Convex Integration in Materials Sciences

Rigidity and Flexibility

Angkana Rüland

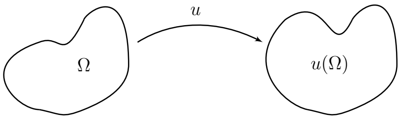
Max Planck Institute for Mathematics in the Sciences

BIRS Worshop on "Convex Integration in PDEs, Geometry, and Variational Calculus"

A Brief Recap of Elasticity

Hyperelastic materials: Consider

$$\mathcal{E}(\nabla u) = \int_\Omega \underbrace{W(\nabla u)}_{\text{energy density}} dx,$$



for deformations $u : \Omega \to \mathbb{R}^3$ in suitable class.

$$T_R(A) = D_A W(A)$$

Modelling ingredients that can lead to mathematical difficulties:

- vector-valued calculus of variations,
- frame indifference,
- symmetry group of materials,
- non-interpenetration of matter,
- ...

Some **basic questions**:

- Existence and Uniqueness,
- Regularity,
- Stability.

Existence Results

- $W(A) \to \infty$, as $\det(A) \to 0^+$,
- $W(A) = \infty$, if $\det(A) \leq 0$.

- implicit functions [Valent],
- direct method with $\mathcal{A} := \{u \in W^{1,1}(\Omega, \mathbb{R}^3) : \mathcal{E}(\nabla u) < \infty, \ u|_{\partial\Omega_1} = u_0\}$ [Ball].

Theorem (Ball '77, Müller-Qi-Yan '94)

Let W satisfy the assumptions

- *W is **polyconvex**, i.e. $W(A) = g(A, \operatorname{cof}(A), \det(A))$ for all $A \in \mathbb{R}^{3\times 3}$ and g **convex**,*
- *$W(A) \geq c_0(|A|^2 + |\operatorname{cof}(A)|^{3/2}) - c_1$ for all $A \in \mathbb{R}^{3\times 3}$, where $c_0 > 0$,*

Then, if $\mathcal{A} \neq \emptyset$, there exists a global minimizer u^* of $\mathcal{E}$ in $\mathcal{A}$.

Existence: Polyconvexity vs Quasiconvexity

Definition

A measurable and bounded below function $f : \mathbb{R}^{m\times n} \rightarrow \mathbb{R} \cup \{+\infty\}$ is *quasiconvex* at $A \in \mathbb{R}^{m\times n}$ if

$$\int\limits_{\Omega} f(A + \nabla\varphi(x))dx \geq \int\limits_{\Omega} f(A)dx$$

for all $\varphi \in C_0^{\infty}(\Omega, \mathbb{R}^m)$.

- Condition is independent of Ω.
- Polyconvexity is strictly stronger than quasiconvexity (Jensen's inequality), quasiconvexity nonlocal notion.
- [Morrey], [Acerbi-Fusco]: Existence results if in addition $C_1|A|^p - C_0 \leq f(A) \leq C_2(|A|^p + 1)$ for all $A \in \mathbb{R}^{m\times n}$, $p > 1$.

Uniqueness and Regularity

- At best partial regularity results [Nečas 77], [Hao-Leonardi-Nečas 96], [Šverák-Yan 00], [Mooney-Savin 15]...
- [Evans 86], [Kristensen-Taheri 01]: partial regularity for global minimizers of strongly quasiconvex functionals.

Satisfaction of Euler-Lagrange equations

$$\operatorname{div}(D_A W(\nabla u)) = 0$$

cannot suffice for partial regularity:

Theorem (Müller-Šverák)

There exists a strongly quasi-convex function $W : \mathbb{R}^{2\times 2} \to \mathbb{R}$ such that there are Lipschitz mappings $u : \Omega \to \mathbb{R}^2$ solving $\operatorname{div}(D_A W(\nabla u)) = 0$ weakly which are on no open set C^1 regular.

Uniqueness and Regularity

Satisfaction of Euler-Lagrange equations

$$\operatorname{div}(D_A W(\nabla u)) = 0$$

cannot suffice for partial regularity:

Theorem (Müller-Šverák)

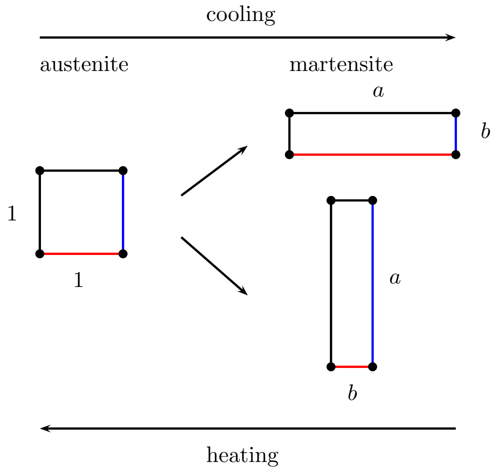
There exists a strongly quasi-convex function $W : \mathbb{R}^{2\times 2} \to \mathbb{R}$ such that there are Lipschitz mappings $u : \Omega \to R^2$ solving $\operatorname{div}(D_A W(\nabla u)) = 0$ weakly which are on no open set C^1 regular.

- Extensions to polyconvex functionals [Székelyhidi], parabolic problems [Müller-Rieger-Šverák].
- Exploits presence of stable T_4 (respectively T_5 configurations).

Question

Does this also happen in equations which are relevant for elasticity?

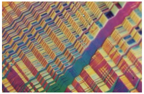
Solid-Solid Phase Transformations in SMA

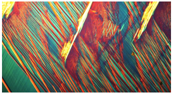


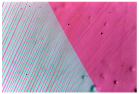
$$SO(2)\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$$

$$SO(2)\begin{pmatrix} b & 0 \\ 0 & a \end{pmatrix}$$

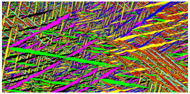
$SO(2) = \{2 \times 2$
rotation matrices$\}$


crossing twins


low hysteresis material


aust.-mart. interface

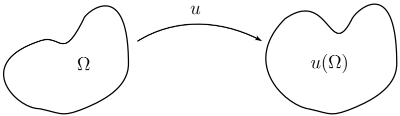

needles


wild microstructures

The Phenomenological Theory

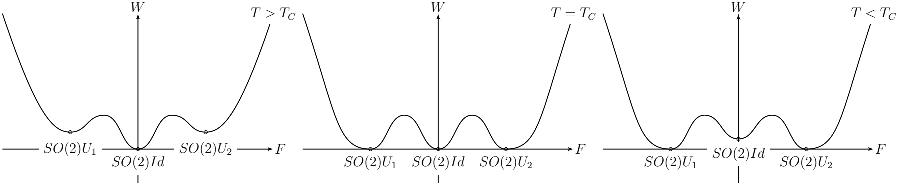
[Ball & James]: Minimize

$$\mathcal{E}(\nabla u, T) = \int_\Omega \underbrace{W_T(\nabla u)}_{\text{energy density}} \, dx,$$



for deformations $u : \Omega \to \mathbb{R}^2$.

$$W_T(QF) = W_T(F) \text{ for all rotations } Q,$$
$$W_T(FR) = W_T(F) \text{ for all material symmetries } R.$$



The High Temperature Regime $\nabla u \in SO(2)$

Theorem (Liouville)

Let $u \in W^{1,\infty}$ be a solution to $\nabla u \in SO(n)$, then $\nabla u = Q$ for some fixed $Q \in SO(n)$.

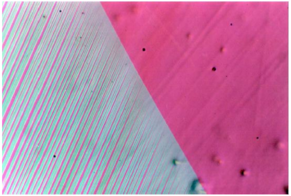
Theorem (Friesecke-James-Müller)

There exists $C = C(\Omega) > 0$ and $Q \in SO(n)$ such that for all $p \in (1, \infty)$

$$\int_{\Omega} |\nabla u - Q|^p dx \leq C \int_{\Omega} \operatorname{dist}^p(\nabla u, SO(n)) dx.$$

- Applications to dimension reduction.
- Extensions to incompatible results ([Müller-Scardia-Zeppieri], [Luckhaus-Lauteri]) $\rightsquigarrow$ discrete-to-continuum limits [Kitavtsev-Luckhaus-Lauteri-Rüland].

Lack of Quasiconvexity: The Low Temperature Regimes



There exists $\{u_k\}_{k\in\mathbb{N}}$ with $\nabla u_k \rightharpoonup Id$ such that

$$W(Id) \geq \liminf_{k\to\infty} W(\nabla u_k).$$

Remedy: **Relaxation**.

Definition (Gradient Young Measure)

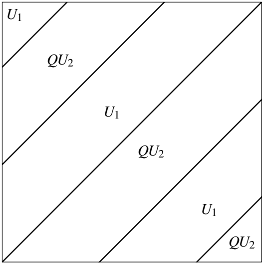
A map $\nu : \Omega \to \mathbb{R}^{n\times n}$ is a $W^{1,p}$ gradient Young measure, if there exists a sequence $u_j : \Omega \to \mathbb{R}^n$ such that

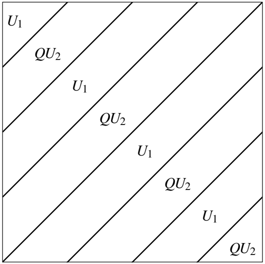
- $u_j \rightharpoonup u$ in $W^{1,p}(\Omega)$,
- $\delta_{\nabla u_j} \rightharpoonup \nu$ weak-$*$ in $L^\infty(\Omega, \mathcal{M}(\mathbb{R}^{n\times n}))$.

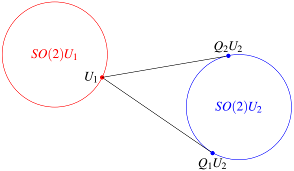
- $\int\limits_{\Omega} f(\nabla u_j)dx \to \int\limits_{\Omega}\int\limits_{\mathbb{R}^{n\times n}} f(A)d\nu_x(A)dx$

Existence of Exactly Stress-Free Solutions

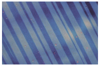
$$\nabla u \in SO(2)U_1 \cup SO(2)U_2$$







rank-one connections



$$\boxed{\begin{aligned} U_1 - Q_1 U_2 &= \sqrt{2}\frac{a^2-b^2}{a^2+b^2}\begin{pmatrix} a \\ -b \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad Q_1 \in SO(2), \\ U_1 - Q_2 U_2 &= \sqrt{2}\frac{a^2-b^2}{a^2+b^2}\begin{pmatrix} a \\ b \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad Q_2 \in SO(2). \end{aligned}}$$

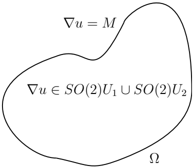
Flexibility

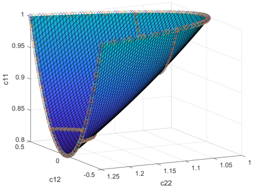
Theorem

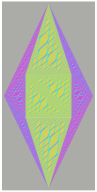
For any $\Omega \subset \mathbb{R}^2$ *and any* $M \in \text{int}(SO(2)U_1 \cup SO(2)U_2)^{lc}$ *there exists a deformation* u *such that*

$$\nabla u \in SO(2)U_1 \cup SO(2)U_2 \text{ a.e. in } \Omega,$$
$$\nabla u = M \text{ in } \mathbb{R}^2 \setminus \Omega.$$

- [Dacorogna-Marcellini] (relaxation property & Baire category)
- [Müller-Šverák] (convex integration)







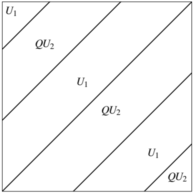
Q: Are these solutions physically relevant?

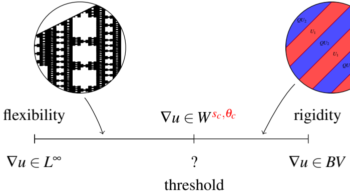
Theorem (Dolzmann-Müller, Rigidity)

Let $\Omega \subset \mathbb{R}^2$, $u : \Omega \to \mathbb{R}^2$ with $\nabla u \in BV(\Omega)$ and

$$\nabla u \in SO(2)U_1 \cup SO(2)U_2 \text{ a.e. in } \Omega.$$

Then ∇u is (locally) a laminate.





Extensions:

- [Dacorogna-Marcellini-Paolini] ($O(2)$, $O(n)$),
- [Kirchheim] & [Conti-Dolzmann-Kirchheim] (cubic-to-tetragonal),
- [R '16] (cubic-to-orthorhombic).

Q: Is there a threshold behaviour between rigidity and flexibility?

Flexibility at Higher Sobolev Regularity

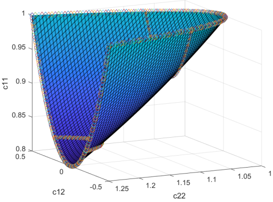
Theorem (Della Porta-R. '19)

For any $\Omega \subset \mathbb{R}^2$ *and any* $M \in \text{int}(SO(2)U_1 \cup SO(2)U_2)^{lc}$ *there exists a deformation* u *and a threshold* $\theta_0 \in (0,1)$ *such that*

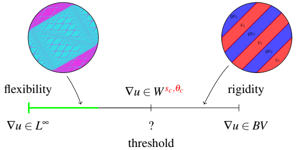
$$\nabla u \in SO(2)U_1 \cup SO(2)U_2 \text{ a.e. in } \Omega,$$
$$\nabla u = M \text{ in } \mathbb{R}^2 \setminus \Omega,$$

and for all $s \in (0,1)$, $p \in (1,\infty)$ *with* $0 < sp < \theta_0$

$$\nabla u \in W^{s,p}(\Omega) \cap L^\infty(\Omega).$$

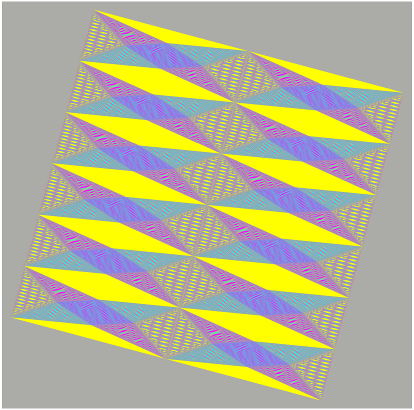


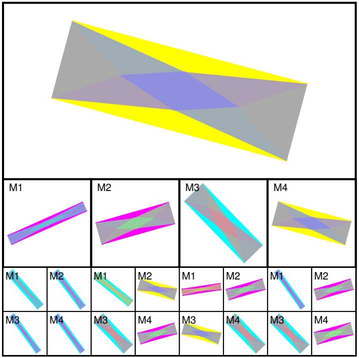
- Building on [Rüland-Zillinger-Zwicknagl].

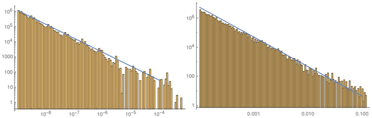


- $K^{lc} = K^c \cap \{M \in \mathbb{R}^{2\times 2} : \det(M) = 1\} \neq K^c$; nonlinear geometry!

Simulations first Algorithm [R.-Taylor-Zillinger '18]







$$\theta_0 \sim 0.132$$

Surface Energies

$$E_\epsilon = \min_{\nabla u = M \text{ a.e. in } \mathbb{R}^n \setminus \overline{\Omega}} \left\{ \int_\Omega \operatorname{dist}^2(\nabla u, K) dx + \epsilon^2 \int_\Omega |\nabla^2 u|^2 dx \right\}.$$

Theorem (Taylor-R.-Zillinger, J. Nonl. Science '18)

Assume that there exist constants $C > 1$ such that for all $\epsilon \in (0, \epsilon_0)$ it holds $E_\epsilon \geq C\epsilon^{2\mu}$. Suppose that u is a solution to

$$\nabla u \in K \textit{ a.e. in } \Omega, \; \nabla u = M \textit{ a.e. in } \mathbb{R}^n \setminus \overline{\Omega}.$$

If $v(x) := u(x) - Mx - b \in H^{s+1}(\mathbb{R}^n)$ for some $b \in \mathbb{R}^n$, $s \in \mathbb{R}$ and $\nabla v \in L^\infty(\mathbb{R}^n)$, then $s \leq \mu$.

[Chan-Conti '14, '15]: Two-well problem, $M = Id$, true for $M \in \partial K^{lc}$.

Excursion: Flexibility for m Incompatible Matrices

Question

Q: *Are there solutions to the differential inclusion $\nabla u \in K$ if $K = \{A_1, \dots, A_m\}$ with affine boundary conditions if $\operatorname{rk}(A_i - A_j) > 1$ for $i \neq j$?*

- If $m < 4$: No!
- If $m = 4$: No, but almost – existence of T_4 deformations, loss of rigidity of approximate solutions.
- If $m = 5$: Yes, [Kirchheim-Preiss], [Pompe].

$$A_1 = \begin{pmatrix} 3 & 0 \\ 0 & -1 \end{pmatrix}, A_2 = \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}, A_3 = \begin{pmatrix} -3 & 0 \\ 0 & 1 \end{pmatrix}, A_4 = \begin{pmatrix} -1 & 0 \\ 0 & -3 \end{pmatrix}.$$

Nemetic Elastomers – Ogden-Type Stored Energy Densities

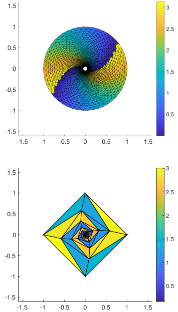
$$W(F) = \sum_{i=1}^{N} \frac{c_i}{\gamma_i} \left[\left(\frac{\lambda_1(F)}{e_1} \right)^{\gamma_i} + \left(\frac{\lambda_2(F)}{e_2} \right)^{\gamma_i} + \left(\frac{\lambda_3(F)}{e_3} \right)^{\gamma_i} - 3 \right], \det(F) = 1$$

Theorem (Agostiniani-Dal Maso-De Simone)

Let $v : \Omega \to \mathbb{R}^3$ *such that* $\det(\nabla v) = 1$ *and*

$$\operatorname{essinf}_{\Omega} \lambda_1(\nabla v) > e_1, \ \operatorname{esssup}_{\Omega} \lambda_3(\nabla v) < e_3.$$

Then for every $\epsilon > 0$ *there exists* $y_\epsilon : \Omega \to \mathbb{R}^3$ *Lipschitz such that* $W(\nabla y_\epsilon) = 0$ *a.e. in* Ω, $y_\epsilon = v$ *on* $\partial\Omega$ *and* $\|y_\epsilon - v\|_{L^\infty(\Omega)} \leq \epsilon$.



- [Cesana-Della Porta-R.-Zillinger-Zwicknagl]: View as limiting setting of highly symmetric martensitic deformations of low energy.

1. Quasiconvex Elasticity

2. Non-Quasiconvex Elasticity – Shape Memory Alloys

3. Constraints

4. Thin Elastic Plates, Folding and Crumpling

5. Conclusions

Non-Interpenetration of Matter

Theorem (Kuomatos-Rindler-Wiedemann)

Let $p \in (1, n)$ and $\nu \subset \mathcal{M}(\mathbb{R}^{n\times n})$ be a p-Young measure. Then the following are equivalent:

- *There exists a sequence $\{\nabla u_j\} \subset L^p(\Omega, \mathbb{R}^{n\times n})$ which generate ν such that $\det(\nabla u_j) > 0$ a.e. for all $j \in \mathbb{N}$.*
- *The following conditions hold:*
  - $\int\limits_{\Omega} \int |A|^p d\nu_x(A) dx < \infty$,
  - *$\exists u$ such that $L^p(\Omega) \ni \nabla u = \int A d\nu_x(A)$ a.e.,*
  - *Jensen: $h(\nabla u(x)) \leq \int h(A) d\nu_x(A)$ for a.e. $x \in \Omega$ and h quasiconvex,*
  - *for a.e. $x \in \Omega$ we have $\operatorname{supp}(\nu_x) \subset \{M \in \mathbb{R}^{n\times n} : \det(M) \geq 0\}$.*

- [Benešová-Kružik-Patho]: invertible gradient Young measures.
- Here only pointwise constraint. [Hencl]: Positivity of Jacobian at low regularity is not necessary for injectivity; rigidity at high regularity.
- Difficulty: Cut-off techniques used in [Pedregal].

Non-Interpenetration of Matter

Corollary (Kuomatos-Rindler-Wiedemann)

Let $u \in W^{1,p}(\Omega)$ *with* $p \in (1,n)$, $\det(\nabla u) = 0$. *Then there exists a sequence* $v_j \in W^{1,p}(\Omega)$ *such that*

- $v_j \to u$ *in* $W^{1,p}(\Omega)$,
- $v_j|_{\partial\Omega} = u|_{\partial\Omega}$,
- *and such that* $\det(\nabla v_j) > 0$.

- For $p > n$ impossible: By Stokes' Theorem

$$\int_{\Omega} \det(\nabla v_j)dx = \int_{\Omega} dv_j^1 \wedge \cdots \wedge dv_j^n = \int_{\partial\Omega} v_j^1 \wedge dv_j^2 \wedge \cdots \wedge dv_j^n$$
$$= \int_{\partial\Omega} u^1 \wedge du^2 \wedge \cdots \wedge du^n = \int_{\Omega} \det(\nabla u)dx.$$

Some Possible Constraints

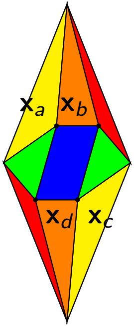
Differential inclusion

$$\nabla u \in K,$$

with $K \subset \mathbb{R}^{n\times n}$.

Possible constraints:

- Incompressibility $\det(\nabla u) = 1$.
- Infinitesimal incompressibility $\operatorname{tr}(\nabla u) = 1$.
- Linear restrictions in K.
- [DeSimone-Dolzmann]: Nonlinear Magnetoelasticity (nonlinear elasticity + Maxwell-type convex integration result).



Question

Q: *How many constraints can you impose without losing existence of convex integration solutions?*

1. Quasiconvex Elasticity

2. Non-Quasiconvex Elasticity – Shape Memory Alloys

3. Constraints

4. Thin Elastic Plates, Folding and Crumpling

5. Conclusions

Monge-Ampère Equations

Nonlinear elastic plates – ansatz for deformation:

$$\phi_\epsilon = id + \epsilon v e_3 + \epsilon^2 w : \Omega \subset \mathbb{R}^2 \to \mathbb{R}^3.$$

- v out-of-plane displacement,
- w in-plane displacement.

$$\begin{aligned}(\nabla\phi_\epsilon)^T\nabla\phi_\epsilon - Id_2 = \epsilon^2 A_0 + o(\epsilon^2) &\Leftrightarrow \frac{1}{2}\nabla v \otimes \nabla v + e(\nabla w) = A_0 \text{ in } \Omega\\ &\Leftrightarrow -\operatorname{curl}\operatorname{curl}(\nabla v \otimes v) = f \text{ in } \Omega\\ &\quad \text{if } -\operatorname{curl}\operatorname{curl}(A_0) = f.\end{aligned}$$

Very weak Hessian $\mathcal{D}et(\nabla^2 v) := -\frac{1}{2}\operatorname{curl}\operatorname{curl}(\nabla v \otimes \nabla v) = f$.

Theorem

Let $f \in L^{\frac{7}{6}}(\Omega)$, $\alpha < \frac{1}{7}$. Then the set of $C^{1,\alpha}(\overline{\Omega})$ solutions to $\mathcal{D}et(\nabla^2 v) = f$ is dense in $C^0(\overline{\Omega})$.

Folding, Crumpling and Origami

$\nabla u \in O(3,2)$

$:= \{M \in \mathbb{R}^{3\times 2}: \; M^T M = Id\}.$

- [Conti-Maggi]: Study of the confinement problem ($u(\Omega) \subset B_r(0)$, $0 < r \ll r_{cri}$): Scaling laws and density of origami constructions in short maps.

$$E_h(\psi, \Omega) := \frac{1}{h} \int\limits_{\Omega\times(0,h)} W(\nabla\psi(x,y,z))dxdydz.$$

- $W(QF) = W(F)$,
- $c\,\mathrm{dist}^2(F, SO(3)) \leq W(F)$,
- $W(F) \leq C\,\mathrm{dist}^2(F, SO(3))$.

"energy per unit thickness"

Folding, Crumpling and Origami

$$I_h(u,\Omega) := \int\limits_{\Omega} \left(|\nabla u^T \nabla u - Id_2|^2 + h^2 |\nabla^2 u|^2 \right) dxdy.$$

Theorem (Conti-Maggi)

Let $\alpha \in (0, 5/3)$. For any short map $u \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ and $h_k \to 0$ there exists a sequence of deformations converging to u uniformly

$$\lim_{k\to\infty} h_k^{-\alpha} E_{h_k}(\psi_k, \Omega) = 0.$$

- Also: upper bounds for origami maps; relevance of convex integration schemes in order to reduce to subclass of origami structures.
- Conjecture: $h^{\frac{5}{3}}$ is the scaling law for the problem.

Folding, Crumpling and Origami

$$I_h(u,\Omega) := \int\limits_{\Omega} \left(|\nabla u^T \nabla u - Id_2|^2 + h^2 |\nabla^2 u|^2 \right) dxdy.$$

Theorem (Conti-Maggi)

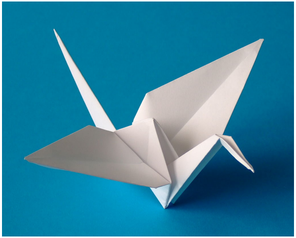
Let $\alpha \in (0, 5/3)$. For any short map $u \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ and $h_k \to 0$ there exists a sequence of deformations converging to u uniformly

$$\lim_{k\to\infty} h_k^{-\alpha} E_{h_k}(\psi_k, \Omega) = 0.$$

A lot of recent work in materials science community on obtaining special origami structures and classifying these, e.g. [Feng-Plucinski-James] "Helical Miura Origami".

Conclusions

- Convex integration produces surprising exact solutions in non-quasiconvex settings (SMA, nematic elastomers, thin sheets).
- Certain constraints can be dealt with.
- Possibly shows that models have to be augmented with additional structure.



Questions

(Q1) *Physical relevance of convex integration in materials? Experimental observations?*

(Q2) *Selection mechanisms to distinguish plethora of "unphysical" from physical solutions?*

(Q3) *Useful in materials design (e.g. origami type structures)?*