UNIVERSITÄT DUISBURG ESSEN

Chair for Nonlinear Analysis and Modelling
Faculty of Mathematics
University of Duisburg-Essen
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Explicit optimal Cosserat rotations

Andreas Fischle and Patrizio Neff

1 Microstructure of materials

The optimal design of the **microstructure** of materials has enormous potential for industrial applications. In the emerging field of computational material design, mathematical modelling needs to reflect physical effects on micro- and nanoscales. Simple material models are insufficient for this task.

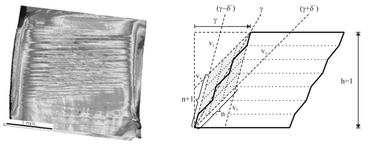


Figure 1: Example: Microbands and Glide planes in Copper [12] as modelled by Cosserat theory.

2 Finite Cosserat Theory (1909)

One of the possible models for microstructured materials is the finite-strain **Cosserat model** [2], which introduces a **rotational (micropolar) microstructure field** $R \in \mathrm{SO}(n)$ in addition to the deformation gradient $F := \nabla\varphi \in \mathrm{GL}^+(n)$. The strain energy $W(F, R)$ depends only on the quantities

$$\overline{U} := R^T F \quad \text{(first Cosserat deformation tensor)}\,,$$
$$\mathfrak{k} := R^T \mathrm{D}_x R \quad \text{(Cosserat curvature tensor)}\,.$$

Intriguing aspects of the Cosserat model include the decoupling of local lattice rotation in crystals as well as a regularized approximation of simple continua.

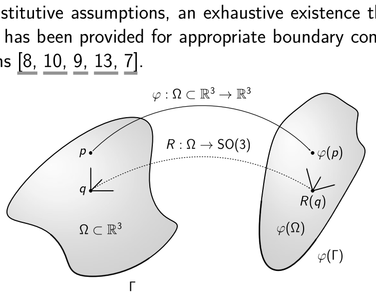
However, some fundamental questions remain; for example, the effect of the Cosserat couple modulus μ_c (see below) is not yet completely understood [10].

3 Size-independent Cosserat hyperelasticity

In Cosserat hyperelasticity, the aim is to minimize the energy

$$I(\varphi, R) := \int_\Omega W(\,\overline{U}\,) + L_c^2 \|\mathfrak{k}\|^2 \,\mathrm{d}V$$

over all admissible deformations $\varphi\colon \Omega \to \mathbb{R}^n$ and micropolar rotation fields $R\colon \Omega \to \mathrm{SO}(n)$. In general, this is a nonlinear and non-convex problem. Under quadratic constitutive assumptions, an exhaustive existence theory has been provided for appropriate boundary conditions [8, 10, 9, 13, 7].



Here, we restrict our attention to the size-independent case $L_c = 0$.

The elastic strain energy is closely connected to the *change of length* in a material. In particular, an *isometry*, i.e. a rigid body motion, has zero elastic energy. This basic observation suggests the characterization of elastic energy functions as **distance measures** to the special orthogonal group $\mathrm{SO}(n)$ of pure rotations.

4 Grioli's Theorem and the polar decomposition

The classical *Euclidean distance* of the deformation gradient $F \in \mathrm{GL}^+(n)$ to $\mathrm{SO}(n)$ is given by *Grioli's theorem* [6, 11]: Let $F \in \mathrm{GL}^+(n)$ and $\|X\|^2 := \mathrm{tr}(X^T X)$. Then

$$\begin{aligned}\underset{R\in\mathrm{SO}(n)}{\operatorname{argmin}} \|R - F\|^2 &= \underset{R\in\mathrm{SO}(n)}{\operatorname{argmin}} \|R^T F - \mathbb{1}\|^2 \\ &= \underset{R\in\mathrm{SO}(n)}{\operatorname{argmin}} \left\{ 1 \cdot \|\,\mathrm{sym}(R^T F - \mathbb{1})\,\|^2 + 1 \cdot \|\mathrm{skew}(R^T F - \mathbb{1})\|^2 \right\} \\ &= \{\mathrm{R_p}(F)\}\,,\end{aligned}$$

where $\mathrm{R_p}(F) \in \mathrm{SO}(n)$ is the orthogonal part of the *polar decomposition* $F = \mathrm{R_p}(F) \cdot U$ with $U = \sqrt{F^T F}$.

In order to find the optimal rotations that minimize the **Cosserat shear-stretch density**

$$\begin{aligned}W_{\mu,\mu_c}(F, R) :&= \mu\,\|\,\mathrm{sym}(R^T F - \mathbb{1})\,\|^2 + \mu_c\,\|\mathrm{skew}(R^T F - \mathbb{1})\|^2 \\ &= \mu\,\|\,\mathrm{sym}(\overline{U} - \mathbb{1})\,\|^2 + \mu_c\,\|\mathrm{skew}(\overline{U} - \mathbb{1})\|^2\,,\end{aligned}$$

where $\mu > 0$ is the Lamé shear modulus and $\mu_c \geq 0$ is the **Cosserat couple modulus**, it is no longer sufficient to consider the classical (squared) Euclidean distance $\|X - Y\|^2$ between $X, Y \in \mathbb{R}^{n\times n}$.

5 Optimal Cosserat rotations

Let

$$\begin{aligned}\mathrm{rpolar}_{\mu,\mu_c}(F) :&= \underset{R\in\mathrm{SO}(n)}{\operatorname{argmin}} W_{\mu,\mu_c}(F, R) \\ &= \mu\,\|\,\mathrm{sym}(R^T F - \mathbb{1})\,\|^2 + \mu_c\,\|\mathrm{skew}(R^T F - \mathbb{1})\|^2\,.\end{aligned}$$

Then in the *classical regime* $\mu_c \geq \mu > 0$, Grioli's Theorem is still applicable: the unique minimizing rotation is $\mathrm{R_p}(F)$. However, in the *non-classical regime* $\mu > \mu_c \geq 0$, a generalization of the theorem is necessary in order to find $\mathrm{rpolar}_{\mu,\mu_c}(F)$.

This task is simplified by two reductions: First, rescaling the deformation gradient F to $\widetilde{F}_{\mu,\mu_c} := \frac{\mu-\mu_c}{\mu} F$ allows us to reduce the case $\mu > \mu_c \geq 0$ to the basic case $\mu = 1,\ \mu_c = 0$ [3]. Second, F can be assumed to be in diagonal form [4, 1], i.e. we can replace F by $D := \mathrm{diag}(\nu_1, \ldots, \nu_n)$, where $\nu_1 > \ldots > \nu_n$ are the singular values of F.

The problem of determining $\mathrm{rpolar}_{\mu,\mu_c}(F)$ requires the characterization of all (possibly nonsymmetric) real square roots of a matrix $S \in \mathrm{Sym}(n)$, i.e. of all $X \in \mathbb{R}^{n\times n}$ such that $X^2 = S$ [1]. It turns out that pitchfork bifurcations between classical and non-classical solutions appear [1, 3] if

$$\nu_{2i-1} + \nu_{2i} \geq \frac{2\mu}{\mu - \mu_c}$$

for the singular values ν_k of F. Furthermore, the global minimizers $\mathrm{rpolar}_{\mu,\mu_c}(F)$ are pairwise symmetric to the polar factor $\mathrm{R_p}(F)$.

6 The relaxed-polar mechanism in 3D

Let $Q = (q_1|q_2|q_3) \in \mathrm{SO}(3)$ denote an eigenframe for $U = \sqrt{F^T F}$. Then the optimal rotation *relative to* $\mathrm{R_p}(F)$ is a rotation around the axis q_3, which is the eigenvector of U corresponding to its smallest eigenvalue ν_3, and the angle of rotation is [4]

$$\alpha_{1,0}^{\pm} = \begin{cases} \pm\arccos\left(\frac{2}{\nu_1+\nu_2}\right) & : \quad \frac{\nu_1+\nu_2}{2} \geq 1 \\ 0 & : \quad \text{otherwise} \end{cases}$$

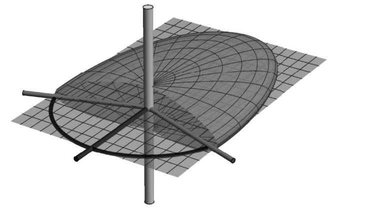
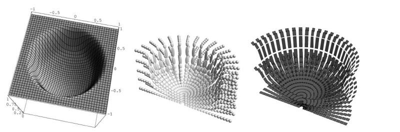
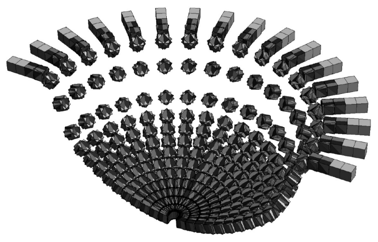


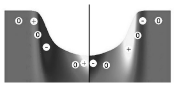
Figure 2: The plane $\mathrm{P^{ms}}(F) := \mathrm{span}(\{q_1, q_2\}) \subset T_x\Omega$ of maximal stretch as defined in [4].

7 Example: Idealized nanoindentation



A possible application of finite Cosserat Theory is the modelling of nanoindentations in copper, which were shown by 3D-EBSD to exhibit counter-rotations of the crystal lattice. The optimal Cosserat rotation $\mathrm{rpolar}_{1,0}^{\pm}(F)$ can reproduce such non-classical counter-rotations in a qualitatively similar way [5].





These results on the explicit nature of the microrotations in a specific Cosserat model are among the first ones since 1909.

8 References

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Dr. rer. nat. Andreas Fischle
Prof. Dr. rer. nat. Patrizio Neff

TU Dresden
Institut für Numerische Mathematik
Zellescher Weg 12-14
01062 Dresden