

# Symmetric Cauchy stresses do not imply symmetric Biot strains in weak formulations of isotropic hyperelasticity with rotational degrees of freedom

P. Neff<sup>1</sup>, A. Fischle<sup>1</sup>, I. Münch<sup>2</sup>

<sup>1</sup>Department of Mathematics, Technische Universität Darmstadt, Darmstadt, Germany

<sup>2</sup>Institute of Structural Analysis, Karlsruhe University of Technology, Karlsruhe, Germany

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**Summary.** We show that symmetric Cauchy stresses do not imply symmetric Biot strains in weak formulations of finite isotropic hyperelasticity with exact rotational degrees of freedom. This is contrary to claims in the literature which are valid, however, in the linear isotropic case.

## 1 Introduction

This article is motivated by the numerous contributions which propose to introduce rotational degrees of freedom in a classical finite elasticity context in order to improve the numerical approximation of classical solutions [2]–[4], [7], [15], [16], [18], [19]. We refer to the introductions in [2] and [7] for the historical development of this specific approach to the numerics of classical finite elasticity<sup>1</sup> and the relevance it has, e.g., in the numerical simulation of thin structures ([5] and [22]). The general idea underlying the approach is to approximate the classical formulation by a weak formulation in which rotational degrees of freedom (also called drilling degrees of freedom) appear as a dedicated numerical intermediary device. Hence, no physical meaning is ascribed to them, as opposed to, e.g., in a Cosserat theory. The contributions of Buefler [2] and [3] are fundamental for the finite strain development in this respect.

The introduction of rotational degrees of freedom gives, in general, rise to a possible asymmetry of the relaxed Biot stretches. In an anisotropic setting, therefore, it is necessary to augment the energetic formulation with a term penalizing this possible asymmetry [3, Eq. (2.9)] in order to still approximate classical solutions with symmetric Biot stretch tensor  $U = \sqrt{F^T F}$ .

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Correspondence: Patrizio Neff, Department of Mathematics, Technische Universität Darmstadt, Schlossgartenstrasse 7, 64289 Darmstadt, Germany  
e-mail: neff@mathematik.tu-darmstadt.de

<sup>1</sup> In the literature this approach is also commonly referred to as a *relaxation* of classical finite elasticity.

However, in the pioneering contribution of Bufler [3, p. 26] it is claimed that this penalization is unnecessary in the case of finite isotropic hyperelasticity similar to the case of isotropic linear elasticity with infinitesimal rotations. From a purely mathematical viewpoint the argument is that all roots of a certain (cubic) polynomial matrix equation are guaranteed to lie in the space of symmetric matrices. Due to the specific structure of the very equation one is intuitively led to accept the correctness of this claim. Had we not a counterexample at our disposal, we admit, our intuition might have led us to the very same belief. From the viewpoint of mechanics, the above mentioned claim amounts to the statement that for an isotropic formulation the moment equilibrium equation enforces automatically the symmetry of the relaxed Biot stretch. Furthermore, it is this automatism which adds to the attractiveness of the numerical proposal [3, Rem. 2].

In this note we clarify that, contrary to appearance and in a certain way counter-intuitive, *penalization is necessary even in the isotropic case*, in order to compute approximately symmetric Biot stretches, i.e., to recover the classical situation.

The paper is organized as follows. Firstly, we recall the isotropic hyperelastic formulation of elasticity in the classical symmetric Biot stretch and derive the corresponding Euler-Lagrange equations. Then, we introduce the formulation with rotational degrees of freedom and establish various connections between solutions of the different models. Moreover, we exhibit the well-known relation of the relaxed model to a finite-strain Cosserat model without curvature energy, see, e.g., the pseudo-polar continuum in [7, p. 158].

By way of a counterexample we show then that symmetry of the relaxed Biot stretch may not be obtained without sufficient penalization. It is noted that in a linearized, isotropic setting the former cannot happen: satisfaction of moment equilibrium (symmetric Cauchy-stresses) implies symmetric infinitesimal stretch in the presence of infinitesimal skew-symmetric degrees of freedom for isotropy [4], [5].

## 2 The classical finite strain isotropic Biot model

### 2.1 The finite strain isotropic Biot model in variational form

For simplicity we restrict the exposition throughout to zero body forces. In a variational framework, the task is to find a deformation  $\varphi : \Omega \subset \mathbb{R}^3 \mapsto \mathbb{R}^3$  minimizing the energy functional  $I$ ,

$$I(\varphi) = \int_{\Omega} W(\nabla\varphi) dV \mapsto \min. \text{ w.r.t. } \varphi, \quad (2.1)$$

together with the Dirichlet boundary condition of place for the deformation  $\varphi$  on some part  $\Gamma$  of the boundary  $\partial\Omega$ :  $\varphi|_{\Gamma} = g_d$ . In the Biot approach, the special constitutive assumptions are

$$W(F) = W^\sharp(U). \quad (2.2)$$

The strain energy  $W$  depends on the deformation gradient  $F = \nabla\varphi \in \mathbf{GL}^+(3)$  only through the *objective symmetric continuum Biot stretch tensor*  $U = R^T F = \sqrt{F^T F} : T_x\Omega \mapsto T_x\Omega$ , where  $R = \text{polar}(F) : T_x\Omega \mapsto T_{\varphi(x)}\varphi(\Omega)$  is the orthogonal part of the polar decomposition of  $F$ , i.e., the continuum rotation and  $U$  is positive definite symmetric. It is well known that every objective free energy, i.e.,  $\forall Q \in \text{SO}(3)$ :  $W(QF) = W(F)$ , can be expressed in this way by a function  $W^\sharp$  defined on the classical stretch  $U$  alone, see, e.g., [6].

In the case of material isotropy, the free energy  $W$  should be right-invariant under the group of special rotations  $\text{SO}(3)$ , i.e.,

$$\begin{aligned} \forall Q \in \text{SO}(3) : \quad W(FQ) &= W(F) \Leftrightarrow \\ \forall Q \in \text{SO}(3) : \quad W^\sharp(Q^T U Q) &= W^\sharp(U). \end{aligned} \quad (2.3)$$

For example, the most general isotropic quadratic energy in  $U$  with zero stresses in the reference configuration is given by

$$W^\sharp(U) = \mu \|U - \mathbb{1}\|^2 + \frac{\lambda}{2} \text{tr}[U - \mathbb{1}]^2, \quad (2.4)$$

where the parameters  $\mu, \lambda > 0$  are the Lamé constants of classical isotropic elasticity.

## 2.2 The Euler-Lagrange equations of the finite Biot model

The following considerations are facilitated by using the representation  $U(F) = R(F)^T F = \text{polar}(F)^T F$ . Moreover, let  $v \in C_0^\infty(\Omega, \mathbb{R}^3)$ . Taking free variations w.r.t.  $\varphi$  in the energy leads to

$$\begin{aligned} \frac{d}{dt}\Big|_{t=0} I(\varphi + tv) &= \int_{\Omega} \langle D_F W(\nabla \varphi), \nabla v \rangle dV = \int_{\Omega} \langle D_F [W^\sharp(U(F))], \nabla v \rangle dV \\ &= \int_{\Omega} \langle D_U W^\sharp(U), D_F U(F) \cdot \nabla v \rangle dV = \int_{\Omega} \langle D_U W^\sharp(U), D_F [R(F)^T F] \cdot \nabla v \rangle dV \\ &= \int_{\Omega} \langle D_U W^\sharp(U), [D_F R(F) \cdot \nabla v]^T F + R(F)^T \nabla v \rangle dV \\ &= \int_{\Omega} \langle D_U W^\sharp(U), [\delta R(F, \nabla v)]^T R(F) R(F)^T F + R(F)^T \nabla v \rangle dV \\ &= \int_{\Omega} \langle R(F) D_U W^\sharp(U), \nabla v \rangle + \langle D_U W^\sharp(U), [\delta R(F, \nabla v)]^T R(F) R(F)^T F \rangle dV \\ &= \int_{\Omega} \langle R(F) D_U W^\sharp(U), \nabla v \rangle + \langle D_U W^\sharp(U) U^T, [\delta R(F, \nabla v)]^T R(F) \rangle dV. \end{aligned} \quad (2.5)$$

Now, we use that on the one hand  $D_U W^\sharp(U) U^T$  is symmetric for isotropic  $W^\sharp$  and that on the other hand  $[\delta R(F, \nabla v)]^T R(F)$  is always skew-symmetric. This implies that the product between them vanishes. Therefore, we obtain in equilibrium

$$\begin{aligned} 0 = \frac{d}{dt}\Big|_{t=0} I(\varphi + tv) &= \int_{\Omega} \langle R(F) D_U W^\sharp(U), \nabla v \rangle dV \\ &= \int_{\Omega} \langle \text{Div}[R(F) D_U W^\sharp(U)], v \rangle dV \quad \forall v \in C_0^\infty(\Omega, \mathbb{R}^3), \end{aligned} \quad (2.6)$$

where we have used the divergence theorem. Thus, the strong form of equilibrium for the classical Biot model reads

$$\text{Div } S_1(F) = \text{Div}[R(F) D_U W^\sharp(U)] = 0, \quad (2.7)$$

with the first Piola-Kirchhoff tensor  $S_1(F) = R(F) D_U W^\sharp(U)$ . Since the second Piola-Kirchhoff tensor is defined as  $S_2(F) = F^{-1} S_1(F)$ , it holds

$$S_2(F) = F^{-1}S_1(F) = F^{-1}R(F)D_U W^\sharp(U) = U^{-1}D_U W^\sharp(U) \in \text{Sym} \quad (2.8)$$

from the fact that for isotropic  $W^\sharp$  the tensors  $D_U W^\sharp$  and  $U^{-1}$  commute and are each symmetric. If we define the Biot stress tensor by  $T = D_U W(U)$ , then the following relation between the Biot stresses (living on the reference configuration) and the Cauchy-stresses in the actual configuration holds:

$$\sigma = \frac{1}{\det[F]} R T F^T = \frac{1}{\det[F]} F S_2(F) F^T \in \text{Sym}. \quad (2.9)$$

We note that the classical Biot model is not known to be well-posed when Eq. (2.4) is used. In this case Legendre-Hadamard ellipticity is lost [1].

Using the polar decomposition we may write equivalently

$$\text{Div}[R D_U W^\sharp(R^T F)] = 0, \quad R = \text{polar}(F). \quad (2.10)$$

A weaker formulation is obtained by replacing the constraint  $R = \text{polar}(F)$  in Eq. (2.10) into

$$\text{Div}[R D_U W^\sharp(R^T F)] = 0, \quad R^T F \in \text{Sym}. \quad (2.11)$$

The difference between Eq. (2.11) and (2.10) is that in (2.10) the stretch  $U = R^T F$  is not only symmetric, but also positive definite symmetric. In fact it holds

$$\forall R \in \text{SO}(3), F \in \text{GL}^+(3) : \quad R^T F \in \text{Sym} \Leftrightarrow R = Q_i \text{polar}(F), \quad (2.12)$$

for

$$Q_1 = 1, \quad Q_2 = \text{diag}(1, -1, -1), \quad Q_3 = \text{diag}(-1, 1, -1), \quad Q_4 = \text{diag}(-1, -1, 1). \quad (2.13)$$

Thus every solution to Eq. (2.10) is a solution to Eq. (2.11) but not vice versa. Despite the difference between the formulations (2.10) and (2.11) it is (2.11) which is sought to be approximated by a formulation with rotational degrees of freedom which we introduce presently.

### 3 The Biot model with rotational degrees of freedom

The Biot model with rotational degrees of freedom is obtained by formally relaxing the constraint on the rotations  $R$  in the previous approach to coincide either with the polar-decomposition or to make  $U = R^T F$  symmetric. Instead, one introduces an independent rotation field  $\bar{R} : \Omega \mapsto \text{SO}(3)$  and writes, cf. [3, 2.3]

$$I^{\text{rel}}(\varphi, \bar{R}) = \int_{\Omega} W^\sharp(\bar{R}^T \nabla \varphi) dV \mapsto \min. \text{ w.r.t. } (\varphi, \bar{R}), \quad (3.1)$$

taking free variations w.r.t  $\varphi$  and  $\bar{R}$ . Let us abbreviate  $\bar{U} = \bar{R}^T F$ , which is in general non-symmetric. Repeating the same steps as before leads us to the balance of forces equation

$$\begin{aligned} 0 &= \frac{d}{dt} \Big|_{t=0} I^{\text{rel}}(\varphi + tv, \bar{R}) = \int_{\Omega} \langle D_F[W^\sharp(\bar{R}^T \nabla \varphi)], \nabla v \rangle dV = \int_{\Omega} \langle D_{\bar{U}} W^\sharp(\bar{R}^T \nabla \varphi), \bar{R}^T \nabla v \rangle dV \\ &= \int_{\Omega} \langle \bar{R} D_{\bar{U}} W^\sharp(\bar{U}), \nabla v \rangle dV = \int_{\Omega} \langle \text{Div}[\bar{R} D_{\bar{U}} W^\sharp(\bar{U}), v] \rangle dV, \quad \forall v \in C_0^\infty(\Omega, \mathbb{R}^3). \end{aligned} \quad (3.2)$$

Free variation w.r.t. to the independent rotations  $\bar{R}$  leads to an algebraic side condition. Since  $\bar{R}^T \bar{R} = \mathbb{1}$  we have  $\delta \bar{R}^T \bar{R} = A \in \mathfrak{so}(3)$  for some arbitrary skew-symmetric matrix  $A$ . Thus for all variations  $\delta \bar{R}$

$$\begin{aligned} 0 &= \langle D_{\bar{R}}[W^\sharp(\bar{R}^T F), \delta \bar{R}] \rangle = \langle DW^\sharp(\bar{R}^T F), \delta \bar{R}^T F \rangle = \langle D_{\bar{U}}W^\sharp(\bar{R}^T F), \underbrace{\delta \bar{R}^T \bar{R}}_A \bar{R}^T F \rangle \\ &= \langle D_{\bar{U}}W^\sharp(\bar{R}^T F), A \bar{U} \rangle = \langle D_{\bar{U}}W^\sharp(\bar{U}) \bar{U}^T, A \rangle \end{aligned} \quad (3.3)$$

and balance of angular momentum follows as

$$\forall A \in \mathfrak{so}(3) : \quad 0 = \langle D_{\bar{U}}W^\sharp(\bar{U}) \bar{U}^T, A \rangle \Leftrightarrow D_{\bar{U}}W^\sharp(\bar{U}) \bar{U}^T \in \text{Sym}. \quad (3.4)$$

Gathering the Euler-Lagrange equations we have for the model with rotational degrees of freedom

$$0 = \text{Div}[\bar{R} D_{\bar{U}}W^\sharp(\bar{U})], \quad D_{\bar{U}}W^\sharp(\bar{U}) \bar{U}^T \in \text{Sym}. \quad (3.5.1, 2)$$

#### 4 The relaxed Biot model for a classical isotropic material

Any classical objective and isotropic strain energy density  $W^\sharp$  can be expressed as depending on the basic invariants (the coefficients of the characteristic polynomial) of the classical symmetric right stretch tensor  $U$ . We follow here closely the notation in [3]. Thus

$$\begin{aligned} W^\sharp(U) &= \Psi(I_1(U), I_2(U), I_3(U)) = \Phi(U), \\ I_1(U) &= \text{tr}[U], \quad I_2(U) = \text{tr}[\text{Cof } U] = \frac{1}{2} [\text{tr}[U]^2 - \text{tr}[U^2]], \quad I_3(U) = \det[U]. \end{aligned} \quad (4.1)$$

We note that, cf. [3, 2.21](including the case that  $X \notin \text{Sym}$ )

$$\frac{\partial I_1(X)}{\partial X} = \mathbb{1}, \quad \frac{\partial I_2(X)}{\partial X} = \text{tr}[X] \mathbb{1} - X^T = I_1(X) - X^T, \quad (4.2.1, 2)$$

$$\frac{\partial [\det[X]]}{\partial X} = \text{Cof } X = \det[X] X^{-T} = \frac{\partial I_3(X)}{\partial X} = I_2(X) \mathbb{1} - I_1(X) X^T + X^{2,T}. \quad (4.2.3)$$

Observe that  $I_3(\bar{R} X) = I_3(X)$  for all  $\bar{R} \in \text{SO}(3)$ . Thus only derivatives of  $\Psi$  with respect to  $I_1, I_2$  need to be taken into account for balance of moment considerations or stated alternatively,

$$\frac{\partial I_3(\bar{U})}{\partial \bar{U}} \bar{U}^T = \det[\bar{U}] \mathbb{1} \in \text{Sym}. \quad (4.3)$$

This can, of course, also be seen from the right hand side in (4.2.2) by considering the Cayley-Hamilton theorem for  $X^T$ .

For the following discussion we consider for arbitrary numbers  $0 \leq \mu_c \leq \mu$

$$\Psi(I_1, I_2, I_3) = \frac{\mu - \mu_c}{2} [I_1^2 - 2I_2] - 2\mu I_1. \quad (4.4)$$

This form is motivated from

$$\begin{aligned}
\|X + X^T - 2\mathbb{1}\|^2 &= \|X + X^T\|^2 - 2\langle X + X^T, 2\mathbb{1} \rangle + 4 \cdot 3 \\
&= 2\|X\|^2 + 2\langle X, X^T \rangle - 8\text{tr}[X] + 12 \\
&= 2\|X\|^2 + 2\text{tr}[X]^2 - 4\text{tr}[\text{Cof}X] - 8\text{tr}[X] + 12, \\
\|X - X^T\|^2 &= 2\|X\|^2 - 2\langle X, X^T \rangle = 2\|X\|^2 - [2\text{tr}[X]^2 - 4\text{tr}[\text{Cof}X]], \\
\frac{\mu}{4}\|X + X^T - 2\mathbb{1}\|^2 + \frac{\mu_c}{4}\|X - X^T\|^2 \\
&= \frac{\mu}{2}\|X\|^2 + \frac{\mu}{4}[2\text{tr}[X]^2 - 4\text{tr}[\text{Cof}X]] - 2\mu\text{tr}[X] + 3\mu \\
&\quad + \frac{\mu_c}{2}\|X\|^2 - \frac{\mu_c}{4}[2\text{tr}[X]^2 - 4\text{tr}[\text{Cof}X]] \\
&= \frac{\mu + \mu_c}{2}\|X\|^2 + \frac{\mu - \mu_c}{4}[2\text{tr}[X]^2 - 4\text{tr}[\text{Cof}X]] - 2\mu\text{tr}[X] + 3\mu \\
&= \frac{\mu + \mu_c}{2}\|X\|^2 + \frac{\mu - \mu_c}{2}[I_1(X)^2 - 2I_2(X)] - 2\mu I_1(X) + 3\mu \\
&= \frac{\mu + \mu_c}{2}\|X\|^2 + \Psi(I_1(X), I_2(X), I_3(X)) + 3\mu. \tag{4.5}
\end{aligned}$$

Abbreviating, as in [3, 2.25],

$$\begin{aligned}
\beta_1 &= \frac{\partial \Psi}{\partial I_1} = (\mu - \mu_c)I_1 - 2\mu, \\
\beta_2 &= \frac{\partial \Psi}{\partial I_2} = -(\mu - \mu_c), \\
\gamma_1 &= \beta_1 + \beta_2 I_1 = (\mu - \mu_c)I_1 - 2\mu + [-(\mu - \mu_c)]I_1 = -2\mu, \\
\gamma_2 &= -\beta_2 = (\mu - \mu_c),
\end{aligned} \tag{4.6}$$

leads to the moment-equation [3, 2.25]

$$\begin{aligned}
0 &= \gamma_1(\bar{U} - \bar{U}^T) + \gamma_2(\bar{U}^2 - \bar{U}^{2,T}) \Leftrightarrow \\
0 &= -2\mu(\bar{U} - \bar{U}^T) + (\mu - \mu_c)(\bar{U}^2 - \bar{U}^{2,T}),
\end{aligned} \tag{4.7}$$

which is nothing else than Eq. (3.5.2) for  $W^\sharp(\bar{U}) = \Psi(I_1(\bar{U}), I_2(\bar{U}), I_3(\bar{U}))$  and  $\Psi$  as in Eq. (4.4). We will come back to the possible (non-symmetric) solutions of Eq. (4.7) in Section 6 following Eq. (6.4).

If we take instead an isotropic potential which is linear in the basic invariants, i.e.,

$$\bar{\Psi}(I_1, I_2, I_3) = \beta_1 I_1 + \beta_2 I_2 + \beta_3 I_3, \tag{4.8}$$

with constants  $\beta_1, \beta_2, \beta_3$ , then the moment equation is equivalent to ( $\beta_3$  disappears)

$$0 = (\beta_1 + \beta_2 \text{tr}[\bar{U}])(\bar{U} - \bar{U}^T) - \beta_2(\bar{U}^2 - \bar{U}^{2,T}). \tag{4.9}$$

In this case the Eq. (4.9) really seems to have only symmetric solutions. Note that the statement of moment of momentum can always be rephrased as a stationarity condition of  $\Psi$  w.r.t. rotations  $\bar{R}$  as a function  $\bar{R} \mapsto \Psi(I_1(\bar{R}^T F), I_2(\bar{R}^T F))$  at given deformation gradient  $F$ . Passing therefore to an appropriate energy expression which delivers the same moment equation, we can show that for  $\beta_1, \beta_2 \geq 0$ , the polar rotation  $\text{polar}(F)$  indeed realizes the global minimum w.r.t.  $\bar{R} \in \text{SO}(3)$ . To see this, consider the energy in  $\bar{U} = \bar{R}^T F$

$$\begin{aligned}
& \beta_1 \|\bar{U} - \mathbb{1}\|^2 + \beta_2 \|\text{Cof } \bar{U} - \mathbb{1}\|^2 \\
&= \beta_1 \|\bar{U}\|^2 + \beta_2 \|\text{Cof } \bar{U}\|^2 + 3(\beta_1 + \beta_2) - 2(\beta_1 \text{tr}[\bar{U}] + \beta_2 \text{tr}[\text{Cof } \bar{U}]) \\
&= \beta_1 \|F\|^2 + \beta_2 \|\text{Cof } F\|^2 + 3(\beta_1 + \beta_2) - 2\bar{\Psi}(I_1(\bar{U}), I_2(\bar{U})).
\end{aligned} \tag{4.10}$$

Since the first terms are invariant w.r.t.  $\bar{R}$  it is obvious that this energy delivers the same stationarity condition as  $\Psi$  does, hence the same moment equation. Moreover,

$$\begin{aligned}
& \inf_{\bar{R} \in \text{SO}(3)} \left( \beta_1 \|\bar{U} - \mathbb{1}\|^2 + \beta_2 \|\text{Cof } \bar{U} - \mathbb{1}\|^2 \right) \\
& \geq \inf_{\bar{R} \in \text{SO}(3)} \beta_1 \|\bar{U} - \mathbb{1}\|^2 + \inf_{\bar{R} \in \text{SO}(3)} \beta_2 \|\text{Cof } \bar{U} - \mathbb{1}\|^2 \\
&= \beta_1 \|U - \mathbb{1}\|^2 + \beta_2 \|\text{Cof } U - \mathbb{1}\|^2,
\end{aligned} \tag{4.11}$$

since both minimum problems are solved by the same  $\bar{R} = \text{polar}(F)$ . For the second term this follows from the optimality of the polar rotation in the sense that

$$\begin{aligned}
& \inf_{\bar{R} \in \text{SO}(3)} \|\text{Cof } \bar{U} - \mathbb{1}\|^2 = \inf_{\bar{R} \in \text{SO}(3)} \|\bar{R}^T \text{Cof } F - \mathbb{1}\|^2 \\
&= \inf_{\bar{R} \in \text{SO}(3)} \|\text{Cof } F - \bar{R}\|^2 = \inf_{\bar{R} \in \text{SO}(3)} \|\det[F]F^{-T} - \bar{R}\|^2 \\
&= \|\det[F]F^{-T} - \text{polar}(\det[F]F^{-T})\|^2 = \|\det[F]F^{-T} - \text{polar}(F^{-T})\|^2 \\
&= \|\det[F]F^{-T} - \text{polar}(F)\|^2 = \|\text{polar}(F)^T \text{Cof } F - \mathbb{1}\|^2 \\
&= \|\text{Cof } \text{polar}(F)^T F - \mathbb{1}\|^2 = \|\text{Cof } U - \mathbb{1}\|^2.
\end{aligned} \tag{4.12}$$

The same consideration for the first term is simpler. Thus  $\text{polar}(F)^T F = U$  is the energy optimal symmetric solution of Eq. (4.9). This suggests that Bufler in [3, 2.25] considered in fact the special situation of Eq. (4.8).

The proposed relaxed Biot model with independent rotations can be viewed as a special case of a nonlinear Cosserat continuum. To see this let us continue by introducing a finite strain Cosserat model.

## 5 The finite strain Cosserat model in variational form

In [11] and [12] a finite-strain, fully frame-indifferent, three-dimensional Cosserat micropolar model is introduced, cf. [21], [17]. The two-field problem has been posed in a variational setting. The task is to find a pair  $(\varphi, \bar{R}) : \Omega \subset \mathbb{R}^3 \mapsto \mathbb{R}^3 \times \text{SO}(3)$  of deformation  $\varphi$  and *independent Cosserat rotation*<sup>2</sup>  $\bar{R} \in \text{SO}(3)$ , minimizing the energy functional  $I$ ,

$$I(\varphi, \bar{R}) = \int_{\Omega} W_{\text{mp}}(\bar{R}^T \nabla \varphi) + W_{\text{curv}}(\bar{R}^T \mathbf{D}_x \bar{R}) dV \mapsto \min. \text{ w.r.t. } (\varphi, \bar{R}), \tag{5.1}$$

together with the Dirichlet boundary condition of place for the deformation  $\varphi$  on  $\Gamma$ :  $\varphi|_{\Gamma} = g_d$  and Neumann conditions on the Cosserat rotations  $\bar{R}$  everywhere on  $\partial\Omega$ . The constitutive assumptions are

<sup>2</sup> The Cosserat rotation  $\bar{R}$  is a homogenized field defined on the macroscale.

$$\begin{aligned}
\bar{R}(x) : T_x \Omega &\mapsto T_{\varphi(x)} \varphi(\Omega), \quad \bar{U}(x) := \bar{R}^T(x) F(x) : T_x \Omega \mapsto T_x \Omega, \\
W_{\text{mp}}(\bar{U}) &= \mu \|\text{sym}(\bar{U} - \mathbb{1})\|^2 + \mu_c \|\text{skew}(\bar{U} - \mathbb{1})\|^2 + \frac{\lambda}{4} \left( \det[\bar{U}] - 1 \right)^2 + \left( \frac{1}{\det[\bar{U}]} - 1 \right)^2, \\
F = \nabla \boldsymbol{\varphi}, \quad W_{\text{curv}}(D_x \bar{R}) &= \mu L_c^q \|\text{Curl} \bar{R}\|^q,
\end{aligned} \tag{5.2}$$

under the minimal requirement  $q \geq 2$ . The total elastically stored energy  $W = W_{\text{mp}} + W_{\text{curv}}$  depends on the generalized stretch  $\bar{U}$  and on the curvature measure  $\text{Curl} \bar{R}$  [14] which describe the interaction of the microstructure on the macroscale. The strain energy  $W_{\text{mp}}$  depends on the deformation gradient  $F = \nabla \boldsymbol{\varphi}$  and the Cosserat rotations  $\bar{R} \in \text{SO}(3)$ , which do not necessarily coincide with the *continuum rotations*  $R = \text{polar}(F) : T_x \Omega \mapsto T_{\varphi(x)} \varphi(\Omega)$ .<sup>3</sup> In general, the *micro-polar stretch tensor*  $\bar{U}$  is *not symmetric* and does not coincide with the *symmetric continuum stretch tensor*  $U = R^T F = \sqrt{F^T F} : T_x \Omega \mapsto T_x \Omega$ .

Here  $\Gamma \subset \partial \Omega$  is that part of the boundary, where Dirichlet conditions  $g_d$  for deformations are prescribed. The parameters  $\mu, \lambda > 0$  are again the Lamé constants of classical isotropic elasticity, the additional parameter  $\mu_c \geq 0$  is called the *Cosserat couple modulus*. For  $\mu_c > 0$  the elastic strain energy density  $W_{\text{mp}}(\bar{U})$  is *uniformly convex* in  $\bar{U}$  and satisfies the *standard growth assumption*

$$\begin{aligned}
\forall F \in \text{GL}^+(3) : W_{\text{mp}}(\bar{U}) = W_{\text{mp}}(\bar{R}^T F) &\geq \min(\mu, \mu_c) \|\bar{R}^T F - \mathbb{1}\|^2 = \min(\mu, \mu_c) \|F - \bar{R}\|^2 \\
&\geq \min(\mu, \mu_c) \inf_{R \in \text{O}(3)} \|F - R\|^2 = \min(\mu, \mu_c) \text{dist}^2(F, \text{O}(3)) \\
&= \min(\mu, \mu_c) \text{dist}^2(F, \text{SO}(3)) = \min(\mu, \mu_c) \|F - \text{polar}(F)\|^2 \\
&= \min(\mu, \mu_c) \|U - \mathbb{1}\|^2,
\end{aligned} \tag{5.3}$$

where  $\text{dist} : \mathbb{M}^{3 \times 3} \mapsto \mathbb{R}$  is the Euclidean distance function on second order tensors. In contrast, for the case  $\mu_c = 0$  the strain energy density is *only convex* w.r.t.  $F$  and does not satisfy (5.3).<sup>4</sup>

The parameter  $L_c > 0$  (with dimension length) introduces an *internal length* which is *characteristic* for the material, e.g., related to the grain size in a polycrystal. The internal length  $L_c > 0$  is responsible for size effects in the sense that smaller samples are relatively stiffer than larger samples.

In the Cosserat model it is still possible to compute a tensor, formally taking on the role of the Cauchy-stresses:

$$\begin{aligned}
\sigma &= \frac{1}{\det[F]} S_1(F, \bar{R}) F^T = \frac{1}{\det[F]} D_F W(F, \bar{R}) F^T \\
&= \frac{1}{\det[F]} \bar{R} D_{\bar{U}} W(\bar{U}) F^T = \frac{1}{\det[F]} \bar{R} T(\bar{U}) F^T.
\end{aligned} \tag{5.4}$$

It is of prime importance to realize that a linearization of this isotropic Cosserat bulk model with  $\mu_c = 0$  for small displacement and small Cosserat rotations completely decouples the two fields of deformation  $\boldsymbol{\varphi}$  and Cosserat rotations  $\bar{R}$  and leads to the classical linear elasticity problem for the deformation. In [9] it is nevertheless shown that  $\mu_c = 0$  is a reasonable choice.<sup>5</sup>

<sup>3</sup> The continuum rotation and the Cosserat rotation rotate infinitesimal volumina and move base points.

<sup>4</sup> The condition  $F \in \text{GL}^+(3)$  is necessary, otherwise  $\|F - \text{polar}(F)\|^2 = \text{dist}^2(F, \text{O}(3)) < \text{dist}^2(F, \text{SO}(3))$ , as can be easily seen for the reflection  $F = \text{diag}(1, -1, 1)$ .

<sup>5</sup> Thinking in the context of an infinitesimal-displacement Cosserat theory one might believe that  $\mu_c > 0$  is necessary also for a ‘‘true’’ finite-strain Cosserat theory.



For more details on the modelling of the three-dimensional Cosserat model we refer the reader to [11]. Extensions to a micromorphic model have been given in [13]. The Cosserat model is well-posed in the sense that the existence of minimizers is obtained for various combinations of constitutive parameters [8], [10], including  $\mu_c = 0$ , provided that  $L_c$  is strictly positive.

The Biot model with independent rotations is obtained from the Cosserat model by neglecting the curvature, i.e., setting  $L_c = 0$ . By a scaling argument it is easy to see that  $L_c = 0$  corresponds to the limit of arbitrarily large samples. Therefore, the proposed Cosserat model can be seen as a regularization of the Biot model with independent rotations. For  $L_c = 0$ , balance of angular momentum is equivalently expressed as  $\sigma \in \text{Sym}$ .

## 6 Symmetry of stresses versus symmetry of stretches

Let us now return to the Euler-Lagrange equations for the Biot model with rotational degrees of freedom (3.5)

$$0 = \text{Div}[\bar{R}D_{\bar{U}}W^\sharp(\bar{U})], \quad D_{\bar{U}}W^\sharp(\bar{U})\bar{U}^T \in \text{Sym}. \quad (6.1)$$

As already remarked, Bufler considers the restricted case  $W^\sharp(\bar{U}) = \Psi(I_1(\bar{U}), I_2(\bar{U}), I_3(\bar{U}))$ . We can be slightly more general by assuming that  $W^\sharp$  also depends on additional invariants intervening for non-symmetric  $\bar{U}$ . In either case, using the representation theorems for isotropic functions of non-symmetric tensor arguments [20] it is easy to see that for isotropic  $W^\sharp$  and for symmetric  $\bar{U}$  the balance of angular momentum (3.4) is automatically satisfied, see, e.g. [18]. We observe, following the fundamental contribution [3] that a (not necessarily unique) solution  $(\varphi, \bar{R})$  of (3.5) cannot solve (2.11) unless  $\bar{U}$  is symmetric.

However, in [3] Bufler proceeds and arrives at

$$\gamma_1(\bar{U} - \bar{U}^T) + \gamma_2(\bar{U}^2 - \bar{U}^{T,2}) + \gamma_3(\bar{U}^3 - \bar{U}^{T,3}) = 0,$$

[3] Eq. (2.25)) for some scalar functions  $\gamma_i = \gamma_i(I_1(\bar{U}), I_2(\bar{U}), I_3(\bar{U}))$ . He concludes: “*The moment equilibrium ... leads to the symmetry condition  $\bar{U} = \bar{U}^T$ . This result, . . . , can be explained as follows: For an isotropic material the stretch  $\bar{U}$  and the stress  $r$  ( $= D_{\bar{U}}W^\sharp(\bar{U})$  our addition) are coaxial; consequently the moment equilibrium in (2.19) is satisfied identically for every symmetrical  $\bar{U}$ . Vice versa the moment equilibrium condition enforces this symmetry under the assumption of an isotropic material as demonstrated in (2.25).*”

This statement is only partially true: symmetric  $\bar{U}$  satisfies, for isotropic  $W^\sharp$ , always the moment equilibrium (3.4). The converse is, however, not necessarily the case. To see this, choose e.g.

$$W^\sharp(\bar{U}) = \mu \|\text{sym}(\bar{U} - \mathbb{1})\|^2 + \mu_c \|\text{skew}(\bar{U} - \mathbb{1})\|^2 + \frac{\lambda}{4} \left( (\det[\bar{U}] - 1)^2 + \left( \frac{1}{\det[\bar{U}]} [\bar{U}] - 1 \right)^2 \right), \quad (6.2)$$

as in the Cosserat model (5.2). Clearly,  $W^\sharp$  is an isotropic scalar valued function of the non-symmetric tensor argument  $\bar{U}$ . Since the volumetric term is independent of  $\bar{R}$  we can concentrate for balance of angular momentum on

$$W_{\mu, \mu_c}(F, \bar{R}) := \mu \|\text{sym}(\bar{U} - \mathbb{1})\|^2 + \mu_c \|\text{skew}(\bar{U} - \mathbb{1})\|^2. \quad (6.3)$$

Balance of angular momentum reads now

$$\begin{aligned}
D_{\bar{U}}W^\sharp(\bar{U})\bar{U}^T \in \text{Sym} &\Leftrightarrow D_{\bar{U}}W_{\mu,\mu_c}(\bar{U})\bar{U}^T \in \text{Sym} \\
&\Leftrightarrow [2\mu(\text{sym}(\bar{U} - \mathbb{1})) + 2\mu_c \text{skew}\bar{U}]\bar{U}^T \in \text{Sym} \\
&\Leftrightarrow [\mu(\bar{U} + \bar{U}^T - 2\mathbb{1}) + \mu_c(\bar{U} - \bar{U}^T)]\bar{U}^T \in \text{Sym} \\
&\Leftrightarrow (\mu - \mu_c)\bar{U}\bar{U} - 2\mu\bar{U} \in \text{Sym} \\
&\Leftrightarrow (\mu - \mu_c)[\bar{U}^2 - \bar{U}^{T,2}] - 2\mu[\bar{U} - \bar{U}^T] = 0.
\end{aligned} \tag{6.4}$$

Note that the last equation coincides with Buffers original equation (4.7). Obviously, for  $\mu_c = \mu$  the symmetric solution is unique. Therefore, assume presently that  $0 \leq \mu_c < \mu$  but we note that the choice  $\mu_c = 0$  is not necessary. Define  $\rho := \frac{2\mu}{\mu - \mu_c}$  and set

$$\begin{aligned}
F &= \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \lambda_1 + \lambda_2 > \rho, \\
\bar{R} &= \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \alpha = \arccos\left(\frac{\rho}{\lambda_1 + \lambda_2}\right) \in \left[0, \frac{\pi}{2}\right].
\end{aligned} \tag{6.5}$$

This yields the explicit forms

$$\begin{aligned}
\bar{R} &= \begin{pmatrix} \frac{\rho}{\lambda_1 + \lambda_2} & -\sqrt{1 - \frac{\rho^2}{(\lambda_1 + \lambda_2)^2}} & 0 \\ \sqrt{1 - \frac{\rho^2}{(\lambda_1 + \lambda_2)^2}} & \frac{\rho}{\lambda_1 + \lambda_2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\
\bar{U} = \bar{R}^T F &= \begin{pmatrix} \frac{\rho \lambda_1}{\lambda_1 + \lambda_2} & \lambda_2 \sqrt{1 - \frac{\rho^2}{(\lambda_1 + \lambda_2)^2}} & 0 \\ -\lambda_1 \sqrt{1 - \frac{\rho^2}{(\lambda_1 + \lambda_2)^2}} & \frac{\rho \lambda_2}{\lambda_1 + \lambda_2} & 0 \\ 0 & 0 & 1 \end{pmatrix},
\end{aligned} \tag{6.6}$$

as can be easily seen from a straight forward calculation. It is obvious that  $\bar{U}$  is in general not symmetric. On the other hand, we obtain

$$\begin{aligned}
\bar{U} - \bar{U}^T &= \begin{pmatrix} 0 & (\lambda_1 + \lambda_2) \sqrt{1 - \frac{\rho^2}{(\lambda_1 + \lambda_2)^2}} & 0 \\ -(\lambda_1 + \lambda_2) \sqrt{1 - \frac{\rho^2}{(\lambda_1 + \lambda_2)^2}} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
\bar{U}^2 - \bar{U}^{T,2} &= \begin{pmatrix} 0 & \rho (\lambda_1 + \lambda_2) \sqrt{1 - \frac{\rho^2}{(\lambda_1 + \lambda_2)^2}} & 0 \\ -\rho (\lambda_1 + \lambda_2) \sqrt{1 - \frac{\rho^2}{(\lambda_1 + \lambda_2)^2}} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\end{aligned} \tag{6.7}$$

Thus,  $\bar{U}^2 - \bar{U}^{T,2} = \frac{2\mu}{\mu - \mu_c} (\bar{U} - \bar{U}^T)$  from which we readily infer

$$(\mu - \mu_c)[\bar{U}^2 - \bar{U}^{T,2}] - 2\mu[\bar{U} - \bar{U}^T] = 0.$$

Hence,  $\bar{U} = \bar{R}^T F \notin \text{Sym}$ , but satisfies the equilibrium equation of angular momentum.

Furthermore, it can be shown by simple evaluation of the corresponding energy levels, that the given rotation  $\bar{R}$  is not only a solution of the balance of momentum equation  $D_{\bar{U}}W^\sharp(\bar{U})\bar{U}^T \in \text{Sym}$

but beats the classical symmetric solution energetically. That the given rotation  $\bar{R}$  realizes indeed the global minimum w.r.t.  $\bar{R}$  of the energy  $W^\sharp$  at given deformation gradient  $F$  will be the subject of a forthcoming contribution.<sup>6</sup>

Moreover, inspection of (6.6) shows that if  $|\lambda_1 - \lambda_2| < \rho$ , then  $\langle \xi, \bar{U} \cdot \xi \rangle_{\mathbb{R}^3}$  defines a positive definite quadratic form. It should also be noted that the always possible classical symmetric solution  $\bar{R} = \text{polar}(F)$  need not even be a local minimizer. Stability considerations do not speak in favour of the polar rotation!

Interestingly enough, if in the former, we choose  $\mu_c \geq \mu$  (a specific kind of penalty) then it is not too difficult to see that the only solution of balance of momentum is indeed a symmetric  $\bar{U}$ . Here, the penalty term enforces exactly the symmetry and not only approximately.

Gathering our findings shows that the remark 2 in [3]: “*The governing variational principle (2.15) and variational equation (2.16), respectively, with displacement- and rotational degrees of freedom can serve as a basis for a discretization in the case of an isotropic material. The corresponding numerical solution approximates not only the force equilibrium condition but also the symmetry of the stretch. This relaxed symmetry proves to be the most advantageous because the strict one would result in a complex coupling of the displacement- and rotation fields  $u$  and  $\varphi$ .*”, must be read with the precaution to use only isotropic free energies in the special format<sup>7</sup>  $W^\sharp(\bar{U}) = \Psi(I_1(\bar{U}), I_2(\bar{U}), I_3(\bar{U}))$  as in Section 4 which have the exceptional property to lead automatically to symmetric relaxed Biot stretches.

## 7 Conclusion

Summarizing the situation, we can say: the Cosserat model turns into a Biot model with independent rotations whenever the internal length scale is absent, i.e.,  $L_c = 0$ . Even in the case of isotropy the equilibrium solutions of the model (3.5) are not necessarily equilibrium solutions of the weak Biot model (2.11). If it is intended to approximate classical solutions by the model with independent rotations, then a sufficiently large penalty term  $\mu_c \|\text{skew} \bar{U}\|^2$  needs to be added. In the investigated isotropic case (6.2), a finite penalty parameter  $\mu_c \geq \mu$  is sufficient to enforce symmetry of the relaxed Biot stretches exactly. If the penalty parameter  $\mu_c$  is small or absent the relation of the relaxed Biot model with independent rotations to the classical isotropic Biot model is lost. Since in the classical Biot model the stretches are not only symmetric but positive definite, the solutions of the relaxed Biot model with sufficient penalty need to be checked w.r.t. positive definiteness in order to maintain their physical relevance.

It remains to find a sufficiently large class of isotropic free energies such that moment equilibrium in the relaxed formulation implies automatically the symmetry of the relaxed Biot stretch  $\bar{U}$ . This question seems to be a formidable challenge. A partial positive answer is provided by restricting attention to energies whose part, effectively depending on rotations, is a linear combination of the three classical invariants  $I_1, I_2, I_3$ .

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<sup>6</sup> This statement is also true with respect to the energy  $\Psi(I_1, I_2, I_3)$  since the difference to  $W^\sharp$  in (6.2) is only an additive term  $\|\bar{U}\|^2 = \|\bar{R}^T F\|^2 = \|F\|^2$  and an additive volumetric contribution which are both invariant w.r.t. rotations  $\bar{R}$ .

<sup>7</sup> Every classical isotropic free energy defined on  $U$  can be used and extended in this way to an isotropic function of the non-symmetric  $\bar{U}$ , but not every isotropic free energy in terms of  $\bar{U}$  has such a representation, since other invariants operating on the skew-symmetric parts of  $\bar{U}$  may intervene.

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