Rend. Lincei Mat. Appl. 28 (2017), 573–600
DOI 10.4171/RLM/777

Continuum Mechanics — *Grioli's theorem with weights and the relaxed-polar mechanism of optimal Cosserat rotations*, by ANDREAS FISCHLE and PATRIZIO NEFF, communicated on February 10, 2017.

This paper is dedicated to the memory of Professor Giuseppe Grioli.

ABSTRACT. — Let $F \in \mathrm{GL}^+(3)$ and consider the right polar decomposition $F = \mathrm{R_p}(F) \cdot U$ into an orthogonal factor $\mathrm{R_p}(F) \in \mathrm{SO}(3)$ and a symmetric, positive definite factor $U = \sqrt{F^T F} \in \mathrm{PSym}(3)$. In 1940 Giuseppe Grioli proved that

$$\underset{R \in \mathrm{SO}(3)}{\arg\min} \|R^T F - \mathbb{1}\|^2 = \{\mathrm{R_p}(F)\} = \underset{R \in \mathrm{SO}(3)}{\arg\min} \|F - R\|^2.$$

This variational characterization of the orthogonal factor $\mathrm{R_p}(F) \in \mathrm{SO}(n)$ holds in any dimension $n \geq 2$ (a result due to Martins and Podio-Guidugli). In a similar spirit, we characterize the optimal rotations

$$\mathrm{rpolar}_{\mu,\mu_c}(F) := \underset{R \in \mathrm{SO}(n)}{\arg\min} \{\mu \|\mathrm{sym}(R^T F - \mathbb{1})\|^2 + \mu_c \|\mathrm{skew}(R^T F - \mathbb{1})\|^2\}$$

for given weights $\mu > 0$ and $\mu_c \geq 0$. We identify a classical parameter range $\mu_c \geq \mu > 0$ for which Grioli's theorem is recovered and a non-classical parameter range $\mu > \mu_c \geq 0$ giving rise to a new type of globally energy-minimizing rotations which can substantially deviate from $\mathrm{R_p}(F)$. In mechanics, the weighted energy subject to minimization appears as the shear-stretch contribution in any geometrically nonlinear, quadratic, and isotropic Cosserat theory.

KEY WORDS: Cosserat, Grioli's theorem, polar media, zero Cosserat couple modulus, euclidean distance to $\mathrm{SO}(n)$

MATHEMATICS SUBJECT CLASSIFICATION: 15A24, 22E30, 74A30, 74A35, 74B20, 74G05, 74G55, 74G65, 74N15

1. INTRODUCTION

In 1940 Giuseppe Grioli proved a variational characterization of the orthogonal factor of the polar decomposition [12]. In order to state this result, let $\mathrm{R_p}(F) \in \mathrm{SO}(n)$ be the unique rotation characterized as the orthogonal factor of the right polar decomposition of

$$F = \mathrm{R_p}(F)U(F), \quad F \in \mathrm{GL}^+(n), \tag{1.1}$$

where $U(F) = \mathrm{R_p}(F)^T F = \sqrt{F^T F} \in \mathrm{PSym}(n)$ denotes the symmetric positive definite factor (which, in mechanics, is referred to as the Biot stretch tensor).

Grioli's original result[1] is the important special case of space dimension $n = 3$ of the following

THEOREM 1.1 (Grioli's theorem [3, 12, 15]). *Let* $n \geq 2$ *and* $\|X\|^2 := \operatorname{tr}[X^T X]$ *the Frobenius norm. Then for any* $F \in \mathrm{GL}^+(n)$*, it holds*

$$\begin{aligned} &\underset{R \in \mathrm{SO}(n)}{\arg\min} \|R^T F - \mathbb{1}\|^2 = \{\mathrm{R_p}(F)\}, \quad \textit{and thus} \\ &\min_{R \in \mathrm{SO}(n)} \|R^T F - \mathbb{1}\|^2 = \|U - \mathbb{1}\|^2. \end{aligned} \tag{1.2}$$

The polar factor $\mathrm{R_p}(F) \in \mathrm{SO}(n)$ is the unique energy-minimizing rotation for any given $F \in \mathrm{GL}^+(n)$ in any dimension $n \geq 2$, see, e.g., [15]. This optimality property has an interesting geometric interpretation following from the orthogonal invariance of the Frobenius norm

$$\|R^T F - \mathbb{1}\|^2 = \|F - R\|^2 = \operatorname{dist}^2_{\text{euclid}}(F, R) \tag{1.3}$$

which reveals a connection to the problem class of matrix distance (or nearness) problems. In elasticity, a distance of a deformation gradient (jacobian matrix) $F := \nabla\varphi \in \mathrm{GL}^+(n)$ to a rotation $\mathrm{SO}(n)$ is of interest as a measure for the energy induced by local changes in length.

In this contribution, we consider a weighted analog of Grioli's theorem motivated by Cosserat theory and present the energy-minimizing (optimal) rotations characterized by

PROBLEM 1.2 (Weighted optimality). *Let* $n \geq 2$. *Compute the set of optimal rotations*

$$\begin{aligned} &\underset{R \in \mathrm{SO}(n)}{\arg\min}\ \mathrm{W}_{\mu,\mu_c}(R; F) \\ &\qquad := \underset{R \in \mathrm{SO}(n)}{\arg\min} \{\mu \|\operatorname{sym}(R^T F - \mathbb{1})\|^2 + \mu_c \|\operatorname{skew}(R^T F - \mathbb{1})\|^2\} \end{aligned} \tag{1.4}$$

for given $F \in \mathrm{GL}^+(n)$ *and weights* $\mu > 0$, $\mu_c \geq 0$. *Here,* $\operatorname{sym}(X) := \frac{1}{2}(X + X^T)$ *and* $\operatorname{skew}(X) := \frac{1}{2}(X - X^T)$ *denote the symmetric and skew-symmetric parts of* $X \in \mathbb{R}^{n \times n}$*, respectively.*

Note that Grioli's theorem stated above is recovered for the case of equal weights $\mu = \mu_c > 0$. In order to express the connection to the variational characterization of the polar factor $\mathrm{R_p}(F)$, we have introduced the following notation

DEFINITION 1.3 (Relaxed polar factor(s)). Let $\mu > 0$ and $\mu_c \geq 0$. We denote the set-valued mapping that assigns to a given parameter $F \in \mathrm{GL}^+(n)$ its associated

[1] An exposition of the original contribution of Grioli in modernized notation has been recently made available in [24].

set of energy-minimizing rotations by

$$\operatorname{rpolar}_{\mu,\mu_c}(F) := \underset{R\in \mathrm{SO}(n)}{\arg\min}\, \mathrm{W}_{\mu,\mu_c}(R;F).$$

In the weighted case, the polar factor $\mathrm{R_p}(F)$ is always critical but *not* always optimal. In general the global minimizers $\operatorname{rpolar}_{\mu,\mu_c}(F)$ depend on the parameters $\mu > 0$ and $\mu_c \geq 0$ and can substantially deviate from $\mathrm{R_p}(F)$.

The optimal rotations in the weighted case $\operatorname{rpolar}_{\mu,\mu_c}(F)$ have been worked out in two and three space dimensions by the present authors in a series of papers [9, 10]; cf. also [8] and [21, 26] for earlier related work. A visualization of the mechanism of optimal Cosserat rotations in dimension $n = 3$ for an idealized nano-indentation was given in [11] and shows that the optimal rotations can produce interesting non-classical patterns. A final proof of optimality in any dimension $n \geq 2$ has been obtained by Borisov and the authors in [2] and is based on a new characterization of real square roots of real symmetric matrices. This contribution presents an overview of these results omitting the proofs for which we refer to the original contributions.

Our study of the energy-minimizing rotations $\operatorname{rpolar}_{\mu,\mu_c}(F)$ is motivated by a particular Cosserat (micropolar) theory [19], i.e., a continuum theory with additional degrees of freedom $R \in \mathrm{SO}(n)$. In this context, the objective function $\mathrm{W}_{\mu,\mu_c}(R;F)$ subject to minimization in Problem 1.2 determines the shear-stretch contribution to the strain energy in any nonlinear, quadratic, and isotropic Cosserat theory, see also [1, 6, 14, 17, 27, 28]. The arguments to the shear-stretch energy $W_{\mu,\mu_c}(R;F)$ are the deformation gradient field $F := \nabla\varphi : \Omega \to \mathrm{GL}^+(n)$ and the microrotation field $R : \Omega \to \mathrm{SO}(n)$ evaluated at a given point of the domain Ω. A full Cosserat continuum model furthermore contains an additional curvature energy term [25] and a volumetric energy term, see, e.g., [20] or [21].

It is always possible to express the local energy contribution in a Cosserat model as $W = W(\overline{U})$, where $\overline{U} := R^T F$ is the first Cosserat deformation tensor. This reduction follows from objectivity requirements and has already been observed by the Cosserat brothers [4, p. 123, eq. (43)], see also [7] and [16]. Since $\overline{U}$ is in general non-symmetric, the most general isotropic and quadratic local energy contribution which is zero at the reference state is given by

$$\underbrace{\mu\|\operatorname{sym}(\overline{U}-\mathbb{1})\|^2 + \mu_c\|\operatorname{skew}(\overline{U}-\mathbb{1})\|^2}_{\text{“shear-stretch energy”}} + \underbrace{\frac{\lambda}{2}\operatorname{tr}[\overline{U}-\mathbb{1}]^2}_{\text{“volumetric energy”}}. \tag{1.5}$$

The last term will be discarded in the following, since it couples the rotational and volumetric response, a feature not present in the well-known isotropic linear Cosserat models.[2]

[2] The Cosserat brothers never proposed any specific expression for the local energy $W = W(\overline{U})$. The chosen quadratic ansatz for $W = W(\overline{U})$ is motivated by a direct extension of the quadratic energy in the linear theory of Cosserat models, see, e.g. [13, 22, 23]. We always consider a true volumetric-isochoric split in our applications.

From the perspective of Cosserat theory, the optimal rotations $\operatorname{rpolar}_{\mu,\mu_c}(F)$ yield insight into the important limit case of vanishing characteristic length $L_c = 0$.[3] In this context, we can interpret the solutions of (1.4) as an energetically optimal mechanical response of the field $R \in \mathrm{SO}(n)$ of Cosserat microrotations to a given deformation gradient $F := \nabla\varphi \in \mathrm{GL}^+(n)$.

Remark 1.4 (Vanishing Cosserat couple modulus μ_c). The correct choice of the so-called Cosserat couple modulus $\mu_c \geq 0$ for specific materials and boundary value problems is an interesting open question. There are indications that a non-vanishing $\mu_c > 0$ has never been experimentally observed and that such a choice is at least debatable [18]. The limit case $\mu_c = 0$ is hence of particular interest.

We want to stress that although the term $\mathrm{W}_{\mu,\mu_c}(R;F)$ subject to minimization in (1.4) is quadratic in the nonsymmetric microstrain tensor $\overline{U} - \mathbb{1} = R^T F - \mathbb{1}$, see, e.g., [6], the associated minimization problem with respect to R is nonlinear due to the multiplicative coupling $R^T F$ and the geometry of $\mathrm{SO}(n)$.

Remark 1.5 (Existence of global minimizers). The energy $\mathrm{W}_{\mu,\mu_c}(R;F)$ is a polynomial in the matrix entries, hence $\mathrm{W}_{\mu,\mu_c} \in C^\infty(\mathrm{SO}(n),\mathbb{R})$. Further, since the Lie group $\mathrm{SO}(n)$ is compact and $\partial\mathrm{SO}(n) = \emptyset$, the global extrema of W_{μ,μ_c} are attained at interior points.

The previous remark hints at a possible solution strategy for Problem 1.2. If *all* the critical points $R_{\mathrm{crit}}(F) \in \mathrm{SO}(n)$ of $\mathrm{W}_{\mu,\mu_c}(R;F)$ can be computed[4], then a direct comparison of the associated critical energy levels $\mathrm{W}_{\mu,\mu_c}(R_{\mathrm{crit}};F)$ allows to determine the critical branches which are energy-minimizing. Clearly, any minimizing critical branch realizes the *reduced* Cosserat shear-stretch energy defined as

$$W^{\mathrm{red}}_{\mu,\mu_c} : \mathrm{GL}^+(n) \to \mathbb{R}^+_0, \quad W^{\mathrm{red}}_{\mu,\mu_c}(F) := \min_{R\in\mathrm{SO}(n)} W_{\mu,\mu_c}(R;F). \tag{1.6}$$

At first, a solution of Problem 1.2 in three space dimensions was out of reach (let alone the n-dimensional problem). Therefore, we first restrict our attention to the planar case, where we can base our computations on the standard

[3] This identification requires that the volume term decouples from the microrotation R, e.g.,

$$W^{\mathrm{vol}}(\overline{U}) := \frac{\lambda}{4}\left[(\det[\overline{U}]-1)^2 + \left(\frac{1}{\det[\overline{U}]}-1\right)^2\right].$$

This requirement is quite natural and is satisfied by all linear Cosserat models [18, 22, 23].

[4] The smooth manifold $\mathrm{SO}(n)$ has empty boundary. This implies that a critical point for given $F \in \mathrm{GL}^+(n)$ satisfies $\frac{\mathrm{d}}{\mathrm{dt}}\mathrm{W}_{\mu,\mu_c}(R(t);F)|_{t=0} = 0$ for every smooth curve of rotations $R(t) : (-\varepsilon,\varepsilon) \to \mathrm{SO}(n)$ passing through $R(0) = R_{\mathrm{crit}}$.

parametrisation

$$R : [-\pi, \pi] \to \mathrm{SO}(2) \subset \mathbb{R}^{2\times 2}, \quad R(\alpha) := \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \tag{1.7}$$

by a rotation angle.[5]

It turns out that there are at most two optimal planar rotations $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$ in the non-classical parameter range $\mu > \mu_c \geq 0$ and we distinguish these by a sign. The corresponding optimal rotation angles of $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$ are denoted by $\alpha^{\pm}_{\mu,\mu_c}(F)$. The non-classical minimizers coincide with the polar factor $\mathrm{R_p}(F)$ in the compressive regime of $F \in \mathrm{GL}^+(2)$, but deviate otherwise.

The computation of the global minimizers in dependence of F is not completely obvious even for the planar case. Hence, the following simplifications of the minimization problem are helpful.

First, it is useful to introduce

DEFINITION 1.6 (Parameter rescaling). Let $\mu > \mu_c \geq 0$. We define the **singular radius** ρ_{μ,μ_c} by

$$\rho_{\mu,\mu_c} := \frac{2\mu}{\mu - \mu_c} > 0, \quad \text{and further define} \quad \lambda_{\mu,\mu_c} := \frac{\rho_{\mu,\mu_c}}{\rho_{1,0}} = \frac{\mu}{\mu - \mu_c}, \tag{1.8}$$

as the **induced scaling parameter**. Note that $\rho_{1,0} = 2$ and $\lambda_{1,0} = 1$. Further, we define the **parameter rescaling** given by

$$\tilde{F}_{\mu,\mu_c} := \lambda^{-1}_{\mu,\mu_c} F = \frac{\mu - \mu_c}{\mu} F \in \mathrm{GL}^+(n). \tag{1.9}$$

For $\mu > 0$ and $\mu_c = 0$, we obtain $\tilde{F}_{\mu,0} = F$, i.e., the rescaling is only effective for $\mu_c > 0$.

Regarding the material parameters, we proved in [9] that for any dimension $n \geq 2$, it is in fact sufficient to restrict our attention to two parameter pairs: $(\mu, \mu_c) = (1, 1)$, the *classical* case, and $(\mu, \mu_c) = (1, 0)$, the *non-classical* case. Hence, somewhat surprisingly, the solutions for arbitrary $\mu > 0$ and $\mu_c \geq 0$ can be recovered from these two limit cases. This is the content of

LEMMA 1.7 (Parameter reduction). *Let $n \geq 2$ and let $F \in \mathrm{GL}^+(n)$, then*

$$\begin{aligned} \mu_c \geq \mu > 0 &\Rightarrow \mathrm{W}_{\mu,\mu_c}(R;F) \sim W_{1,1}(R;F), \quad \textit{and} \\ \mu > \mu_c \geq 0 &\Rightarrow \mathrm{W}_{\mu,\mu_c}(R;F) \sim \mathrm{W}_{1,0}(R;\tilde{F}_{\mu,\mu_c}). \end{aligned} \tag{1.10}$$

Here, the equivalence notation means that the energies give rise to the same global minimizers which we can also state as

[5] Note that π and $-\pi$ are mapped to the same rotation. In this text, we implicitly choose π over $-\pi$ for the rotation angle whenever uniqueness is an issue.

COROLLARY 1.8.

$$\operatorname{rpolar}_{\mu,\mu_c}(F) = \begin{cases} \operatorname{rpolar}_{1,1}(F) = \{\mathrm{R_p}(F)\}, & \text{if } \mu_c \geq \mu > 0 \\ \operatorname{rpolar}_{1,0}(\tilde{F}_{\mu,\mu_c}), & \text{if } \mu > \mu_c \geq 0 \end{cases}. \tag{1.11}$$

Another important observation can be made introducing the rotation

$$\hat{R} := Q^T R^T \mathrm{R_p} Q \tag{1.12}$$

which acts *relative* to the polar factor $\mathrm{R_p}(F)$ in the coordinate system given by the columns of Q which span a positively oriented frame of principal directions of U. This allows us to transform

$$\begin{aligned} Q^T(\operatorname{sym}(R^T F) - \mathbb{1})Q &= Q^T(\operatorname{sym}(R^T \mathrm{R_p} Q D Q^T) - \mathbb{1}))Q \\ &= \operatorname{sym}(Q^T R^T \mathrm{R_p} Q D Q^T Q - Q^T Q) \\ &= \operatorname{sym}(\underbrace{Q^T R^T \mathrm{R_p} Q}_{=:\hat{R}} D - \mathbb{1}) = \operatorname{sym}(\hat{R} D - \mathbb{1}). \end{aligned} \tag{1.13}$$

For fixed choice of $Q \in \mathrm{SO}(n)$, the inverse transformation allows to reconstruct the absolute rotation uniquely

$$R = (Q\hat{R}Q^T \mathrm{R}_\mathrm{p}^T)^T = \mathrm{R_p} Q \hat{R}^T Q^T. \tag{1.14}$$

Hence, in the non-classical parameter range represented by the limit case $(\mu, \mu_c) = (1, 0)$, the minimization problem can be reduced to the following problem for the optimal relative rotations.

PROBLEM 1.9. *Let $n \geq 2$. Compute the set of energy-minimizing relative rotations*

$$\operatorname{rpolar}_{1,0}(D) := \underset{\hat{R} \in \mathrm{SO}(n)}{\arg\min}\, W_{1,0}(\hat{R}; D) = \underset{\hat{R} \in \mathrm{SO}(n)}{\arg\min}\, \|\operatorname{sym}(\hat{R}D - \mathbb{1})\|^2 \subseteq \mathrm{SO}(n). \tag{1.15}$$

The decisive point in the solution of Problem 1.9 in dimensions $n \geq 3$ is the characterization of the set of relative rotations $\hat{R} \in \mathrm{SO}(n)$ satisfying the particular symmetric square condition

$$(\hat{R}D - \mathbb{1})^2 \in \mathrm{Sym}(n)$$

which is equivalent to the Euler-Lagrange equations.

After having set the stage of the optimization problem on $\mathrm{SO}(n)$, this overview is now structured as follows: in the next Section 2, we consider in some detail the planar problem which allows for a complete solution by elementary techniques and which presents already the essential geometry which unfolds in dimensions $n \geq 3$. In Section 3, we provide the complete solution for the three-dimensional case as well as the corresponding reduced energy expression in terms of singular values of F. We also provide a geometrical interpretation that allows to view the minimization problem for $\mu_c = 0$ as a distance problem. Furthermore, we provide a discussion for which deformation gradients we can only have the classical response $\mathrm{R_p}(F)$. Finally, in Section 4, we present our results for the general n-dimensional case.

2. Optimal rotations in two space dimensions

In this section, we consider

Problem 2.1 (The planar minimization problem). *Let $F \in \mathrm{GL}^+(2)$, $\mu > 0$ and $\mu_c \geq 0$. The task is to compute the set of optimal microrotation angles*

$$\operatorname*{arg\,min}_{\alpha \in [-\pi,\pi]} \{\mu \|\mathrm{sym}(R(\alpha)^T F - \mathbb{1}_2)\|^2 + \mu_c \|\mathrm{sym}(R(\alpha)^T F - \mathbb{1}_2)\|^2\}, \tag{2.1}$$

where

$$R(\alpha) := \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \in \mathrm{SO}(2) \quad \textit{and} \quad \begin{pmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{pmatrix} \in \mathrm{GL}^+(2).$$

In this case we can compute explicit representations of optimal planar rotations for the Cosserat shear-stretch energy by elementary means. The parameter reduction strategy described by Lemma 1.7 allows us to concentrate our efforts towards the construction of explicit solutions to Problem 2.1 on two representative pairs of parameter values μ and μ_c. The classical regime is characterized by the limit case $(\mu, \mu_c) = (1, 1)$ and the unique minimizer is given by the polar factor $\mathrm{R_p}(F)$ for any dimension $n \geq 2$.

The non-classical case represented by $(\mu, \mu_c) = (1, 0)$ turns out to be much more interesting and we compute all global non-classical minimizers $\mathrm{rpolar}_{1,0}(F)$ for $n = 2$. This is the main contribution of this section. Furthermore, we derive the associated reduced energy levels $W^{\mathrm{red}}_{1,1}(F)$ and $W^{\mathrm{red}}_{1,0}(F)$ which are realized by the corresponding optimal Cosserat microrotations. Finally, we reconstruct the minimizing rotation angles for general values of μ and μ_c from the classical and non-classical limit cases.

2.1. *Explicit solution for the classical parameter range: $\mu_c \geq \mu > 0$*

The polar factor $\mathrm{R_p}(F)$ is uniquely optimal for the classical parameter range in any dimension $n \geq 2$. Let us give an explicit representation for $n = 2$ in terms of $\alpha_\mathrm{p} \in (-\pi, \pi]$. In view of the parameter reduction, distilled in Lemma 1.7, it suffices to compute the set of optimal rotation angles for the representative limit case $(\mu, \mu_c) = (1, 1)$.

Thus, to obtain an explicit representation of $\alpha_\mathrm{p} \in (-\pi, \pi]$ which characterizes the polar factor $\mathrm{R_p}(F)$ in dimension $n = 2$, we consider

$$\begin{aligned}(2.2)\qquad &\operatorname*{arg\,min}_{\alpha\in[-\pi,\pi]} W_{1,1}(R(\alpha);F)\\ &= \operatorname*{arg\,min}_{\alpha\in[-\pi,\pi]}\left\|\left[\begin{pmatrix}\cos\alpha & -\sin\alpha\\ \sin\alpha & \cos\alpha\end{pmatrix}^T\begin{pmatrix}F_{11} & F_{12}\\ F_{21} & F_{22}\end{pmatrix}-\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\right]\right\|^2.\end{aligned}$$

Let us introduce the rotation $J := \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} \in \mathrm{SO}(2)$. Its application to a vector $v \in \mathbb{R}^2$ corresponds to multiplication with the imaginary unit $i \in \mathbb{C}$. In what follows, the quantities $\mathrm{tr}[F] = F_{11} + F_{22}$ and $\mathrm{tr}[JF] = -F_{21} + F_{12}$ play a particular role and we note the identity

$$\mathrm{tr}[F]^2 + \mathrm{tr}[JF]^2 = \|F\|^2 + 2\det[F] = \mathrm{tr}[U]^2. \tag{2.3}$$

The reduced energy $W_{1,1}^{\mathrm{red}}(F) := \min_{R\in\mathrm{SO}(n)} W_{1,1}(R;F)$ realized by the polar factor $\mathrm{R_p}(F)$ can be shown to be the euclidean distance of an arbitrary F in $\mathbb{R}^{n\times n}$ to $\mathrm{SO}(n)$. For $n = 2$, we obtain

THEOREM 2.2 (Euclidean distance to planar rotations). *Let $F \in \mathrm{GL}^+(2)$, then*

$$W_{1,1}^{\mathrm{red}}(F) = \mathrm{dist}^2(F,\mathrm{SO}(2)) = \|U - \mathbb{1}\|^2 = \|F\|^2 - 2\sqrt{\|F\|^2 + 2\det[F]} + 2. \tag{2.4}$$

The unique optimal rotation angle realizing this minimial energy level satisfies the equation

$$\begin{pmatrix}\sin\alpha_{\mathrm{p}}\\ \cos\alpha_{\mathrm{p}}\end{pmatrix} = \frac{1}{\mathrm{tr}[U]}\begin{pmatrix}-\mathrm{tr}[JF]\\ \mathrm{tr}[F]\end{pmatrix}. \tag{2.5}$$

In particular, we have $\alpha_{\mathrm{p}}(F) = -\mathrm{sign}(\mathrm{tr}[JF]) \cdot \arccos\left(\frac{\mathrm{tr}[F]}{\mathrm{tr}[U]}\right) \in [-\pi,\pi]$.

COROLLARY 2.3 (Explicit formula for $\mathrm{R_p}(F)$). *Let $F \in \mathrm{GL}^+(2)$, then the polar factor $\mathrm{R_p}(F)$ has the explicit representation*

$$\mathrm{R_p}(F) = R(\alpha_p) := \begin{pmatrix}\cos\alpha_p & -\sin\alpha_p\\ \sin\alpha_p & \cos\alpha_p\end{pmatrix} = \frac{1}{\mathrm{tr}[U]}\begin{pmatrix}\mathrm{tr}[F] & \mathrm{tr}[JF]\\ -\mathrm{tr}[JF] & \mathrm{tr}[F]\end{pmatrix}. \tag{2.6}$$

2.2. *The limit case* $(\mu,\mu_c) = (1,0)$ *for* $\mu > \mu_c \geq 0$

We now approach the more interesting non-classical limit case $(\mu,\mu_c) = (1,0)$ and compute the optimal rotations for $W_{\mu,\mu_c}(R;F)$. Note that, due to Lemma 1.7, this limit case represents the entire non-classical parameter range $\mu > \mu_c \geq 0$.

THEOREM 2.4 (The formally reduced energy $W_{1,0}^{\mathrm{red}}(F)$). *Let $F \in \mathrm{GL}^+(2)$. Then, the* **formally reduced energy**

$$W_{1,0}^{\mathrm{red}}(F) := \min_{R\in\mathrm{SO}(2)} W_{1,0}(R;F) := \min_{R\in\mathrm{SO}(2)} \|\mathrm{sym}(R^TF - \mathbb{1})\|^2 \tag{2.7}$$

is given by

$$W_{1,0}^{\mathrm{red}}(F) = \begin{cases} \|U - \mathbb{1}\|^2 = \mathrm{tr}[(U-\mathbb{1})^2] = \mathrm{dist}^2(F, \mathrm{SO}(2)), & \text{if } \mathrm{tr}[U] < 2 \\ \frac{1}{2}\|F\|^2 - \det[F] = \frac{1}{2}\,\mathrm{tr}[U]^2 - 2\det[U], & \text{if } \mathrm{tr}[U] \geq 2. \end{cases} \tag{2.8}$$

It is well-known that any orthogonally invariant energy density $W(F)$ admits a representation in terms of the singular values of F, i.e., in the eigenvalues of U. Let us give this representation.

Corollary 2.5 (Representation of $W_{1,0}^{\mathrm{red}}(F)$ in the singular values of F). *Let $F \in \mathrm{GL}^+(2)$ and denote its singular values by ν_i, $i = 1, 2$. The representation of $W_{1,0}^{\mathrm{red}}(F)$ in the singular values of F is given by*

$$W_{1,0}^{\mathrm{red}}(F) = W_{1,0}^{\mathrm{red}}(\nu_1, \nu_2) = \begin{cases} (\nu_1 - 1)^2 + (\nu_2 - 1)^2, & \text{if } \nu_1 + \nu_2 < 2 \\ \frac{1}{2}(\nu_1 - \nu_2)^2, & \text{if } \nu_1 + \nu_2 \geq 2. \end{cases} \tag{2.9}$$

Note that the previous formulae are independent of the enumeration of the singular values.

2.2.1. Optimal relative rotations for $\mu = 1$ and $\mu_c = 0$. Our next goal is to compute explicit representations of the rotations $\mathrm{rpolar}_{1,0}^{\pm}(F)$ which realize the minimal energy level in the non-classical limit case $(\mu, \mu_c) = (1, 0)$. This is the content of the next theorem for which we now prepare the stage with the following

Lemma 2.6. *Let $D = \mathrm{diag}(\nu_1, \nu_2) > 0$, i.e, a diagonal matrix with strictly positive diagonal entries. Then, assuming $\mathrm{tr}[D] \geq 2$, the equation $\mathrm{tr}[R(\beta)D] = 2$ has the following solutions*

$$\beta^{\pm} = \pm\arccos\left(\frac{2}{\mathrm{tr}[D]}\right) \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]. \tag{2.10}$$

For $\mathrm{tr}[D] < 2$, there exists no solution, but we can define $\beta = \beta^{\pm} := 0$ by continuous extension.

Our Figure 2.1 shows a plot of the optimal relative rotation angle $\beta(\mathrm{tr}[U])$. In the classical parameter range $0 < \mathrm{tr}[U] \leq 2$, $\alpha_{\mathrm{p}}(F)$ is uniquely optimal and β vanishes identically. In $\mathrm{tr}[U] = 2$, a classical pitchfork bifurcation occurs. In particular, due to $\mathrm{tr}[U(\mathbb{1}_2)] = \mathrm{tr}[\mathbb{1}_2] = 2$, the identity matrix is a bifurcation point of $\beta^{\pm}(F)$. Further, we note that the branches $\beta^{\pm}(\mathrm{tr}[U]) = \pm\arccos(2/\mathrm{tr}[U])$ *are not differentiable* at $\mathrm{tr}[U] = 2$. This has implications on the interaction of the Cosserat shear-stretch energy with the Cosserat curvature energy W_{curv}.

Theorem 2.7 (Optimal non-classical microrotation angles $\alpha_{1,0}^{\pm}$). *Let $F \in \mathrm{GL}^+(2)$ and consider $(\mu, \mu_c) = (1, 0)$. The optimal rotation angles for* $\mathrm{W}_{1,0}$

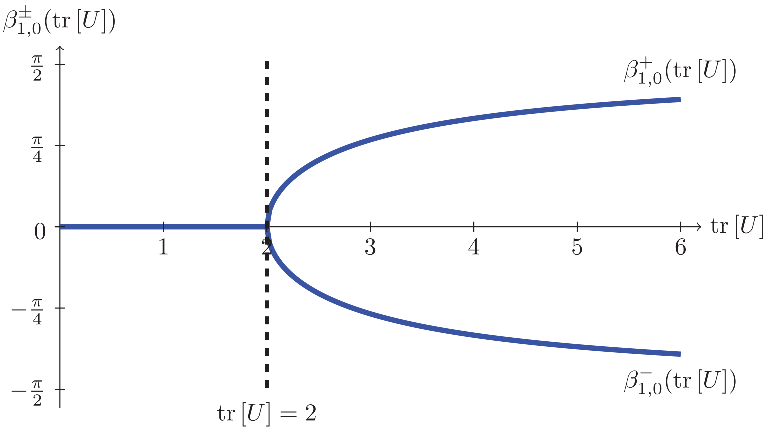


Figure 2.1. Plot of the two optimal relative rotation angles $\beta^{\pm}_{1,0} = \pm\arccos\left(\frac{2}{\mathrm{tr}[U]}\right)$ for the non-classical limit case $(\mu, \mu_c) = (1, 0)$. Note the pitchfork bifurcation in $\mathrm{tr}[U] = \rho_{1,0} = 2$. For $0 < \mathrm{tr}[U] < 2$, the polar angle α_{p} is uniquely optimal and the relative rotation angle β vanishes identically.

are given by

$$\alpha^{\pm}_{1,0}(F) = \begin{cases} \alpha_p(F) = \arccos\left(\frac{\mathrm{tr}[F]}{\mathrm{tr}[U]}\right), & \textit{if } \mathrm{tr}[U] < 2 \\ \alpha_p(F) \pm \arccos\left(\frac{2}{\mathrm{tr}[U]}\right), & \textit{if } \mathrm{tr}[U] \geq 2. \end{cases} \tag{2.11}$$

2.3. Expressions for general non-classical parameter choices

The reduction for μ and μ_c in Lemma 1.7 asserts that the optimal rotations for arbitrary values of $\mu > 0$ and $\mu_c \geq 0$ can be reconstructed from the limit cases $(\mu, \mu_c) = (1, 1)$ and $(\mu, \mu_c) = (1, 0)$. We now detail this procedure which essentially exploits Definition 1.6.

Note first that the rescaled deformation gradient $\tilde{F}_{\mu,\mu_c} := \lambda^{-1}_{\mu,\mu_c} F$ induces a rescaled stretch tensor

$$\tilde{U}_{\mu,\mu_c} = \sqrt{(\tilde{F}_{\mu,\mu_c})^T \tilde{F}_{\mu,\mu_c}} = \lambda^{-1}_{\mu,\mu_c} \cdot U. \tag{2.12}$$

The right polar decomposition takes the form $\tilde{F}_{\mu,\mu_c} = \mathrm{R_p}(\tilde{F}_{\mu,\mu_c})\tilde{U}_{\mu,\mu_c}$. From $\mathrm{R_p}(\tilde{F}_{\mu,\mu_c}) = \tilde{F}_{\mu,\mu_c}\tilde{U}^{-1}_{\mu,\mu_c}$ follows the scaling invariance $\mathrm{R_p}(\tilde{F}_{\mu,\mu_c}) = \mathrm{R_p}(F)$. For the non-classical parameter range $\mu > \mu_c \geq 0$, the quantity

$$\mathrm{tr}[\tilde{U}_{\mu,\mu_c}] = \mathrm{tr}[\lambda^{-1}_{\mu,\mu_c} \cdot U] = \frac{\rho_{1,0}}{\rho_{\mu,\mu_c}}\,\mathrm{tr}[U] \tag{2.13}$$

plays an essential role. This leads us to

$$\mathrm{tr}[\tilde{U}_{\mu,\mu_c}] \geq 2 = \rho_{1,0} \quad \Leftrightarrow \quad \mathrm{tr}\left[\frac{\rho_{1,0}}{\rho_{\mu,\mu_c}} \cdot U\right] \geq \rho_{1,0} \quad \Leftrightarrow \quad \mathrm{tr}[U] \geq \rho_{\mu,\mu_c}. \tag{2.14}$$

In particular, this implies that the bifurcation in $\operatorname{tr}[U]$ allowing for non-classical optimal planar rotations is characterized by the singular radius $\rho_{\mu,\mu_c} := \frac{2\mu}{\mu-\mu_c}$.

THEOREM 2.8. *Let $F \in \mathrm{GL}^+(2)$. For $\mu_c \geq \mu > 0$ the optimal microrotation angle is given by*

$$\alpha_{\mu,\mu_c}(F) = \alpha_p(\tilde{F}_{\mu,\mu_c}) = \alpha_p(F) = \arccos\left(\frac{\operatorname{tr}[F]}{\operatorname{tr}[U]}\right). \tag{2.15}$$

For $\mu > \mu_c \geq 0$, the two optimal rotation angles are given by

$$\alpha^{\pm}_{\mu,\mu_c}(F) = \alpha^{\pm}_{1,0}(\tilde{F}_{\mu,\mu_c}) = \begin{cases} \alpha_p(F) = \arccos\left(\frac{\operatorname{tr}[F]}{\operatorname{tr}[U]}\right), & \textit{if } \operatorname{tr}[U] < \rho_{\mu,\mu_c} \\ \alpha_p(F) \mp \arccos\left(\frac{\rho_{\mu,\mu_c}}{\operatorname{tr}[U]}\right), & \textit{if } \operatorname{tr}[U] \geq \rho_{\mu,\mu_c}. \end{cases} \tag{2.16}$$

2.4. *Optimal rotations for planar simple shear*

We now apply our previous optimality results to simple shear deformations

$$F_\gamma := \begin{pmatrix} 1 & \gamma \\ 0 & 1 \end{pmatrix}, \quad \gamma \in \mathbb{R}. \tag{2.1}$$

The energy-minimizing rotation angles $\alpha_{\mu,\mu_c}(\gamma) := \alpha_{\mu,\mu_c}(F_\gamma)$ for simple shear can be explicitly computed; see also [26] for previous results.

In the classical parameter range $\mu_c \geq \mu > 0$ represented by the limit case $(\mu,\mu_c) = (1,1)$ the polar rotation $\mathrm{R_p}(F_\gamma)$ is uniquely optimal.

Let us collect some properties of simple shear F_γ. We have $\|F_\gamma\|^2 = 2 + \gamma^2$ and $\det[F_\gamma] = 1$, i.e., simple shear is volume preserving for any amount γ. This allows us to compute

$$\operatorname{tr}[U_\gamma] = \sqrt{\|F_\gamma\|^2 + 2\det[F_\gamma]} = \sqrt{4+\gamma^2} \geq 2. \tag{2.2}$$

Thus, we have

COROLLARY 2.9 (Optimal non-classical Cosserat rotations for simple shear). *Let $(\mu,\mu_c) = (1,0)$ and let $F_\gamma \in \mathrm{GL}^+(2)$ be a simple shear of amount $\gamma \in \mathbb{R}$. Then,*

$$\gamma \neq 0 \quad \Rightarrow \quad \operatorname{rpolar}^{\pm}_{1,0}(F_\gamma) \neq \mathrm{R_p}(F_\gamma). \tag{2.3}$$

REMARK 2.10 (Symmetry of the first Cosserat deformation tensor $\overline{U}$ in simple shear). A simple shear F_γ by a non-zero amount $\gamma \neq 0$ automatically generates an optimal microrotational response $\operatorname{rpolar}^{\pm}(F_\gamma)$ which deviates from the continuum rotation $\mathrm{R_p}(F)$. This implies that the associated first Cosserat deformation tensor $\overline{U}^{\pm}_{1,0}(F_\gamma) := \operatorname{rpolar}^{\pm}_{1,0}(F_\gamma)^T F_\gamma$ is not symmetric for any $\gamma \neq 0$.

3. OPTIMAL ROTATIONS IN THREE SPACE DIMENSIONS

In this section, we discuss

PROBLEM 3.1 (Weighted optimality in dimension $n = 3$). *Let $\mu > 0$ and $\mu_c \geq 0$. Compute the set of optimal rotations*

$$\begin{aligned}(3.1)\qquad &\underset{R\in\mathrm{SO}(3)}{\arg\min}\, \mathrm{W}_{\mu,\mu_c}(R;F)\\ &\quad := \underset{R\in\mathrm{SO}(3)}{\arg\min}\{\mu\|\mathrm{sym}(R^TF-\mathbb{1})\|^2+\mu_c\|\mathrm{skew}(R^TF-\mathbb{1})\|^2\}\end{aligned}$$

for given parameter $F \in \mathrm{GL}^+(3)$ with distinct singular values $\nu_1 > \nu_2 > \nu_3 > 0$.

The polar factor $\mathrm{R_p}(F)$ is the *unique* minimizer for $W_{\mu,\mu_c}(R;F)$ in the *classical* parameter range $\mu_c \geq \mu > 0$, in all dimensions $n \geq 2$, see [15, 24].

Since the classical parameter domain $\mu_c \geq \mu > 0$ is very well understood, we focus entirely on the non-classical parameter range $\mu > \mu_c \geq 0$. Furthermore, due to the parameter reduction described by Lemma 1.7, which holds for all dimensions $n \geq 2$, it suffices to solve the non-classical limit case $(\mu, \mu_c) = (1, 0)$, since

$$(3.2)\qquad \underset{R\in\mathrm{SO}(3)}{\arg\min}\, W_{\mu,\mu_c}(R;F) = \underset{R\in\mathrm{SO}(3)}{\arg\min}\, W_{1,0}(R;\tilde{F}_{\mu,\mu_c}).$$

On the right hand side, we notice a *rescaled deformation gradient*

$$\tilde{F}_{\mu,\mu_c} := \lambda_{\mu,\mu_c}^{-1}\cdot F \in \mathrm{GL}^+(3)$$

which is obtained from $F \in \mathrm{GL}^+(3)$ by multiplication with the inverse of the *induced scaling parameter* $\lambda_{\mu,\mu_c} := \frac{\mu}{\mu-\mu_c} > 0$. We note that we use the previous notation throughout the text and further introduce the *singular radius* $\rho_{\mu,\mu_c} := \frac{2\mu}{\mu-\mu_c}$.

It follows that the set of optimal Cosserat rotations can be described by

$$(3.3)\qquad \mathrm{rpolar}_{\mu,\mu_c}(F) = \mathrm{rpolar}_{1,0}(\tilde{F}_{\mu,\mu_c})$$

for the entire non-classical parameter range $\mu > \mu_c \geq 0$. We are therefore mostly concerned with the case $\mu_c = 0$ in the present text. Note that for all $\mu > 0$, we have the equality

$$(3.4)\qquad \mathrm{rpolar}^{\pm}_{\mu,0}(F) = \mathrm{rpolar}^{\pm}_{1,0}(F).$$

3.1. The locally energy-minimizing Cosserat rotations $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$

We briefly present the geometric characterization of the optimal Cosserat rotations $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$ obtained in [10]. Let $R \in \mathrm{SO}(3)$ and let $\mathbb{S}^2 \subset \mathbb{R}^3$ denote the unit 2-sphere. We make use of the well-known angle-axis parametrization of rotations which we write as $[\alpha, r]$[6], where $\alpha \in (-\pi, \pi]$ denotes the rotation angle and $r \in \mathbb{S}^2$ specifies the oriented rotation axis.

We recall that it is sufficient to solve for the relative rotation, i.e., we consider

[6] The angle-axis parametrization is singular, but this is not an issue for our exposition.

PROBLEM 3.2 (Diagonal form of weighted optimality in $n = 3$). *Let $\mu > 0$ and $\mu_c \geq 0$ and let $D = \mathrm{diag}(\nu_1, \nu_2, \nu_3)$ with $\nu_1 > \nu_2 > \nu_3 > 0$. Compute the set of optimal relative rotations*

$$\arg\min_{\hat{R}\in\mathrm{SO}(3)} \mathrm{W}_{\mu,\mu_c}(\hat{R}^T; D) := \arg\min_{\hat{R}\in\mathrm{SO}(3)} \{\mu\|\mathrm{sym}(\hat{R}D - \mathbb{1})\|^2 + \mu_c\|\mathrm{skew}(\hat{R}D - \mathbb{1})\|^2\}. \tag{3.5}$$

We stress that the rotation angle of the relative rotation $\hat{R}$ is implicitly reversed due to the correspondence $R^T \leftrightarrow \hat{R}$.

The computation of the solutions to Problem 3.2 by computer algebra together with a statistical verification are the core results obtained in [10] which we present next.

PROPOSITION 3.3 (Energy-minimizing relative rotations for $(\mu, \mu_c) = (1, 0)$). *Let $\nu_1 > \nu_2 > \nu_3 > 0$ be the singular values of $F \in \mathrm{GL}^+(3)$. Then the energy-minimizing relative rotations solving Problem 3.2 are given by*

$$\hat{R}^{\pm}_{1,0}(F) := \begin{pmatrix} \cos\hat{\beta}^{\pm}_{1,0} & -\sin\hat{\beta}^{\pm}_{1,0} & 0 \\ \sin\hat{\beta}^{\pm}_{1,0} & \cos\hat{\beta}^{\pm}_{1,0} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{3.6}$$

where the optimal rotation angles $\hat{\beta}^{\pm}_{1,0} \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right]$ are given by

$$\hat{\beta}^{\pm}_{1,0}(F) := \begin{cases} 0, & \text{if } \nu_1 + \nu_2 \leq 2, \\ \pm\arccos\left(\frac{2}{\nu_1+\nu_2}\right), & \text{if } \nu_1 + \nu_2 \geq 2. \end{cases} \tag{3.7}$$

Thus, in the non-classical regime $\nu_1 + \nu_2 \geq 2$, we obtain the explicit expression

$$\hat{R}^{\pm}_{1,0}(F) := \begin{pmatrix} \frac{2}{\nu_1+\nu_2} & \mp\sqrt{1 - \left(\frac{2}{\nu_1+\nu_2}\right)^2} & 0 \\ \pm\sqrt{1 - \left(\frac{2}{\nu_1+\nu_2}\right)^2} & \frac{2}{\nu_1+\nu_2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.8}$$

In the classical regime $\nu_1 + \nu_2 \leq 2$, we simply obtain the relative rotation $\hat{R}^{\pm}_{1,0}(F) = \mathbb{1}$, and there is no deviation from the polar factor $\mathrm{R_p}(F)$ at all.

Note that, due to the parameter reduction Lemma 1.7, it is always possible to recover the optimal rotations $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$ for general non-classical parameter choices $\mu > \mu_c \geq 0$ from the non-classical limit case $(\mu, \mu_c) = (1, 0)$; cf. [9] and [10] for details.

3.2. Geometric and mechanical aspects of optimal Cosserat rotations

It seems natural to introduce

DEFINITION 3.4 (Maximal mean planar stretch and strain). Let $F \in \mathrm{GL}^+(3)$ with singular values $\nu_1 \geq \nu_2 \geq \nu_3 > 0$. We introduce the **maximal mean planar stretch** u_{mmp} and the **maximal mean planar strain** s_{mmp} as follows:

$$
\begin{aligned}
u_{\mathrm{mmp}}(F) &:= \frac{\nu_1 + \nu_2}{2}, \quad \text{and} \\
s_{\mathrm{mmp}}(F) &:= \frac{(\nu_1 - 1) + (\nu_2 - 1)}{2} = u_{\mathrm{mmp}}(F) - 1.
\end{aligned} \tag{3.9}
$$

In order to describe the bifurcation behavior of $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$ as a function of the parameter $F \in \mathrm{GL}^+(3)$, it is helpful to partition the parameter space $\mathrm{GL}^+(3)$.

DEFINITION 3.5 (Classical and non-classical domain). To any pair of material parameters (μ, μ_c) in the non-classical range $\mu > \mu_c \geq 0$, we associate a **classical domain** $\mathrm{D}^{\mathrm{C}}_{\mu,\mu_c}$ and a **non-classical domain** $\mathrm{D}^{\mathrm{NC}}_{\mu,\mu_c}$. Here,

$$
\begin{aligned}
\mathrm{D}^{\mathrm{C}}_{\mu,\mu_c} &:= \{F \in \mathrm{GL}^+(3) \,|\, s_{\mathrm{mmp}}(\tilde{F}_{\mu,\mu_c}) \leq 0\}, \quad \text{and} \\
\mathrm{D}^{\mathrm{NC}}_{\mu,\mu_c} &:= \{F \in \mathrm{GL}^+(3) \,|\, s_{\mathrm{mmp}}(\tilde{F}_{\mu,\mu_c}) \geq 0\},
\end{aligned} \tag{3.10}
$$

respectively.

It is straight-forward to derive the following equivalent characterizations

$$
\begin{aligned}
\mathrm{D}^{\mathrm{C}}_{\mu,\mu_c} &= \{F \in \mathrm{GL}^+(3) \,|\, u_{\mathrm{mmp}}(F) \leq \lambda_{\mu,\mu_c}\} \\
&= \left\{F \in \mathrm{GL}^+(3) \,|\, \nu_1 + \nu_2 \leq \rho_{\mu,\mu_c} := \frac{2\mu}{\mu - \mu_c}\right\}, \\
\mathrm{D}^{\mathrm{NC}}_{\mu,\mu_c} &= \{F \in \mathrm{GL}^+(3) \,|\, u_{\mathrm{mmp}}(F) \geq \lambda_{\mu,\mu_c}\} \\
&= \left\{F \in \mathrm{GL}^+(3) \,|\, \nu_1 + \nu_2 \geq \rho_{\mu,\mu_c} := \frac{2\mu}{\mu - \mu_c}\right\}.
\end{aligned} \tag{3.11}
$$

On the intersection $\mathrm{D}^{\mathrm{C}}_{\mu,\mu_c} \cap \mathrm{D}^{\mathrm{NC}}_{\mu,\mu_c} = \{F \in \mathrm{GL}^+(3) \,|\, s_{\mathrm{mmp}}(F) = 0\}$, the minimizers $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$ coincide with the polar factor $\mathrm{R_p}(F)$. This can be seen from the form of the optimal relative rotations in Proposition 3.3. More explicitly, in dimension $n = 3$ and in the non-classical limit case $(\mu, \mu_c) = (1, 0)$, we have:

$$
\begin{aligned}
\mathrm{D}^{\mathrm{C}}_{1,0} &:= \{F \in \mathrm{GL}^+(3) \,|\, s_{\mathrm{mmp}}(F) \leq 0\}, \quad \text{and} \\
\mathrm{D}^{\mathrm{NC}}_{1,0} &:= \{F \in \mathrm{GL}^+(3) \,|\, s_{\mathrm{mmp}}(F) \geq 0\}.
\end{aligned} \tag{3.12}
$$

Since the maximal mean planar strain $s_{\mathrm{mmp}}(F)$ is related to strain, this indicates a particular (possibly new) type of tension-compression asymmetry.

Towards a geometric interpretation of the energy-minimizing Cosserat rotations $\mathrm{rpolar}^{\pm}_{1,0}(F)$ in the non-classical limit case $(\mu, \mu_c) = (1, 0)$, we reconsider the spectral decomposition of $U = QDQ^T$ from the principal axis transformation in Section 1. Let us denote the columns of $Q \in \mathrm{SO}(3)$ by $q_i \in \mathbb{S}^2$, $i = 1, 2, 3$. Then

q_1 and q_2 are orthonormal eigenvectors of U which correspond to the largest two singular values ν_1 and ν_2 of $F \in \mathrm{GL}^+(3)$. More generally, we introduce the following

DEFINITION 3.6 (Plane of maximal stretch). The **plane of maximal stretch** is the linear subspace

$$\mathrm{P}^{\mathrm{ms}}(F) := \mathrm{span}(\{q_1, q_2\}) \subset \mathbb{R}^3$$

spanned by the two eigenvectors q_1, q_2 of U associated with the two largest singular values $\nu_1 > \nu_2 > \nu_3 > 0$ of the deformation gradient $F \in \mathrm{GL}^+(3)$.

We recall that, due to the parameter reduction Lemma 1.7, it is always possible to recover the optimal rotations

$$\mathrm{rpolar}_{\mu,\mu_c}(F) := \underset{R\in \mathrm{SO}(3)}{\arg\min}\, W_{\mu,\mu_c}(R;F) \tag{3.13}$$

for a general choice of non-classical parameters $\mu > \mu_c \geq 0$ from the non-classical limit case $(\mu, \mu_c) = (1, 0)$. However, we defer the explicit procedure for a bit since it is quite instructive to interpret this distinguished non-classical limit case first.

REMARK 3.7 ($\mathrm{rpolar}^{\pm}_{1,0}(F)$ in the classical domain). For $s_{\mathrm{mmp}}(F) \leq 0$ the maximal mean planar strain is non-expansive. By definition, we have $F \in \mathrm{D}^{\mathrm{C}}_{1,0}$ in the classical domain, for which the energy-minimizing relative rotation is given by $\hat{R}_{1,0}(F) = \mathbb{1}$ and there is no deviation from the polar factor. In short $\mathrm{rpolar}^{\pm}_{1,0}(F) = \mathrm{R_p}(F)$.

Let us now turn to the more interesting non-classical case $F \in \mathrm{D}^{\mathrm{NC}}_{1,0}$.

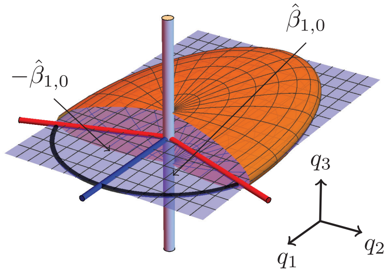


Figure 3.1. Action of $\mathrm{rpolar}^{\pm}_{1,0}(F)$ in axes of principal stretch for a stretch ellipsoid with half-axes $(\nu_1, \nu_2, \nu_3) = (4, 2, 1/2)$. The plane of maximal stretch $\mathrm{P}^{\mathrm{ms}}(F)$ is depicted in blue. The cylinder along $q_3 \perp \mathrm{P}^{\mathrm{ms}}(F)$ illustrates that the axis of rotation is the eigenvector q_3 of U associated with the smallest singular value $\nu_3 = 1/2$ of F. The thin cylinder [blue] bisecting the opening represents the relative rotation angle $\hat{\beta} = 0$ and corresponds to $\mathrm{R_p}(F)$. The outer two cylinders [red] correspond to the two non-classical minimizers $\mathrm{rpolar}^{\pm}_{1,0}(F)$. The enclosed angles $\hat{\beta}^{\pm}_{1,0} = \pm\arccos\left(\frac{2}{\nu_1+\nu_2}\right)$ are the optimal relative rotation angles. This reveals the major symmetry of the non-classical minimizers.

REMARK 3.8 ($\mathrm{rpolar}^{\pm}_{1,0}(F)$ in the non-classical domain). If $F \in \mathrm{D}^{\mathrm{NC}}_{1,0}$, then by definition $s_{\mathrm{mmp}}(F) > 0$ and the maximal mean planar strain is expansive. The deviation of the non-classical energy-minimizing rotations $\mathrm{rpolar}^{\pm}_{1,0}(F)$ from the polar factor $\mathrm{R_p}$ is measured by a rotation in the plane of maximal stretch $\mathrm{P}^{\mathrm{ms}}(F)$ given by $\mathrm{R_p}(F)^T\, \mathrm{rpolar}^{\pm}_{1,0}(F) = Q(F)\hat{R}^{\mp}_{1,0}(F)Q(F)^T$. The rotation axis is the eigenvector q_3 associated with the smallest singular value $\nu_3 > 0$ of F and the relative rotation angle is given by $\hat{\beta}^{\mp}_{1,0}(F) = \mp \arccos(1/u_{\mathrm{mmp}}(F))$. The rotation angles increase monotonically towards the asymptotic limits

$$\lim_{u_{\mathrm{mmp}}(F)\to\infty} \hat{\beta}^{\pm}_{1,0}(F) = \pm\frac{\pi}{2}.$$

In axis-angle representation, we obtain

$$\hat{R}^{\pm}_{1,0}(F) \equiv [\pm\arccos(1/u_{\mathrm{mmp}}(F)), (0,0,1)], \quad \text{and} \tag{3.14}$$

$$\mathrm{R_p^T}\, \mathrm{rpolar}^{\pm}_{1,0}(F) \equiv [\mp\arccos(1/u_{\mathrm{mmp}}(F)), q_3]. \tag{3.15}$$

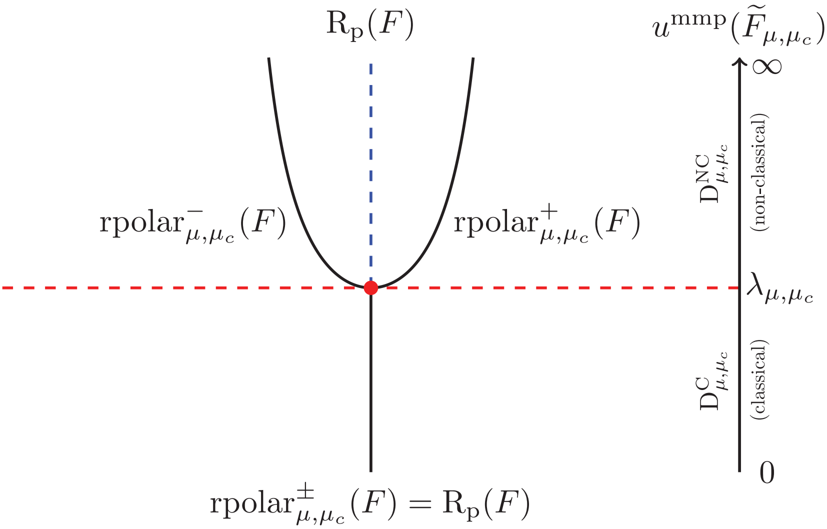


Figure 3.2. Pitchfork bifurcation diagram for $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$ for $\mu > \mu_c \geq 0$. Let us express the energy-minimizers $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$ in terms of the maximal mean planar stretch $u_{\mathrm{mmp}}(\tilde{F}_{\mu,\mu_c})$ of the rescaled deformation gradient $\tilde{F}_{\mu,\mu_c} := \lambda^{-1}_{\mu,\mu_c}F$. For values $F \in \mathrm{D}^{\mathrm{C}}_{\mu,\mu_c}$, we have $0 < u_{\mathrm{mmp}} \leq \lambda_{\mu,\mu_c}$ and the polar factor $\mathrm{R_p}(F)$ is uniquely energy-minimizing. In contrast, for $F \in \mathrm{D}^{\mathrm{NC}}_{\mu,\mu_c}$, $\lambda_{\mu,\mu_c} \leq u_{\mathrm{mmp}} < \infty$, there are two non-classical minimizers $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$. In this regime, the polar factor is no longer optimal but it is still a critical point. At the branching point $u_{\mathrm{mmp}}(\tilde{F}_{\mu,\mu_c}) = \lambda_{\mu,\mu_c}$ the minimizers all coincide: $\mathrm{rpolar}^{-}_{\mu,\mu_c}(F) = \mathrm{R_p}(F) = \mathrm{rpolar}^{+}_{\mu,\mu_c}(F)$. For $\mu_c \to \mu$, the branching point escapes to infinity which asymptotically recovers the behavior in the classical parameter range $\mu_c \geq \mu > 0$.

COROLLARY 3.9 (An explicit formula for $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$). *For the non-classical limit case* $(\mu,\mu_c)=(1,0)$ *we have the following formula for the energy-minimizing Cosserat rotations:*

$$\mathrm{rpolar}^{\pm}_{1,0}(F) := \begin{cases} \mathrm{R_p}(F), & \text{if } F \in \mathrm{D}^{\mathrm{C}}_{1,0}, \\ \mathrm{R_p}(F)Q(F)\hat{R}^{\mp}_{1,0}(F)Q(F)^T, & \text{if } F \in \mathrm{D}^{\mathrm{NC}}_{1,0}. \end{cases} \tag{3.16}$$

For general values of the weights in the non-classical range $\mu > \mu_c \geq 0$, *we obtain*

$$\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F) := \mathrm{rpolar}^{\pm}_{1,0}(\tilde{F}_{\mu,\mu_c}), \tag{3.17}$$

where $\tilde{F}_{\mu,\mu_c} := \lambda^{-1}_{\mu,\mu_c}F$ *is obtained by rescaling the deformation gradient with the inverse of the* induced scaling parameter $\lambda_{\mu,\mu_c} := \frac{\mu}{\mu-\mu_c} > 0$.

Note that the previous definition is relative to a fixed choice of the orthonormal factor $Q(F) \in \mathrm{SO}(3)$ in the spectral decomposition of $U = QDQ^T$. Further, right from their variational characterization, one easily deduces that the energy-minimizing rotations satisfy $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(QF) = Q\,\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$, for any $Q \in \mathrm{SO}(3)$, i.e., they are objective functions; cf. Remark 3.10.

The domains of the piecewise definition of $\mathrm{rpolar}^{\pm}_{1,0}(F)$ in Corollary 3.9 indicate a certain tension-compression asymmetry in the material model characterized by the Cosserat shear-stretch energy $W_{1,0}(R;F)$. We can also make a second important observation. To this end, consider a smooth curve $F(t) : (-\varepsilon,\varepsilon) \to \mathrm{GL}^+(3)$. If the eigenvector $q_3(t) \in \mathbb{S}^2$ associated with the smallest singular value $\nu_3(t)$ changes its orientation along this curve, then the rotation axis of $\mathrm{rpolar}^{\pm}_{1,0}(F)$ flips as well. Effectively, the sign of the relative rotation angle $\hat{\beta}^{\pm}_{1,0}(F)$ is negated which may lead to jumps. This can happen, e.g., if $F(t)$ passes through a deformation gradient with a non-simple singular value, but it may also depend on details of the specific algorithm used for the computation of the eigenbasis.

For the classical range $\mu_c \geq \mu > 0$, the polar factor and the relaxed polar factor(s) coincide and trivially share all properties. This is no longer true for the non-classical parameter range $\mu_c \geq \mu > 0$ and we compare the properties for that range in our next remark. More precisely, we present a detailed comparison of the well-known features of the polar factor $\mathrm{R_p}$ which are of fundamental importance in the context of mechanics.

REMARK 3.10 ($\mathrm{R_p}(F)$ vs. $\mathrm{rpolar}(F)$ for the non-classical range $\mu > \mu_c \geq 0$). Let $n \geq 2$ and $F \in \mathrm{GL}^+(n)$. The polar factor $\mathrm{R_p}(F) \in \mathrm{SO}(n)$ obtained from the polar decomposition $F = \mathrm{R_p}(F)U$ is *always unique* and satisfies:

$$\begin{array}{lll} \text{(Objectivity)} & \mathrm{R_p}(Q\cdot F) = Q\cdot \mathrm{R_p}(F) & (\forall Q \in \mathrm{SO}(n)), \\ \text{(Isotropy)} & \mathrm{R_p}(F\cdot Q) = \mathrm{R_p}(F)\cdot Q & (\forall Q \in \mathrm{SO}(n)), \\ \text{(Scaling invariance)} & \mathrm{R_p}(\lambda\cdot F) = \mathrm{R_p}(F) & (\forall \lambda > 0), \\ \text{(Inversion symmetry)} & \mathrm{R_p}(F^{-1}) = \mathrm{R_p}(F)^{-1}. & \end{array} \tag{3.18}$$

The relaxed polar factor(s) $\mathrm{rpolar}_{\mu,\mu_c}(F) \subset \mathrm{SO}(n)$ is *in general multi-valued* and, due to its variational characterization, satisfies:

$$\begin{array}{lll} \text{(Objectivity)} & \mathrm{rpolar}_{\mu,\mu_c}(Q \cdot F) = Q \cdot \mathrm{rpolar}_{\mu,\mu_c}(F) & (\forall Q \in \mathrm{SO}(n)), \\ \text{(Isotropy)} & \mathrm{rpolar}_{\mu,\mu_c}(F \cdot Q) = \mathrm{rpolar}_{\mu,\mu_c}(F) \cdot Q & (\forall Q \in \mathrm{SO}(n)). \end{array} \tag{3.19}$$

For the particular dimensions $k = 2, 3$, our explicit formulae imply that there exist particular instances $\lambda^* > 0$ and $F^* \in \mathrm{GL}^+(k)$, for which we have

$$\begin{array}{lll} (\underline{\text{Broken}}\text{ scaling invariance}) & \mathrm{rpolar}^{\pm}_{\mu,\mu_c}(\lambda^* \cdot F^*) \neq \mathrm{rpolar}(F^*), & \text{and} \\ (\underline{\text{Broken}}\text{ inversion symmetry}) & \mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F^{*-1}) \quad \neq \mathrm{rpolar}(F^*)^{-1}. & \end{array} \tag{3.20}$$

This can be directly inferred from the partitioning of $\mathrm{GL}^+(k) = \mathrm{D}^{\mathrm{C}}_{\mu,\mu_c} \cup \mathrm{D}^{\mathrm{NC}}_{\mu,\mu_c}$ and the respective piecewise definition of the relaxed polar factor(s), see Corollary 3.9.

We interpret these broken symmetries as a (generalized) tension-compression asymmetry.

3.3. The reduced Cosserat shear-stretch energy

We now introduce the notion of a reduced energy as the energy level realized by the energy-minimizing rotations $\mathrm{rpolar}_{\mu,\mu_c}(F)$.

Definition 3.11 (Reduced Cosserat shear-stretch energy). The **reduced Cosserat shear-stretch energy** is defined as

$$W^{\mathrm{red}}_{\mu,\mu_c} : \mathrm{GL}^+(n) \to \mathbb{R}^+_0, \quad W^{\mathrm{red}}_{\mu,\mu_c}(F) := \min_{R \in \mathrm{SO}(n)} W_{\mu,\mu_c}(R; F). \tag{3.21}$$

Besides the previous definition, we also have the following equivalent means for the explicit computation of the reduced energy

$$\begin{aligned} &W^{\mathrm{red}}_{\mu,\mu_c}(F) = W_{\mu,\mu_c}(\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F); F), \quad \text{and} \\ &W^{\mathrm{red}}_{\mu,\mu_c}(F) = W^{\mathrm{red}}_{\mu,\mu_c}(D) := \min_{\hat{R} \in \mathrm{SO}(n)} W_{\mu,\mu_c}(\hat{R}; D) = W_{\mu,\mu_c}(\hat{R}^{\pm}_{\mu,\mu_c}; D). \end{aligned} \tag{3.22}$$

Lemma 3.12 (The reduced Cosserat shear-stretch energy $\mathrm{W}^{\mathrm{red}}_{1,0}(F)$ in terms of singular values). *Let $F \in \mathrm{GL}^+(3)$ and $\nu_1 > \nu_2 > \nu_3 > 0$ the ordered singular values of F. Then the reduced Cosserat shear-stretch energy $\mathrm{W}^{\mathrm{red}}_{1,0}(F)$ admits the following piecewise representation*

$$\mathrm{W}^{\mathrm{red}}_{1,0}(F) = \begin{cases} (\nu_1 - 1)^2 + (\nu_2 - 1)^2 + (\nu_3 - 1)^2 = \|U - \mathbb{1}\|^2, \\ \quad \textit{if } \nu_1 + \nu_2 \leq 2, \textit{ i.e., } F \in \mathrm{D}^{\mathrm{C}}_{1,0}, \\ \frac{1}{2}(\nu_1 - \nu_2)^2 + (\nu_3 - 1)^2, \\ \quad \textit{if } \nu_1 + \nu_2 \geq 2, \textit{ i.e., } F \in \mathrm{D}^{\mathrm{NC}}_{1,0}. \end{cases}$$

Our next step is to reveal the form of the reduced energy for the entire non-classical parameter range $\mu > \mu_c \geq 0$ which involves the parameter reduction lemma, but we have to be a bit careful.

REMARK 3.13 (Reduced energies and the parameter reduction lemma). The parameter reduction in Lemma 1.7 is the key step in the computation of the minimizers for general non-classical material parameters $\mu > \mu_c \geq 0$. It might be tempting, but we have to stress that the general form of the reduced energy cannot be obtained by rescaling the singular values $\nu_i \mapsto \lambda_{\mu,\mu_c}^{-1} \nu_i$ in the singular value representation of $W_{1,0}^{\mathrm{red}}$.

THEOREM 3.14 ($W_{\mu,\mu_c}^{\mathrm{red}}$ as a function of the singular values). *Let $F \in \mathrm{GL}^+(n)$ and $\nu_1 > \nu_2 > \nu_3 > 0$, the ordered singular values of F and let $\mu > \mu_c \geq 0$, i.e., a non-classical parameter set. Then the reduced Cosserat shear-stretch energy $W_{\mu,\mu_c}^{\mathrm{red}} : \mathrm{GL}^+(3) \to \mathbb{R}_0^+$ admits the following explicit representation*

$$W_{\mu,\mu_c}^{\mathrm{red}}(F) = \begin{cases} \mu((\nu_1-1)^2 + (\nu_2-1)^2 + (\nu_3-1)^2) = \mu\|U - \mathbb{1}\|^2, & F \in \mathrm{D}_{\mu,\mu_c}^{\mathrm{C}}, \\ \frac{\mu}{2}(\nu_1-\nu_2)^2 + \mu(\nu_3-1)^2 + \frac{\mu_c}{2}((\nu_1+\nu_2) - \rho_{\mu,\mu_c})^2 - \frac{\mu_c}{2}\cdot\rho_{\mu,\mu_c}^2, & F \in \mathrm{D}_{\mu,\mu_c}^{\mathrm{NC}}. \end{cases}$$

REMARK 3.15 (On μ_c as a penalty weight). Let us consider the contribution of the skew-term to $W_{\mu,\mu_c}^{\mathrm{red}}$ given by

$$\frac{\mu_c}{2}((\nu_1+\nu_2) - \rho_{\mu,\mu_c})^2$$

as a penalty term for $F \in \mathrm{GL}^+(3)$ arising for material parameters in the non-classical parameter range $\mu > \mu_c \geq 0$. This leads to a simple but interesting observation for strictly positive $\mu_c > 0$. The minimizers $F \in \mathrm{GL}^+(3)$ *for the penalty term* satisfy the bifurcation criterion

$$\nu_1 + \nu_2 = \rho_{\mu,\mu_c}$$

for $\mathrm{rpolar}_{\mu,\mu_c}^{\pm}(F)$. In this case $\hat{R}_{\mu,\mu_c}^{\pm} = \mathbb{1}$ which implies that $\hat{R}_{\mu,\mu_c}^{\pm} D - \mathbb{1} \in \mathrm{Sym}(3)$, i.e., it is symmetric. Hence, the skew-part vanishes entirely which minimizes the penalty. In numerical applications, a rotation field R approximating $\mathrm{rpolar}^{\pm}(F)$ can be expected to be unstable in the vicinity of the branching point $\nu_1 + \nu_2 \approx \rho_{\mu,\mu_c}$. Hence, a penalty which explicitly rewards an approximation to the bifurcation point seems to be a delicate property. In strong contrast, for the case when the Cosserat couple modulus is zero, i.e., $\mu_c = 0$, the penalty term vanishes entirely. This hints at a possibly more favorable qualitative behavior of the model in that case; cf. [18].

We recall that the tangent bundle $T\,\mathrm{SO}(n)$ is isomorphic to the product $\mathrm{SO}(n) \times \mathfrak{so}(n)$ as a vector bundle. This is commonly referred to as the left trivialization, see, e.g., [5]. With this we can minimize over the tangent bundle in the following

LEMMA 3.16. *Let $F \in \mathbb{R}^{n\times n}$. Then*

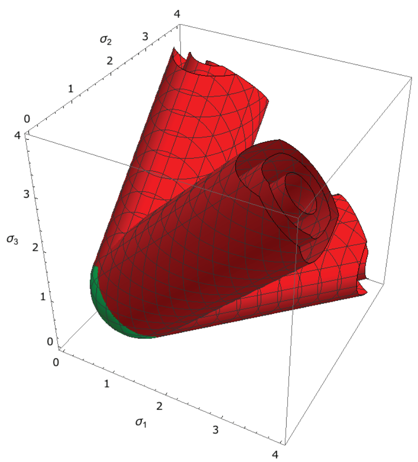
$$\inf_{\substack{R\in \mathrm{SO}(n)\\ A\in \mathfrak{so}(n)}} \|R^T F - \mathbb{1} - A\|^2 = \min_{R\in \mathrm{SO}(n)} \|\mathrm{sym}(R^T F - \mathbb{1})\|^2 =: \min_{R\in \mathrm{SO}(n)} W_{1,0}(R;F).$$

In the non-classical limit case $(\mu,\mu_c) = (1,0)$, the preceding lemma yields a geometric characterization of the *reduced* Cosserat shear-stretch energy as a distance which we find remarkable.

COROLLARY 3.17 (Characterization of $W^{\mathrm{red}}_{1,0}$ as a distance). *Let $n \geq 2$ and consider $F \in \mathrm{GL}^+(n)$ with singular values $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_n > 0$, i.e., not necessarily distinct. Then the reduced Cosserat shear-stretch energy $W^{\mathrm{red}}_{1,0} : \mathrm{GL}^+(n) \to \mathbb{R}^+_0$ admits the following characterization as a distance*

$$W^{\mathrm{red}}_{1,0}(F) = \mathrm{dist}^2_{\mathrm{euclid}}(F, \mathrm{SO}(n)(\mathbb{1} + \mathfrak{so}(n))). \tag{3.23}$$

Here, $\mathrm{dist}_{\mathrm{euclid}}$ *denotes the euclidean distance function.*



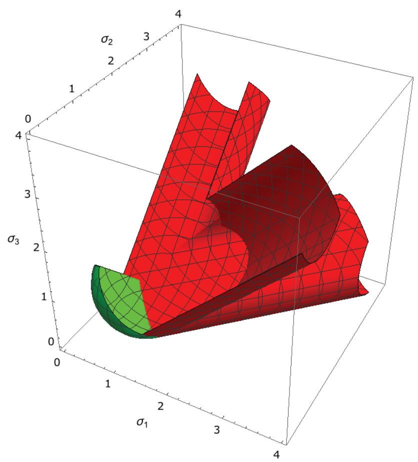


Figure 3.3. Energy isosurfaces of $W^{\mathrm{red}}_{1,0}$ considered as a function of the *unordered* singular values $\nu_1, \nu_2, \nu_3 > 0$ of $F \in \mathrm{GL}^+(3)$. The displayed contour levels are 0.1, 0.4 and 0.8. On the right, we have removed a piece from the non-classical cylindrical parts (red) of the energy level 0.8 which reveals the spherical shell of the classical part (green). Note that a computation of these level surfaces via Monte Carlo minimization yields the same result (but at a much lower resolution).

3.4. Alternative criteria for the existence of non-classical solutions

For $\mu > \mu_c > 0$, i.e., for strictly positive $\mu_c > 0$, the singular radius satisfies $\rho_{\mu,\mu_c} := \frac{2\mu}{\mu-\mu_c} > 2$. We now define a quite similar constant, namely

$$\zeta_{\mu,\mu_c} := \rho_{\mu,\mu_c} - \rho_{1,0} = \frac{2\mu_c}{\mu - \mu_c} > 0. \tag{3.24}$$

Furthermore, we define the ε-neighborhood of a set $\mathscr{X} \subseteq \mathbb{R}^{n\times n}$ relative to the euclidean distance function as

$$N_\varepsilon(\mathscr{X}) := \{ Y \in \mathbb{R}^{n\times n} \,|\, \mathrm{dist}_{\mathrm{euclid}}(Y, \mathscr{X}) < \varepsilon \}.$$

LEMMA 3.18 (Classical SO(3)-neighborhood for $\mu_c > 0$). *Let $\mu > \mu_c > 0$, $F \in \mathrm{GL}^+(3)$ and $\zeta_{\mu,\mu_c} := \frac{2\mu_c}{\mu-\mu_c} > 0$. Then we have the following inclusion*

$$N_{\frac{1}{2}\zeta^2_{\mu,\mu_c}}(\mathrm{SO}(3)) \subset \mathrm{D}^{\mathrm{C}}_{\mu,\mu_c}. \tag{3.25}$$

In other words, for all $F \in \mathrm{GL}^+(3)$ satisfying $\mathrm{dist}_{\mathrm{euclid}}(F, \mathrm{SO}(3)) = \|U - \mathbb{1}\|^2 < \frac{1}{2}\zeta^2_{\mu,\mu_c}$, the polar factor $\mathrm{R_p}$ is the unique minimizer of $W_{\mu,\mu_c}(R; F)$.

LEMMA 3.19. *Let $F \in \mathrm{SL}(3)$, i.e., $\det[F] = \nu_1\nu_2\nu_3 = 1$, where $\nu_1 \geq \nu_2 \geq \nu_3 > 0$ are ordered singular values of F, not necessarily distinct. Then*

$$\mathrm{SL}(3) \subset \mathrm{D}^{\mathrm{NC}}_{1,0}, \tag{3.26}$$

i.e., F induces a strictly non-classical minimizer. Equivalently, $\det[F] = 1$ implies the estimate $\nu_1 + \nu_2 \geq 2$.

REMARK 3.20. If we make the stronger assumption $\nu_1 > \nu_2 > \nu_3 > 0$, we obtain a strict inequality $\nu_1 + \nu_2 > 2$. In that case, $F \in \mathrm{D}^{\mathrm{NC}}_{1,0} \backslash \mathrm{D}^{\mathrm{C}}_{1,0}$ is strictly non-classical.

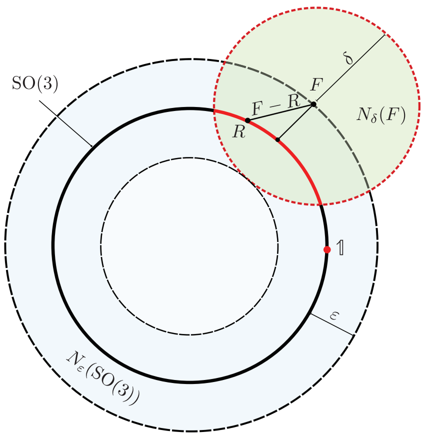


Figure 3.4. Illustration of a euclidean ε-neighborhood of $\mathrm{SO}(3) \subset \mathbb{R}^{3\times 3}$.

Corollary 3.21. *Let* $\mu > 0$, $F \in \mathrm{SL}^+(3)$ *and assume that* $\nu_1 > \nu_2 > \nu_3 > 0$. *Then*

$$F \in \mathrm{D}^{\mathrm{NC}}_{\mu,0} \setminus \mathrm{D}^{\mathrm{C}}_{\mu,0}, \tag{3.27}$$

i.e., the minimizers $\mathrm{rpolar}^{\pm}_{\mu,0}(F) \neq \mathrm{R_p}$ *are* strictly *non-classical.*

4. Optimal rotations in general dimension

The key insight for the solution of the minimization problem in general dimension $n \geq 2$ is a new approach to the analysis of the critical points. The Euler-Lagrange equations for $W_{1,0}(R;F)$ are equivalent to

$$(\hat{R}D - \mathbb{1})^2 \in \mathrm{Sym}(n). \tag{4.1}$$

This is a *symmetric square condition* for the relative rotation $\hat{R}$, since

$$(X(\hat{R}))^2 = S \in \mathrm{Sym}(n), \quad \text{where } X(\hat{R}) := \hat{R}D - \mathbb{1} \in \mathbb{R}^{n \times n}. \tag{4.2}$$

As it is sufficient to compute the optimal relative rotation $\hat{R}$, we simply set $R = \hat{R}$ for the rest of this section.

One might suspect that the critical points of $W_{1,0}(R;D)$ are connected to real matrix square roots of real symmetric matrices. And indeed, the structure of the set of critical points of $W_{1,0}(R;D)$ can be revealed quite elegantly by a specific characterization of the set of real matrix square roots of real symmetric matrices. Note that this characterization [2, Thm. 2.13], which is similar in spirit to the standard representation theorem for orthogonal matrices $\mathrm{O}(n)$ as block matrices, seems not to be known in the literature. Due to this representation, the square roots of interest can always be orthogonally transformed into a block-diagonal representation which reduces the minimization problem from arbitrary dimension $n > 2$ into decoupled one- and two-dimensional subproblems. These can then be solved independently. From this point of view, a non-classical minimizer in $n = 3$, simultaneously solves a one-dimensional and a two-dimensional subproblem. The one-dimensional problem determines the rotation axis of the optimal rotations, while the two-dimensional subproblem determines the optimal rotation angles.

The degenerate cases of optimal Cosserat rotations arising for recurring parameter values ν_i, $i = 1, 2, 3$, in the diagonal parameter matrix $D \in \mathrm{Diag}(n)$ has not been treated previously in [10], but is also accessible with the general approach. Note that this case corresponds to the special case of two or more equal principal stretches ν_i which is an important highly symmetric corner case in mechanics.

Combining the results of the two preceding sections, we can now describe the critical values of the Cosserat shear-stretch energy $W_{1,0}(R;D)$ which are attained at the critical points. The main result of this section is a procedure (algorithm) which traverses the set of critical points in a way that reduces the

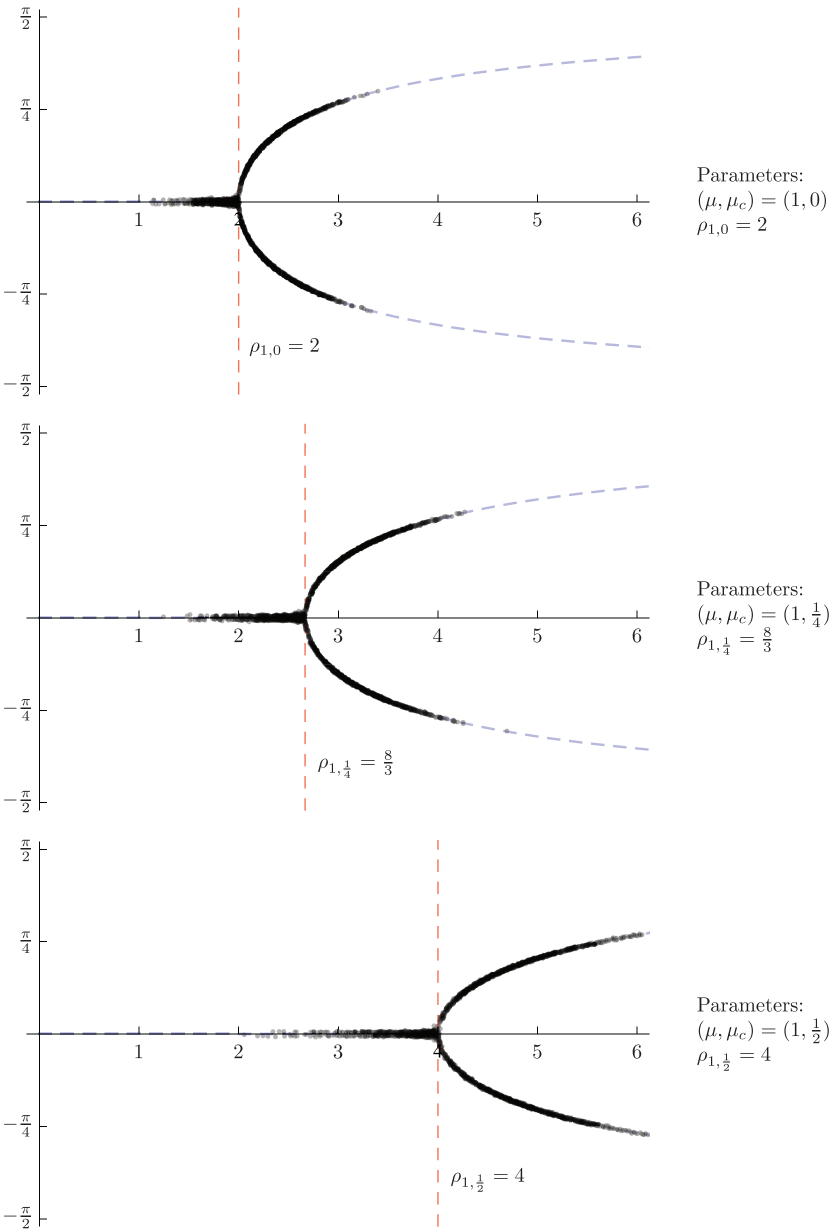


Figure 3.5. Optimal relative rotation angles $\hat{\beta}^{\mathrm{MC}}_{\mu,\mu_c}$ for multiple non-classical values $\mu > \mu_c \geq 0$. The angles are obtained by stochastic (Monte Carlo) minimization of $W_{\mu,\mu_c}(R; F)$. The dashed blue curve shows the predicted value for $\hat{\beta}^{\pm}_{1,0}(\nu_1 + \nu_2)$ and the dashed red line marks the expected bifurcation point at ρ_{μ,μ_c}. For a direct comparison, we provide Figure 3.6 on page 596 which shows the classical limit case $(\mu, \mu_c) = (1, 1)$; see also Figure 3.2 on page 588 for an illustration and a more precise description of the bifurcation behavior predicted by our proposed formula $\mathrm{rpolar}^{\pm}_{\mu,\mu_c}(F)$.

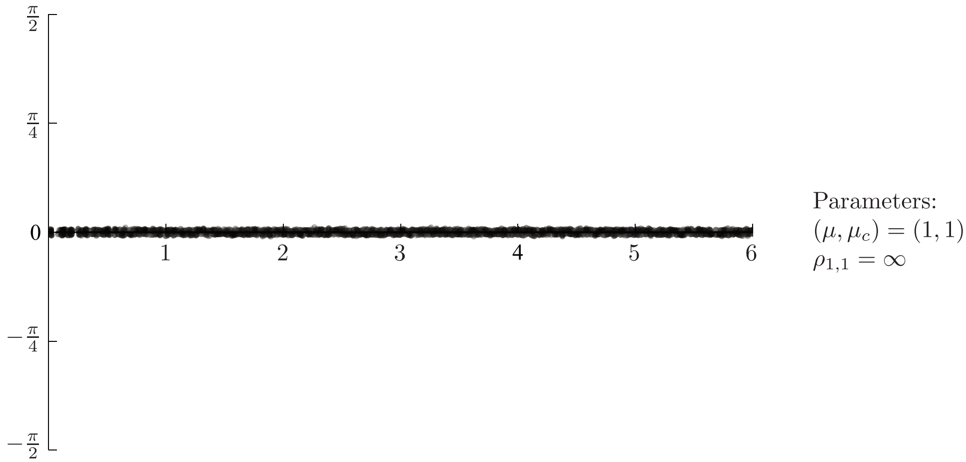


Figure 3.6. Optimal relative rotation angle $\hat{\beta}^{\mathrm{MC}}_{1,1}$ obtained from stochastic (Monte Carlo) minimization for the classical limit case $\mu = \mu_c = 1$. We observe that the relative rotation angle vanishes up to numerical accuracy, since the polar factor $\mathrm{R_p}(F)$ is always optimal in perfect accordance with Grioli's theorem, see [24] and [9, Cor. 2.4, p. 5]. More precisely, this corresponds to the prediction $\hat{\beta}^{\pm}_{1,1}(\nu_1 + \nu_2) = 0$.

energy at every step of the procedure and finally terminates in the subset of global minimizers.

Technically, we label the critical points by certain partitions of the index set $\{1, \ldots, n\}$ containing only subsets I with one or two elements. We note that the subsets I and a choice of sign for $\det[R_I]$ uniquely characterize a critical point $R \in \mathrm{SO}(n)$.

Let us give an outline of the energy-decreasing traversal strategy starting from a given labeling partition (i.e., critical point):

1. Choose the positive sign $\det[R_I] = +1$ for each subset of the partition.
2. Disentangle all overlapping blocks for $n > 3$ (cf. Lemma 4.5).
3. Successively shift all 2×2-blocks to the lowest possible index, i.e., collect the blocks of size two as close to the upper left corner of the matrix R as possible (cf. Lemma 4.3).
4. Introduce as many additional 2×2-blocks by joining adjacent blocks of size 1 as the constraint $\nu_i + \nu_j > 2$ allows (cf. Lemma 4.3).

The next theorem connects the value of $W_{1,0}(R; D)$ realized by a critical point with its labeling partition and the choice of determinants $\det[R_I]$ which characterize it.

Theorem 4.1 (Characterization of critical points and values). *Let the entries $\nu_1 > \nu_2 > \ldots > \nu_n > 0$ of $D \in \mathrm{Diag}(n)$. Then the critical points $R \in \mathrm{SO}(n)$ can be classified according to partitions of the index set $\{1, \ldots, n\}$ into subsets of size one or two and choices of signs for the determinant* $\det[R_I]$ *for each subset I. The sub-*

sets of size two $I = \{i, j\}$ *satisfy*

$$\begin{cases} v_i + v_j > 2, & \det[R_I] = +1, \quad \textit{and} \\ |v_i - v_j| > 2, & \det[R_I] = -1. \end{cases}$$

The corresponding critical values are given by

$$\begin{aligned} W_{1,0}(R; D) = &\sum_{\substack{I=\{i\} \\ \det[R_I]=1}} (v_i - 1)^2 + \sum_{\substack{I=\{i\} \\ \det[R_I]=-1}} (v_i + 1)^2 \\ &+ \sum_{\substack{I=\{i,j\} \\ \det[R_I]=1}} \frac{1}{2}(v_i - v_j)^2 + \sum_{\substack{I=\{i,j\} \\ \det[R_I]=-1}} \frac{1}{2}(v_i + v_j)^2. \end{aligned}$$

Remark 4.2 (On non-distinct entries of D). If we allow

$$v_1 \geq v_2 \geq \cdots \geq v_n > 0$$

for the entries of D, then the D- and R-invariant subspaces V_i are not necessarily coordinate subspaces. This produces non-isolated critical points but does not change the formula for the critical values.

In order to compute the global minimizers $R \in \mathrm{SO}(n)$ for the Cosserat shear-stretch energy $W_{1,0}(R; D)$, we have to compare all the critical values which correspond to the different partitions and choices of the signs of the determinants in the statement of Theorem 4.1. We may, however, assume that $\det[R_I] = +1$ for all subsets I, see [2] for further details.

The following lemma shows that blocks of size two are always favored *whenever they exist*.

Lemma 4.3 (Comparison lemma). *If* $v_i + v_j > 2$ *then the difference between the critical values of* $W_{1,0}(R; D)$ *corresponding to the choice of a size two subset* $I = \{i, j\}$ *as compared to the choice of two size one subsets* $\{i\}$, $\{j\}$ *is given by*

$$-\frac{1}{2}(v_i + v_j - 2)^2.$$

Let us rewrite $W_{1,0}(R; D)$ in a slightly different form in order to distill the contributions of the size two blocks in the partition.

Corollary 4.4. *For the choices of* $\det[R_I] = 1$ *there holds*

$$W_{1,0}(R; D) = \|\mathrm{sym}(RD - \mathbb{1})\|^2 = \sum_{i=1}^{n} (v_i - 1)^2 - \frac{1}{2} \sum_{I=\{i,j\}} (v_i + v_j - 2)^2.$$

To study the global minimizers for the Cosserat shear-stretch energy in arbitrary dimension $n \geq 4$, we need to investigate the relative location of the size two subsets of the partition.

LEMMA 4.5. *Let $R \in \mathrm{SO}(n)$ be a global minimizer for $W_{1,0}(R;D)$. Then R cannot contain overlapping size two subsets, i.e., $I = \{i_1, i_4\}$, $J = \{i_2, i_3\}$, with $i_1 < i_2 < i_3 < i_4$.*

We are now ready to state the result in the general n-dimensional case.

THEOREM 4.6. *Let $\nu_1 > \nu_2 > \cdots \nu_n > 0$ be the entries of D. Let us fix the maximum k for which $\nu_{2k-1} + \nu_{2k} > 2$. Any global minimizer $R \in \mathrm{SO}(n)$ corresponds to the partition of the form*

$$\{1,2\} \sqcup \{3,4\} \sqcup \cdots \sqcup \{2k-1, 2k\} \sqcup \{2k+1\} \sqcup \cdots \sqcup \{n\}$$

and the global minimum of $W_{1,0}(R;D)$ is given by

$$W_{1,0}^{\mathrm{red}}(D) := \min_{R \in \mathrm{SO}(n)} \|\mathrm{sym}(RD - \mathbb{1})\|^2 = \sum_{i=1}^{n} (\nu_i - 1)^2 - \frac{1}{2}\sum_{i=1}^{k} (\nu_{2i-1} + \nu_{2i} - 2)^2$$
$$= \frac{1}{2}\sum_{i=1}^{k} (\nu_{2i-1} - \nu_{2i})^2 + \sum_{i=2k+1}^{n} (\nu_i - 1)^2.$$

REMARK 4.7. The number of global minimizers in the above theorem is 2^k, where k is the number of blocks of size two in the preceding characterization of a global minimizer as a block diagonal matrix. All global minimizers are block diagonal, similar to the previously discussed $n = 3$ case.

REFERENCES

[1] C. G. BÖHMER - P. NEFF - B. SEYMENOGLU, *Soliton-like solutions based on geometrically nonlinear Cosserat micropolar elasticity*, Wave Motion, 60:158–165, 2016.

[2] L. BORISOV - A. FISCHLE - P. NEFF, *Optimality of the relaxed polar factors by a characterization of the set of real square roots of real symmetric matrices*, arXiv preprint arXiv:1606.09085, 2016. https://arxiv.org/abs/1606.09085 (submitted to SIAM Journal on Applied Algebra and Geometry (SIAGA)).

[3] C. BOUBY - D. FORTUNÉ - W. PIETRASZKIEWICZ - C. VALLÉE, *Direct determination of the rotation in the polar decomposition of the deformation gradient by maximizing a Rayleigh quotient*, Z. Angew. Math. Mech., 85:155–162, 2005.

[4] E. COSSERAT - F. COSSERAT, *Théorie des corps déformables*, Librairie Scientifique A. Hermann et Fils (engl. translation by D. Delphenich 2007, available online at https://www.uni-due.de/~hm0014/Cosserat_files/Cosserat09_eng.pdf), reprint 2009 by Hermann Librairie Scientifique, ISBN 978 27056 6920 1, Paris, 1909.

[5] J. J. DUISTERMAAT - J. A. C. KOLK, *Lie Groups*, Universitext. Springer, 2012.

[6] V. A. EREMEYEV - L. P. LEBEDEV - H. ALTENBACH, *Foundations of Micropolar Mechanics*, Springer, 2012.

[7] A. C. Eringen, *Microcontinuum Field Theories. Vol. I: Foundations and Solids*, Springer, 1999.

[8] A. Fischle, *The planar Cosserat model: minimization of the shear energy on* SO(2) *and relations to geometric function theory*, (diploma thesis). 2007. (available online: http://www.uni-due.de/~hm0014/Supervision_files/dipl_final_online.pdf).

[9] A. Fischle - P. Neff, *The geometrically nonlinear Cosserat micropolar shear–stretch energy*, Part I: A general parameter reduction formula and energy-minimizing microrotations in 2D. Z. Angew. Math. Mech., 97(7):828–842, 2017.

[10] A. Fischle - P. Neff, *The geometrically nonlinear Cosserat micropolar shear–stretch energy*, Part II: Nonclassical energy-minimizing microrotations in 3D and their computational validation. Z. Angew. Math. Mech., 97(7):843–871, 2017.

[11] A. Fischle - P. Neff - D. Raabe, *The relaxed-polar mechanism of locally optimal Cosserat rotations for an idealized nanoindentation and comparison with 3D-EBSD experiments*. Z. Angew. Math. Phys. (2017) 68: 90. https://link.springer.com/article/10.1007/s00033-017-0834-4.

[12] G. Grioli, *Una proprieta di minimo nella cinematica delle deformazioni finite*, Boll. Un. Math. Ital., 2:252–255, 1940.

[13] J. Jeong - H. Ramézani - I. Münch - P. Neff, *A numerical study for linear isotropic Cosserat elasticity with conformally invariant curvature*, Z. Angew. Math. Mech., 89(7):552–569, 2009.

[14] J. Lankeit - P. Neff - F. Osterbrink, *Integrability conditions between the first and second Cosserat deformation tensor in geometrically nonlinear micropolar models and existence of minimizers*, Z. Angew. Math. Phys., 68(1):11, Dec 2016.

[15] L. C. Martins - P. Podio-Guidugli, *An elementary proof of the polar decomposition theorem*, Amer. Math. Month., 87:288–290, 1980.

[16] G. A. Maugin, *On the structure of the theory of polar elasticity*, R. Soc. Lond. Philos. Trans. Ser. A Math. Phys. Eng. Sci., 356(1741):1367–1395, 1998.

[17] P. Neff, *Finite multiplicative plasticity for small elastic strains with linear balance equations and grain boundary relaxation*, Cont. Mech. Thermod., 15(2):161–195, 2003.

[18] P. Neff, *The Cosserat couple modulus for continuous solids is zero viz the linearized Cauchy-stress tensor is symmetric*, Z. Angew. Math. Mech., 86:892–912, 2006.

[19] P. Neff, *A finite-strain elastic-plastic Cosserat theory for polycrystals with grain rotations*, Int. J. Engng. Sci., 44:574–594, 2006.

[20] P. Neff - M. Bîrsan - F. Osterbrink, *Existence theorem for geometrically nonlinear Cosserat micropolar model under uniform convexity requirements*, J. Elasticity, 121, Issue 1:1–23, 2015.

[21] P. Neff - A. Fischle - I. Münch, *Symmetric Cauchy-stresses do not imply symmetric Biot-strains in weak formulations of isotropic hyperelasticity with rotational degrees of freedom*, Acta Mech., 197:19–30, 2008.

[22] P. Neff - J. Jeong, *A new paradigm: the linear isotropic Cosserat model with conformally invariant curvature energy*, Z. Angew. Math. Mech., 89(2):107–122, 2009.

[23] P. Neff - J. Jeong - A. Fischle, *Stable identification of linear isotropic Cosserat parameters: bounded stiffness in bending and torsion implies conformal invariance of curvature*, Acta Mech., 211(3-4):237–249, 2010.

[24] P. Neff - J. Lankeit - A. Madeo, *On Grioli's minimum property and its relation to Cauchy's polar decomposition*, Int. J. Engng. Sci., 80:209–217, 2014.

[25] P. Neff - I. Münch, *Curl bounds Grad on* SO(3), ESAIM: COCV, 14(1):148–159, 2008.

[26] P. Neff - I. Münch, *Simple shear in nonlinear Cosserat elasticity: bifurcation and induced microstructure*, Cont. Mech. Thermod., 21(3):195–221, 2009.

[27] W. Pietraszkiewicz - V. A. Eremeyev, *On vectorially parameterized natural strain measures of the non-linear Cosserat continuum*, Int. J. Solids Struct., 46(11):2477–2480, 2009.

[28] C. Sansour - S. Skatulla, *A non-linear Cosserat continuum-based formulation and moving least square approximations in computations of size-scale effects in elasticity*, Comp. Mat. Sci., 41(4):589–601, 2008.

Received 11 January 2017,
and in revised form 28 January 2017.

Andreas Fischle
Institut für Numerische Mathematik
TU Dresden
Zellescher Weg 12-14
01069 Dresden, Germany
andreas.fischle@tu-dresden.de

Patrizio Neff
Lehrstuhl für Nichtlineare Analysis und Modellierung
Fakultät für Mathematik
Universität Duisburg-Essen
Thea-Leymann Str. 9
45127 Essen, Germany
patrizio.neff@uni-due.de