

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

Patrizio Neff

TU DARMSTADT



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.
- $F = \nabla\varphi \in \text{GL}^+(3, \mathbb{R})$, the deformation gradient, $\mathbb{1}$ the identity.
- $\overline{R} : \Omega \mapsto \text{SO}(3, \mathbb{R})$ true rotation, $R = \text{polar}(F)$ 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.
- $\|A\|$, $\langle A, B \rangle$, $\text{tr}[A]$ norm, scalar product and trace.
- $F = RU = \text{polar}(F)U$, $R \in \text{SO}(3)$, polar decomposition.



The classical linear elasticity problem

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

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

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

$\mu, \lambda > 0$, 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:

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

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

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

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:**

$$\varphi_k \rightharpoonup \varphi \Rightarrow \int_{\Omega} W(\nabla \varphi) \, dV \leq \liminf_k \int_{\Omega} W(\nabla \varphi_k) \, dV$$

- **W quasiconvex:** $\int_{\Omega} W(B) \, dV \leq \int_{\Omega} W(\nabla \varphi) \, dV$, $\varphi(x)_{\partial\Omega} = B \cdot x$,
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: $D_F^2 W(x, F) \cdot (\xi \otimes \eta, \xi \otimes \eta) < 0$
- 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

$$W(F) = \|F^T F - \mathbb{1}\|^2$$

$$D_F W(F).H = 2\langle F^T F - \mathbb{1}, F^T H + H^T F \rangle$$

$$D_F^2 W(F).(H, H) = 4\langle F^T F - \mathbb{1}, H^T H \rangle + 2\|F^T H + H^T F\|^2$$

$$D_F^2 W(F_0).(\xi \otimes \eta, \xi \otimes \eta) < 0, \quad \langle \xi, \eta \rangle = 0, \quad F_0 = m \cdot \mathbb{1}, \quad m < 1$$

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:

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

$$W(U) = \mu \|\text{sym}(U - \mathbb{1})\|^2 + \frac{\lambda}{2} \text{tr} [\text{sym}(U - \mathbb{1})]^2$$

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

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

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

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** $\text{polar}(\nabla\varphi)$. Allow for **independent (micro) rotations** $\overline{R}$ (Cosserat 1906)
- Attribute energy to spatial variations of rotations (curvature):

$$W_{\text{curv}}(\text{D}_x \overline{R}) = \mu L_c^p \|\text{D}_x \overline{R}\|^p.$$
- Look for independent fields $\varphi, \overline{R}$ in the minimization problem.
 $\overline{R} \in \text{SO}(3, \mathbb{R})$ **nonlinear manifold**



The finite **Cosserat** problem in variational form

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

$$W_{\text{mp}}(\bar{U}) = \mu \|\text{sym}(\bar{U} - \mathbb{1})\|^2 + \frac{\lambda}{2} \text{tr} [\text{sym}(\bar{U} - \mathbb{1})]^2 \\ + \mu_c \|\text{skew}(\bar{U} - \mathbb{1})\|^2$$

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

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

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

$$D_x \bar{R} = (\nabla(\bar{R}.e_1), \nabla(\bar{R}.e_2), \nabla(\bar{R}.e_3)) .$$

Coercivity of curvature

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

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

$$\Rightarrow p > 1$$

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



The infinitesimal, linear **Cosserat** problem

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

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

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

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

$L_c = 0 \Rightarrow$ linear elasticity.



The Cosserat couple modulus μ_c

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



Cases for the **finite Cosserat model**

- I: $\mu_c > 0$, $\mathbf{p} \geq 2$, existence of minimizers trivial. **Fracture excluded.**
- II: $\mu_c = 0$, $\mathbf{p} > 3$, existence of minimizers. **Fracture excluded.**
- IV: $\mu_c = 0$, $1 < \mathbf{p} \leq 3$, possibly $\varphi \notin W^{1,1}(\Omega)$. **Fracture included.**
- V: $\mu_c = 0$, $\mathbf{L}_c = 0$, **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 $g_d \in H^1(\Omega, \mathbb{R}^3)$ and $\bar{R}_d \in W^{1,p}(\Omega, \text{SO}(3, \mathbb{R}))$. 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 $(\varphi, \bar{R}) \in H^1(\Omega, \mathbb{R}^3) \times W^{1,p}(\Omega, \text{SO}(3, \mathbb{R}))$.*

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 $\overline{R}^k \rightarrow \overline{R}$ in L^p .
- $\mu_c > 0$: elastic energy estimates strain part: $\|\overline{R}^{k,T} \nabla \varphi_k - \mathbb{1}\|^2 = \|\overline{R}^{k,T} \nabla \varphi_k\|^2 - 2\langle \overline{R}^k, \nabla \varphi_k \rangle + 3 \geq \|\nabla \varphi_k\|^2 - 2\sqrt{3}\|\nabla \varphi_k\| + 3$



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 $\overline{R}^{k,T} \nabla \varphi_k \rightharpoonup \tilde{U} \in L^2(\Omega)$
- $p \geq 2$: $\overline{R}^k \rightarrow \overline{R} \in L^2(\Omega) \Rightarrow \overline{R}^{k,T} \nabla \varphi_k \rightharpoonup \overline{R}^T \nabla \varphi \in L^1(\Omega)$
- $\tilde{U} = \overline{R}^T \nabla \varphi \in L^2(\Omega)$
- Energy is convex in $D_x \overline{R}$ and $\tilde{U} = \overline{R}^T \nabla \varphi$



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 $g_d \in H^1(\Omega, \mathbb{R}^3)$ and $\bar{R}_d \in W^{1,p}(\Omega, \text{SO}(3, \mathbb{R}))$. 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 $(\varphi, \bar{R}) \in H^1(\Omega, \mathbb{R}^3) \times W^{1,p}(\Omega, \text{SO}(3, \mathbb{R}))$.*



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

- Take infimizing sequences of deformations φ_k and rotations $\overline{R}^k$.
- Since $\|D_x \overline{R}\|^p$ 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 $\overline{R}^k \rightarrow \overline{R}$ 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 $\varphi_k = x + u_k(x)$

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

Use **extended Korn's inequality** (**coercivity** of deformations) along $\overline{R}^k \rightarrow \overline{R}$ 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 $\bar{R}^k \rightharpoonup \bar{R}$ in $W^{1,p}(\Omega)$.
- Energy is convex in $D_x \bar{R}$ and $\bar{U} = \bar{R}^T \nabla \varphi$
- Use extended convexity arguments to show that the limit $\varphi, \bar{R}$ 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** $\text{Curl } F_p \in C^1(\overline{\Omega}, \mathbb{M}^{3 \times 3})$. Then

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

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

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

Reminder: **Classical Korn's first inequality:**

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



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

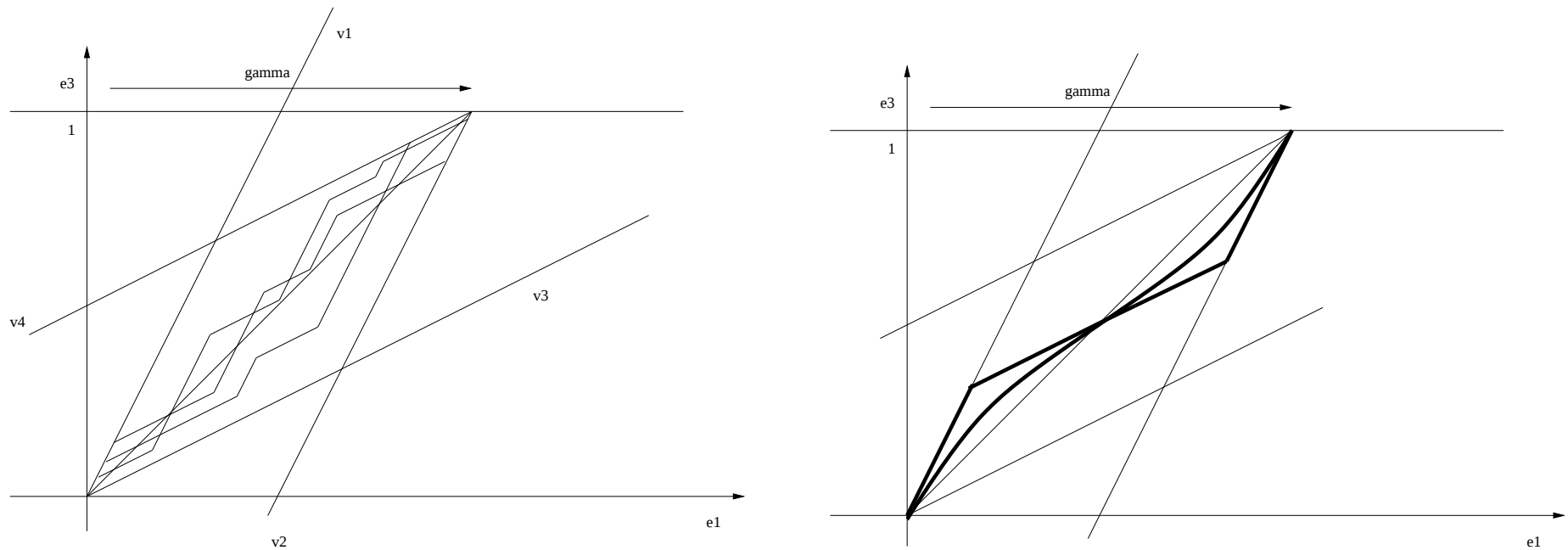


Figure 1: Left: Constructed equilibrium microstructure for $\mu_c = 0$, $L_c = 0$. Right: minimizing microstructure and regularized profile for $L_c > 0$.



Open problems

- Limit case Sobolev embedding: $\mu_c = 0$ and curvature control with bounded $\|\bar{R}\|_{W^{1,p}(\Omega)} < K$ for $2 \leq p \leq 3$ suffices? Note: $\|\bar{R}\|_\infty = \sqrt{3}$.
- How much control of curvature is really needed: would $\|\text{Curl } \bar{R}\|_{L^p(\Omega)} < K$, $p > 3$ suffice instead of $\|D_x \bar{R}\|_{L^p(\Omega)} < K$?
- Linearized version: $\|\text{Curl } \bar{A}\|^2 \geq c^+ \|D_x \bar{A}\|^2$ 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

