(\nabla y_k(x), \nabla \mathrm{cof}\, \nabla y_k(x), \nabla \det \nabla y_k(x))\,\mathrm{d}x$$

- exploit *convexity* in $\nabla \det(\cdot)$ and $\nabla \mathrm{cof}(\cdot)$
- need at least pointwise convergence in the first term (or convergence in measure)

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Use the information on cofactor and determinant!

Sketch of proof III

- We know that the determinant and the cofactor converge pointwise

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By Cramer's rule we have

$$(\nabla y_k(x))^{-1} = \frac{(\mathrm{cof}\,\nabla y_k(x))^\top}{\det \nabla y_k(x)}$$

and thus,

$$(\nabla y_k(x))^{-1} \longrightarrow (\nabla y(x))^{-1}.$$

Consequently,

$$\begin{aligned}\nabla y_k(x) &= (\mathrm{cof}\,\nabla y_k(x))^{-\top} \det \nabla y_k(x) \\ &\longrightarrow (\mathrm{cof}\,\nabla y(x))^{-\top} \det \nabla y(x) = \nabla y(x),\end{aligned}$$

Apply Fatou lemma

What we have proved...

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Remark: Ciarlet-Nečas condition

We can additionally impose Ciarlet-Nečas condition

$$\int_\Omega \det \nabla y(x)\,\mathrm{d}x \le \mathcal{L}^3(y(\Omega)) \tag{1}$$

$\rightsquigarrow$ Injectivity almost everywhere in the deformed configuration

[Ciarlet, Nečas, 1985], [Hencl, Koskela, 2014]

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$$\Updownarrow$$

the distortion is in $L^{n-1+\delta}$ which implies that y is an open map

[Ciarlet, Nečas, 1985], [Hencl, Koskela, 2014]

Remark: Lower bound on the determinant

We can strengthen the coercivity as

$$\hat{W}(F,\Delta_1,\Delta_2) \geq \begin{cases} c\big(|F|^p + (\det F)^{-s} + |\Delta_1|^q + |\Delta_2|^r\big) & \text{if } \det F > 0, \\ \infty & \text{otherwise.} \end{cases}$$

Proposition (BB, MK, AS)

Take a gradient polyconvex energy with a coercivity according to $r > 3$ and $s > \frac{3r}{r-3}$. (And have the same assumptions as above.) Then, for every $y \in \mathcal{A}$, there is

$$\varepsilon > 0 \text{ such that } \det \nabla y \geq \varepsilon \quad \text{on} \quad \overline{\Omega}$$

This ε depends just on the bound on the energy. In this case $y \in W^{2,1}(\Omega;\mathbb{R}^3)$.

[Healey, Krömer, 2009]

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$\rightsquigarrow$ because under these assumptions the Jacobian is positive up to the boundary!

[Healey, Krömer, 2009]

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This ε depends just on the bound on the energy.

If there is a lower bound on the determinant one may derive a Euler-Lagrange equation.

[Healey, Krömer, 2009]

Strong compactness

Proposition (B.B., M.K., A.S.)
Let $\Omega \subset \mathbb{R}^n$, $n \geq 2$, be a Lipschitz bounded domain and let $\{y_k\}_{k\in\mathbb{N}} \subset W^{1,p}(\Omega;\mathbb{R}^n)$ for $p > n$ be such that for some $s > 0$

$$\sup_{k\in\mathbb{N}} \big(\|y_k\|_{W^{1,p}(\Omega;\mathbb{R}^n)} + \|\mathrm{cof}\,\nabla y_k\|_{\mathrm{BV}(\Omega;\mathbb{R}^{n\times n})} + \|\det\nabla y_k\|_{\mathrm{BV}(\Omega)} + \||\det\nabla y_k|^{-s}\|_{L^1(\Omega)}\big) < \infty\ .$$

Then there is a (nonrelabeled) subsequence and $y \in W^{1,p}(\Omega;\mathbb{R}^n)$ such that for $k \to \infty$ we have the following convergence results: $y_k \to y$ in $W^{1,d}(\Omega;\mathbb{R}^n)$ for every $1 \leq d < p$, $\det\nabla y_k \to \det\nabla y$ in $L^r(\Omega)$ for every $1 \leq r < p/n$, $\mathrm{cof}\,\nabla y_k \to \mathrm{cof}\,\nabla y$ in $L^q(\Omega;\mathbb{R}^{n\times n})$ for every $1 \leq q < p/(n-1)$, and $|\det\nabla y_k|^{-t} \to |\det\nabla y|^{-t}$ in $L^1(\Omega)$ for every $0 \leq t < s$.

Take-home message

- Many requirements of mechanics cannot be fulfilled by CoV
- New variational principle for elasticity (non-standard elliptic regularization)
- We exploit weak continuity of subdeterminants (but in Sobolev spaces), control of $1/\det\nabla y$
- If $n=2$, gradient polyconvexity is the same like adding the full 2nd gradient
- Immediate applications to plasticity, SMA modeling (Mielke's energetic solution)
- Locking/strain-limiting materials ($L(\nabla y(x)) \leq 0$)

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References

1/ Benešová, B., Kružík, M.: Weak lower semicontinuity of integral functionals and applications. *SIAM Review* **59** (2017), 703–766. Preprint arXiv:1601.00390.

2/ Benešová, B., Kružík, M., Schlömerkemper, A.: A note on locking materials and gradient polyconvexity. *Math. Mod. Meth. Appl. Sci.* (2018). Preprint arXiv:1706.04055.