A Geometrically Exact Cosserat Model Including Sharp Interfaces And Fracture. Mathematical Analysis.

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Plan of the talk

- Introduction
- Classical linear and finite elasticity as minimization problems
- Ellipticity, quasiconvexity, material failure and fracture
- The finite Cosserat approach
- Mathematical analysis of the Cosserat model: Existence results
- Analytical example for microstructure in simple glide
- Open problems
- Conclusions

Introduction

- Continuum mechanical models relating macroscopic (averaged) quantities.
- Need to describe large deformation and failure (picture): shear bands, localization, fracture
- Necessary: finite deformations, geometrically exact formulation (frame-indifferent, not necessarily covariant)
- Classical linear models not suitable: non-convexity, non-linearity, non-uniqueness, non-smoothness, non-homogeneity

Notation

- $\varphi : \Omega \subseteq \mathbb{R}^3 \mapsto \mathbb{R}^3$, the deformation, Ω reference configuration.
- $F = \nabla\varphi \in \mathrm{GL}^+(3, \mathbb{R})$, the deformation gradient, $1\!\!1$ the identity.
- $\overline{R} : \Omega \mapsto \mathrm{SO}(3, \mathbb{R})$ true rotation, $R = \mathrm{polar}(F)$ orthogonal part.
- $W(F)$ elastic free energy density, $D_F W(F)$ first P. K. stresses.
- $D_F^2 W(F).(H, H)$ bilinear form of second differential.
- $\|A\|$, $\langle A, B\rangle$, $\mathrm{tr}\,[A]$ norm, scalar product and trace.
- $F = R\,U = \mathrm{polar}(F)\,U, \quad R \in \mathrm{SO}(3)$, polar decomposition.

The classical linear elasticity problem

Write $\varphi(x) = x + u(x)$, $F = 1\!\!1 + \nabla u$, u displacement:

$$\int_\Omega W(\nabla u) - \langle f, u\rangle \,\mathrm{dV} \mapsto \min . \text{ w.r.t. } u,\ u_{|_\Gamma} = u_\mathrm{d}$$

$$W(\nabla u) = \mu \,\|\operatorname{sym} \nabla u\|^2 + \frac{\lambda}{2} \operatorname{tr}\left[\operatorname{sym} \nabla u\right]^2$$

$$\mu,\ \lambda > 0, \quad \text{Lamé constants}$$

Existence, uniqueness, regularity classical. Korn's first inequality.
Euler-Lagrange equations linear elliptic system of second order PDE, constant coefficients.
Not frame-indifferent, physically irrelevant model

The St. Venant-Kirchhoff finite elasticity model as minimization problem

Frame-indifferent extension to finite deformations:

$$\int W(F) - \langle f, \varphi \rangle \,\mathrm{dV} \mapsto \min . \text{ w.r.t. } \varphi, \quad \varphi_{|\Gamma} = g_{\mathrm{d}}$$

$$W(F) = \frac{\mu}{4} \|F^T F - 1\!\!1\|^2 + \frac{\lambda}{8} \operatorname{tr}\left[F^T F - 1\!\!1\right]^2$$

$$1\mathrm{dim} : (|\varphi'|^2 - 1)^2 \text{ non-convex on } \varphi' \geq 0$$

Finite elasticity: Nonlinear Euler-Lagrange equations of no help.

Least action: Find minimizers $\varphi \in W^{1,4}(\Omega, \mathbb{R}^3)$, φ continuous.

Direct methods of variations (Ball'77): weak convergence, ellipticity

Ellipticity conditions

- uniform convexity: $D_F^2 W(x,F).(H,H) \geq c^+ \|H\|^2$, inappropriate!
- uniform Legendre-Hadamard elliptic (stable material, elliptic regularity): $D_F^2 W(x,F).(\xi\otimes\eta,\xi\otimes\eta) \geq c^+ \|\xi\|^2 \|\eta\|^2$
- Hadamard's jump condition: $\varphi \in W^{1,1}(\Omega,\mathbb{R}^3)$, φ continuous across hyperplane, if $\nabla\varphi = \begin{cases} A \\ B \end{cases}$ jumps across hyperplane $\mathcal{H} \Rightarrow$ $A - B = \xi\otimes\eta$.
- φ minimizer and solution of E-L: $\nabla\varphi$ cannot jump across hyperplane $\Leftrightarrow\ D_F^2 W(\nabla\varphi).(\xi\otimes\eta,\xi\otimes\eta) \geq c^+\|\xi\|^2 \|\eta\|^2$

Weak convergence

- **weak lower semicontinuity**:
  $\varphi_k \rightharpoonup \varphi \Rightarrow \int\limits_{\Omega} W(\nabla\varphi)\,\mathrm{dV} \leq \liminf_k \int\limits_{\Omega} W(\nabla\varphi_k)\,\mathrm{dV}$

- W **quasiconvex**: $\int\limits_{\Omega} W(B)\,\mathrm{dV} \leq \int\limits_{\Omega} W(\nabla\varphi)\,\mathrm{dV}, \quad \varphi(x)_{\partial\Omega} = B.x,$
  homogeneous response is energy optimal

- **convex, polyconvex** $\Rightarrow$ **weak lower semicontinuity**

- **quasiconvex** $\Leftrightarrow$ **weak lower semicontinuity**

- **quasiconvex** $\Rightarrow$ **Legendre-Hadamard ellipticity** (not reverse!)

Failure and microstructure

- material failure: $D_F^2 W(x,F).(\xi \otimes \eta, \xi \otimes \eta) < 0$
- sharp interfaces: $\varphi \in H^{1,2}(\Omega) \setminus H^2(\Omega)$
- fracture: $\varphi \notin W^{1,1}(\Omega)$
- Microstructure: non-homogeneous response to homogeneous data
- goal: allow for microstructure without leaving $H^{1,2}(\Omega)$
- slide (overhead: possible response to simple glide)

Non-ellipticity of St. Venant-Kirchhoff

$$W(F) = \|F^T F - 1\!\!1\|^2$$
$$D_F W(F).H = 2\langle F^T F - 1\!\!1, F^T H + H^T F\rangle$$
$$D_F^2 W(F).(H,H) = 4\langle F^T F - 1\!\!1, H^T H\rangle + 2\|F^T H + H^T F\|^2$$
$$D_F^2 W(F_0).(\xi\otimes\eta, \xi\otimes\eta) < 0, \quad \langle \xi, \eta\rangle = 0,\ F_0 = m\cdot 1\!\!1,\ m < 1$$

material failure already under pressure, expect microstructure $\Rightarrow$
no mathematical existence for St. Venant-Kirchhoff.
Wrong Sobolev space?

The Biot finite elasticity model

Deformations in $W^{1,2}(\Omega, \mathbb{R}^3)$, φ not necessarily continuous:

$$\int W(U) - \langle f, \varphi \rangle \, \mathrm{dV} \mapsto \min . \text{ w.r.t. } \varphi, \quad \varphi_{|_\Gamma} = g_{\mathrm{d}}$$

$$W(U) = \mu \, \| \, \mathrm{sym}(U - 1\!\!1) \|^2 + \frac{\lambda}{2} \mathrm{tr} \left[\mathrm{sym}(U - 1\!\!1) \right]^2$$

$1\mathrm{dim} : (|\varphi'| - 1)^2$ convex on $\varphi' \geq 0$

$U = R(F)^T \, F = \sqrt{F^T F}$ symmetric stretch tensor

$R(\nabla\varphi) = \mathrm{polar}(\nabla\varphi)$ continuum rotation

not Legendre-Hadamard elliptic, material failure only due to continuum rotations $R(F)$, no mathematical results for Biot

Regularization alternatives

- higher gradient theories: introduce $D_x^2\varphi$: problem: fourth order system of pde, computationally prohibitive

- viscoelasticity

- quasiconvexification: modify energy, keep first gradient structure: problem: no precise information on the deformation, φ is probability measure

- Cosserat continua, micromorphic-continua

The Cosserat approach

- Idea: relax constraint on the rotations $R(\nabla\varphi)$ to coincide with continuum rotations $\operatorname{polar}(\nabla\varphi)$. Allow for independent (micro) rotations $\overline{R}$ (Cosserat 1906)

- Attribute energy to spatial variations of rotations (curvature): $W_{\text{curv}}(\mathrm{D_x}\overline{R}) = \mu\, {L_c}^p \|\mathrm{D_x}\overline{R}\|^p$.

- Look for independent fields $\varphi, \overline{R}$ in the minimization problem. $\overline{R} \in \mathrm{SO}(3,\mathbb{R})$ nonlinear manifold

The finite Cosserat problem in variational form

$$\int W_{\mathrm{mp}}(\overline{U}) + \mu\, L_c{}^p \|\mathrm{D_x}\overline{R}\|^p - \langle f, \varphi\rangle\, \mathrm{dV} \mapsto \min\,.\ \text{w.r.t.}\ (\varphi, \overline{R}),$$

$$W_{\mathrm{mp}}(\overline{U}) = \mu\, \|\,\mathrm{sym}(\overline{U} - 1\!\!1)\|^2 + \frac{\lambda}{2}\,\mathrm{tr}\left[\mathrm{sym}(\overline{U} - 1\!\!1)\right]^2$$

$$+ \mu_c\, \|\mathrm{skew}(\overline{U} - 1\!\!1)\|^2$$

$\overline{U} = \overline{R}^T F,$ non-symmetric micropolar stretch tensor.

No previous mathematical results.

E-L: linear momentum+angular momentum: nonlinear second order PDE, non-constant coefficients

The Cosserat curvature energy

The curvature term has the form

$$W_{\text{curv}}(\mathrm{D_x}\overline{R}) = \mu\, L_c{}^{p}\, \|\mathrm{D_x}\overline{R}\|^{p}\,,$$

$$\mathrm{D_x}\overline{R} = \left(\nabla(\overline{R}.e_1), \nabla(\overline{R}.e_2), \nabla(\overline{R}.e_3)\right)\ .$$

Coercivity of curvature

$$\exists\, c^{+} > 0\ \exists\, r > 1:\ \forall\, \mathfrak{K} \in \mathfrak{T}(3):\quad W_{\text{curv}}(\mathfrak{K}) \geq c^{+}\,\|\mathfrak{K}\|^{r}$$

$$\exists\, r > 1:\quad \frac{W_{\text{curv}}(\mathfrak{K})}{\|\mathfrak{K}\|^{r}} \to \infty \quad \text{as } \|\mathfrak{K}\| \to \infty$$

$$\Rightarrow \quad p > 1$$

$L_c > 0$: internal length, characteristic for the material (grain size).

The infinitesimal, linear Cosserat problem

Expand $F = 1\!\!1 + \nabla u$, $\overline{R} = 1\!\!1 + \overline{A} + \ldots$, $\overline{A} \in \mathfrak{so}(3, \mathbb{R})$

$$\int_\Omega W_{\mathrm{mp}}(\nabla u, \overline{A}) + \mu\, L_c{}^2\, \|\mathrm{D_x}\overline{A}\|^2 - \langle f, u\rangle\,\mathrm{dV} \mapsto \min.\ \text{w.r.t. } (u, \overline{A}),$$

$$W_{\mathrm{mp}}(\nabla u, \overline{A}) = \mu\, \|\,\mathrm{sym}\,\nabla u\|^2 + \frac{\lambda}{2}\,\mathrm{tr}\,[\mathrm{sym}\,\nabla u]^2 + \mu_c\, \|\mathrm{skew}\,\nabla u - \overline{A}\|^2$$

Cosserat couple modulus $\mu_c = 0 \Rightarrow$ no coupling, linear elasticity.

$L_c = 0 \Rightarrow$ linear elasticity.

The Cosserat couple modulus μ_c

- $\mu_c > 0: \quad D_F^2 W_{\mathrm{mp}}(\overline{R}^T F).(H,H) \geq 2\,\mu_c\,\|H\|^2$
- $\mu_c = 0: \quad D_F^2 W_{\mathrm{mp}}(\overline{R}^T F).(H,H) \geq 2\,\mu\|\frac{1}{2}(\overline{R}^T H + H^T\overline{R})\|^2$
- $\mu_c = 0: \quad D_F^2 W_{\mathrm{mp}}(\overline{R}^T F).(\xi\otimes\eta,\xi\otimes\eta) \geq \mu\,\|\xi\|^2\|\eta\|^2$
- $\mu_c = 0$: uniformly Legendre-Hadamard independent of $\overline{R}(x)$
- $\mu_c = 0$: linearization coincides with classical linear elasticity!
- engineers, thinking linear believe: $\mu_c > 0$ necessary

Cases for the finite Cosserat model

I: $\mu_{\mathbf{c}} > \mathbf{0}$, $\mathbf{p} \geq \mathbf{2}$, existence of minimizers trivial. **Fracture excluded**.

II: $\mu_{\mathbf{c}} = \mathbf{0}$, $\mathbf{p} > \mathbf{3}$, existence of minimizers. **Fracture excluded**.

IV: $\mu_{\mathbf{c}} = \mathbf{0}$, $\mathbf{1} < \mathbf{p} \leq \mathbf{3}$, possibly $\varphi \notin W^{1,1}(\Omega)$. **Fracture included**.

V: $\mu_{\mathbf{c}} = \mathbf{0}, \mathbf{L}_{\mathbf{c}} = \mathbf{0}$, weak solutions of Biot finite elasticity are stationary points of the Cosserat variational problem. **Sharp interfaces**.

Existence for $\mu_c > 0$, $p \geq 2$

Theorem 0.1. **[$\mu_c > 0$, $p \geq 2$]** *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain and assume for the boundary data $g_{\mathrm{d}} \in H^1(\Omega, \mathbb{R}^3)$ and $\overline{R}_{\mathrm{d}} \in W^{1,p}(\Omega, \mathrm{SO}(3,\mathbb{R}))$. Moreover, let $f \in L^2(\Omega, \mathbb{R}^3)$. Then the Cosserat problem with material constants conforming to case I admits at least one minimizing solution pair $(\varphi, \overline{R}) \in H^1(\Omega, \mathbb{R}^3) \times W^{1,p}(\Omega, \mathrm{SO}(3,\mathbb{R}))$.*

Direct methods of variations, Ball 1977 (polyconvexity)

Sketch of proof $\mu_c > 0$: part 1

- Take infimizing sequences of deformations φ_k and rotations $\overline{R}^k$.
- Since $\|\mathrm{D_x}\overline{R}\|^p$ in the energy, control $\overline{R}^k$ in $W^{1,p}(\Omega)$.
- Take strongly convergent subsequence of rotations $\overline{R}^k \to \overline{R}$ in L^p.
- $\mu_c > 0$: elastic energy estimates strain part: $\|\overline{R}^{k,T}\nabla\varphi_k - 1\!\!1\|^2 = \|\overline{R}^{k,T}\nabla\varphi_k\|^2 - 2\langle\overline{R}^k, \nabla\varphi_k\rangle + 3 \geq \|\nabla\varphi_k\|^2 - 2\sqrt{3}\|\nabla\varphi_k\| + 3$

Sketch of proof $\mu_c > 0$: part 2

- Boundedness of deformations $\varphi_k \in H^{1,2}(\Omega)$ independent of spatial features of microrotations $\overline{R}(x)$!
- Extract weakly convergent subsequence of deformations $\varphi_k \rightharpoonup \varphi$
- Choose $\overline{R}^k \rightharpoonup \overline{R}$ in $W^{1,p}(\Omega)$.
- Subsequence $(\varphi_k, \overline{R}^k)$ with $\overline{R}^{k,T} \nabla\varphi_k \rightharpoonup \tilde{\overline{U}} \in L^2(\Omega)$
- $p \geq 2: \ \overline{R}^k \to \overline{R} \in L^2(\Omega) \Rightarrow \overline{R}^{k,T} \nabla\varphi_k \rightharpoonup \overline{R}^T \nabla\varphi \in L^1(\Omega)$
- $\tilde{\overline{U}} = \overline{R}^T \nabla\varphi \in L^2(\Omega)$
- Energy is convex in $\mathrm{D_x}\overline{R}$ and $\overline{U} = \overline{R}^T \nabla\varphi$

Existence for: $\mu_c = 0,\ p > 3$

Theorem 0.2. **[$\mu_c = 0,\ p > 3$]** *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain and assume for the boundary data $g_{\mathrm{d}} \in H^1(\Omega, \mathbb{R}^3)$ and $\overline{R}_{\mathrm{d}} \in W^{1,p}(\Omega, \mathrm{SO}(3, \mathbb{R}))$. Moreover, let $f \in L^2(\Omega, \mathbb{R}^3)$. Then the Cosserat problem with material constants conforming to case II admits at least one minimizing solution pair $(\varphi, \overline{R}) \in H^1(\Omega, \mathbb{R}^3) \times W^{1,p}(\Omega, \mathrm{SO}(3, \mathbb{R}))$.*

Sketch of proof $\mu_c = 0$, $p > 3$: part 1

- Take infimizing sequences of deformations φ_k and rotations $\overline{R}^k$.
- Since $\|\mathrm{D_x}\overline{R}\|^p$ in the energy, control $\overline{R}^k$ in $W^{1,p}(\Omega)$.
- Sobolev embedding $p > n = 3$: $W^{1,p} \subset C^0(\overline{\Omega})$: take strongly convergent subsequence of rotations $\overline{R}^k \to \overline{R}$ in $C(\overline{\Omega})$.
- Strain part: $\|\overline{R}^{k,T}\nabla\varphi_k + \nabla\varphi_k^T\overline{R}^k - 2\mathbb{1}\|^2$ is bounded.

Sketch of proof $\mu_c = 0$, $p > 3$: part 2

Consider $\varphi_k = x + u_k(x)$

$$\begin{aligned} &\|\overline{R}^{k,T}\,\nabla\varphi_k + \nabla\varphi_k^T\,\overline{R}^k - 2\mathbb{1}\|^2 \\ &\geq \|\overline{R}^{k,T}\,\nabla u_k + \nabla u_k^T\,\overline{R}^k\|^2 - C\,\|\nabla u_k\| - C \\ &\geq c_K^+\,\|u_k\|^2_{H^{1,2}(\Omega)} - C\,\|u_k\|_{H^{1,2}(\Omega)} - C \end{aligned}$$

Use extended Korn's inequality (**coercivity** of deformations) along $\overline{R}^k \to \overline{R}$ to establish boundedness of deformations φ_k in $H^{1,2}(\Omega)$.

Sketch of proof $\mu_c = 0$, $p > 3$: part 3

- Extract weakly convergent subsequence of deformations $\varphi_k \rightharpoonup \varphi$ in $H^{1,2}(\Omega)$.
- Choose $\overline{R}^k \rightharpoonup \overline{R}$ in $W^{1,p}(\Omega)$.
- Energy is convex in $\mathrm{D_x}\overline{R}$ and $\overline{U} = \overline{R}^T \nabla\varphi$
- Use extended convexity arguments to show that the limit $\varphi, \overline{R}$ is a minimizer.

Extended Korn's first inequality

Let $F_p, F_p^{-1} \in C^1(\overline{\Omega}, GL^+(3,\mathbb{R}))$ be given with $\det[F_p(x)] \geq c > 0$. Suppose dislocation density $\operatorname{Curl} F_p \in C^1(\overline{\Omega}, \mathbb{M}^{3\times 3})$. Then

$$\exists\, c^+ > 0 \quad \forall\, \phi \in H_0^1(\Omega):$$

$$\|\nabla\phi\, F_p^{-1}(x) + F_p^{-T}(x)\, \nabla\phi^T\|^2_{L^2(\Omega)} \geq c^+\ \|\phi\|^2_{H^{1,2}(\Omega)}\,.$$

Proof: [Neff'02], recent improvement: $F_p \in C^0(\overline{\Omega})$. But work in progress suggests $F_p \in L^\infty(\Omega), \operatorname{Curl} F_p \in L^{3+\delta}(\Omega)$ suffices. Counterexample for $F_p \in L^\infty(\Omega)$.

Reminder: Classical Korn's first inequality:

$$\exists\, c^+ > 0 \quad \forall\, \phi \in H_0^1(\Omega): \quad \|\nabla\phi + \nabla\phi^T\|^2_{L^2(\Omega)} \geq c^+\ \|\phi\|^2_{H^{1,2}(\Omega)}\,.$$

Example: Microstructure in simple glide

- Simple glide: infinite layer of material with unit height, attached at the bottom, sheared with amount γ at the top.
- Question: profile $u(x_3)$ as a function of the height x_3.
- Classical finite/linear elasticity: unique energy minimizing solution is always homogeneous response $u(x_3) = \gamma\, x_3$.
- Finite Cosserat model with $\mu_c = 0$, $L_c = 0$: possible equilibrium solution: homogeneous response **and** microstructure.
- energy minimizing solution with least number of weak discontinuities is microstructure with S-type profile.

Microstructure

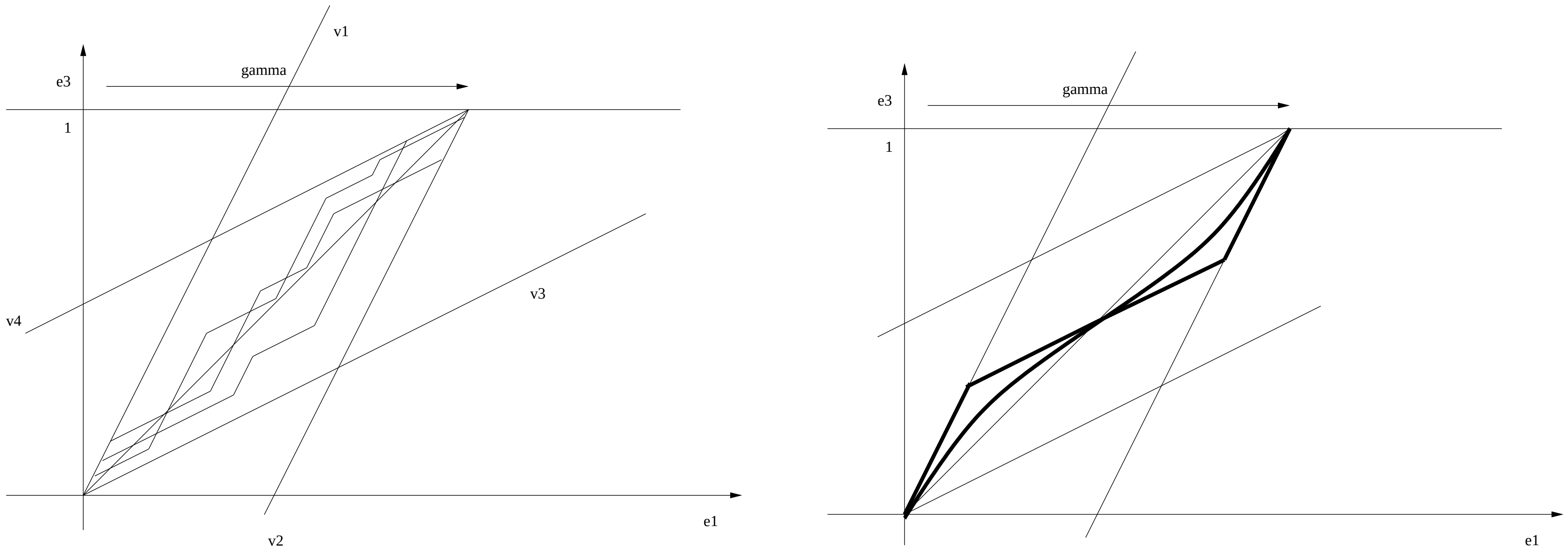

Figure 1: Left: Constructed equilibrium microstructure for $\mu_c = 0$, $L_c = 0$. Right: minimizing microstructure and regularized profile for $L_c > 0$.

Open problems

- Limit case Sobolev embedding: $\mu_c = 0$ and curvature control with bounded $\|\overline{R}\|_{W^{1,p}(\Omega)} < K$ for $2 \leq p \leq 3$ suffices? Note: $\|\overline{R}\|_\infty = \sqrt{3}$.

- How much control of curvature is really needed: would $\|\operatorname{Curl} \overline{R}\|_{L^p(\Omega)} < K$, $p > 3$ suffice instead of $\|\mathrm{D_x}\overline{R}\|_{L^p(\Omega)} < K$?

- Linearized version: $\|\operatorname{Curl} \overline{A}\|^2 \geq c^+ \|\mathrm{D_x}\overline{A}\|^2$ algebraically.

- Find sharp result for extended Korn's inequality.

- Investigate true fracture case $\mu_c = 0$, $p > 1$.

Conclusion

- Fundamentally new behaviour of finite Cosserat model compared to infinitesimal, linear Cosserat model for couple modulus $\mu_c = 0$
- Circumvent limits of quasiconvexity
- restore Legendre-Hadamard ellipticity, weak lower semicontinuity
- Introduce internal length scale $L_c > 0$, characteristic for the material, regularize shear failure
- Incorporate size effects: small samples of the material behave comparatively stiffer than large samples, experimental fact
- $L_c = 0$ allows for sharp interfaces and fracture