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Construction of polyconvex, anisotropic free-energy functions

The existence of minimizers of some variational principles in finite elasticity is based on the concept of quasiconvexity, introduced by Morrey [6]. This integral inequality is rather complicated to handle. Thus, the sufficient condition for quasiconvexity, the polyconvexity condition in the sense of Ball [1], is a more important concept for practical applications, see also Ciarlet [4] and Dacorogna [5]. In the case of isotropy there exist some models which satisfy this condition. Furthermore, there does not exist a systematic treatment of anisotropic, polyconvex free-energies in the literature. In the present work we discuss some aspects of the formulation of polyconvex, anisotropic free-energy functions in the framework of the invariant formulation of anisotropic constitutive equations and focus on transverse isotropy.

1. Continuum Mechanical and Mathematical Foundations

Let $\mathcal{B} \subset \mathbb{R}^3$ be the body in the reference configuration parametrized in $\boldsymbol{X}$. The deformation gradient $\boldsymbol{F}$ is defined by $\boldsymbol{F} := \mathrm{Grad}\boldsymbol{\varphi}_t(\boldsymbol{X})$ with $\det \boldsymbol{F} > 0$, where $\boldsymbol{\varphi}_t$ denotes the nonlinear deformation map at time t. The fundamental deformation tensor is the right Cauchy–Green tensor $\boldsymbol{C} := \boldsymbol{F}^T\boldsymbol{F}$. As mentioned before we are interested in polyconvex free-energy functions. Let $W \in C^2(M^{3\times3}, \mathbb{R})$ be a scalar–valued energy density, where $M^{3\times3}$ denotes the set of real 3×3 matrices, then

Definition: $\boldsymbol{F} \mapsto W(\boldsymbol{F})$ is polyconvex if and only if there exists a function $P : M^{3\times3} \times M^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ such that

$$W(\boldsymbol{F}) = P(\boldsymbol{F}, \mathrm{Adj}\boldsymbol{F}, \det \boldsymbol{F})$$

and $\mathbb{R}^{19} \mapsto \mathbb{R},\ (X, Y, Z) \mapsto P(X, Y, Z)$ is convex for all points $\boldsymbol{X} \in \mathbb{R}^3$.

It should be noted that the individual arguments $(\boldsymbol{F}, \mathrm{Adj}\boldsymbol{F}, \det \boldsymbol{F})$ in the above definition can be physically interpreted. $\boldsymbol{F}$ controls the deformation of an infinitesimal line element, $(\mathrm{Adj}\boldsymbol{F})^T$ the deformation of an infinitesimal vectorial area element and $\det \boldsymbol{F}$ the deformation of an infinitesimal volume element. In order to fulfill the principle of objectivity a priori we focus on the so-called reduced constitutive equations for the second Piola-Kirchhoff stresses $\boldsymbol{S} = 2\partial_C\hat{\psi}(\boldsymbol{C})$. In the case of transverse isotropy we introduce a material symmetry group $\mathcal{G}_{ti} \subset \mathrm{SO}(3)$ with respect to a local reference configuration, here SO(3) characterizes the special orthogonal group. Furthermore the concept of material symmetry states that

$$\hat{\psi}(\boldsymbol{C}) = \hat{\psi}(\boldsymbol{Q}^T\boldsymbol{C}\boldsymbol{Q}) \quad \forall\, \boldsymbol{Q} \,\in\, \mathcal{G}_{ti}, \boldsymbol{C}\ . \tag{1}$$

We say that the function ψ in Equation (1) is a $\mathcal{G}_{ti}$-invariant function. The material symmetry group is defined by

$$\mathcal{G}_{ti} := \{\boldsymbol{1};\ \boldsymbol{Q}(\alpha, \boldsymbol{a}) \mid 0 < \alpha < 2\,\pi\}\ , \tag{2}$$

where $\boldsymbol{Q}(\alpha, \boldsymbol{a})$ represents all rotations about the prefered direction $\boldsymbol{a}$. In order to extend the $\mathcal{G}_{ti}$-invariant function into a function which is invariant under the special orthogonal group we introduce a so-called structural tensor $\boldsymbol{M}$. The invariance group of $\boldsymbol{M}$ has to preserve the material symmetry group $\mathcal{G}_{ti}$. For the considered anisotropy class we arrive at $\boldsymbol{M} := \boldsymbol{a} \otimes \boldsymbol{a}$, with $||\boldsymbol{a}|| = 1$. This leads to a scalar–valued isotropic tensor function of the form

$$\psi = \hat{\psi}(\boldsymbol{C}, \boldsymbol{M}) = \hat{\psi}(\boldsymbol{Q}^T\boldsymbol{C}\boldsymbol{Q}, \boldsymbol{Q}^T\boldsymbol{M}\boldsymbol{Q})\ \ \forall\, \boldsymbol{Q} \,\in\, \mathrm{SO}(3)\ . \tag{3}$$

Thus it is possible to formulate the free-energy in terms of the so-called principal invariants and the mixed invariants:

$$I_1 = \mathrm{tr}\,\boldsymbol{C},\ I_2 = \mathrm{tr}[\mathrm{Cof}\boldsymbol{C}],\ I_3 = \mathrm{det}\boldsymbol{C},\ I_4 = \mathrm{tr}[\boldsymbol{C}\boldsymbol{M}],\ I_5 = \mathrm{tr}[\boldsymbol{C}^2\boldsymbol{M}]\ , \tag{4}$$

in this context see e.g. [2], [3] and [9]. For the free-energy function we assume the general form $\psi = \hat{\psi}(I_i|i = 1, ...5) + c$, where we have introduced the constant $c \in \mathbb{R}$ in order to fulfill the non-essential normalization condition $\psi(\boldsymbol{1}, \boldsymbol{M}) = 0$. Furthermore, the condition $\psi = \hat{\psi}(\boldsymbol{C}, \boldsymbol{M}) = \hat{\psi}(\boldsymbol{Q}^T\boldsymbol{C}\boldsymbol{Q}, \boldsymbol{M})$ holds for all $\boldsymbol{Q} \,\in\, \mathcal{G}_{ti}$, which reflects (1).

2. Polyconvex Anisotropic Free-Energies

In the following we assume an additive decomposition of the free-energy function in isotropic terms ψ_i^{iso} and anisotropic terms ψ_j^{ti}, i.e.

$$\psi = \sum_i \psi_i^{iso}(I_1, I_2, I_3) + + \sum_j \psi_j^{ti}(I_1, I_2, I_3, I_4, I_5) \ . \tag{5}$$

For the isotropic ones we can choose some well–known formulations from the literature, see e.g. [4]. Some anisotropic terms are discussed in the following, for details see [7] and [8]. It should be noted that direct extensions of the small strain theory to large strain formulations by replacing the linear strain tensor with the Green-Lagrange strain tensor $\boldsymbol{E} := \frac{1}{2}(\boldsymbol{C} - \boldsymbol{1})$ are a priori not polyconvex. Furthermore, the often used polynomial invariants

$$\boldsymbol{F} \mapsto \mathrm{tr}\,(\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{M})\mathrm{tr}\,(\boldsymbol{F}^T\boldsymbol{F}) = \mathrm{tr}\,[\boldsymbol{C}\boldsymbol{M}]\mathrm{tr}\,\boldsymbol{C} = I_1\,I_4 \quad \text{and} \quad \boldsymbol{F} \mapsto \mathrm{tr}\,[\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{M}] = \mathrm{tr}\,[\boldsymbol{C}^2\boldsymbol{M}] = I_5 \tag{6}$$

are not polyconex, see [7], [8]. That means that the functions c^+I_5 and $c^+I_1I_4$ can not be used in this form. In order to derive further ansatz functions it seems reasonable to construct a convex polynomial mixed invariant with respect to Adj$\boldsymbol{F}$, which reflects the deformation of a preferred area element in some sense. For this we take into account the Cayley-Hamilton theorem and multiply the characteristic polynomial in $\boldsymbol{C}$ with $\boldsymbol{C}^{-1}\boldsymbol{M}$. This leads with Cof$\boldsymbol{C}$ = Adj$\boldsymbol{C}$ to the expression

$$\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M} = \boldsymbol{C}^2\boldsymbol{M} - I_1\boldsymbol{C}\boldsymbol{M} + I_2\boldsymbol{M} \ . \tag{7}$$

Note that Cof$[\boldsymbol{C}]$ is a quadratic function in the $\boldsymbol{C}$. The trace of Equation (7) is the polyconvex polynomial invariant

$$K_1 := \mathrm{tr}\,[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M}] = I_5 - I_1\,I_4 + I_2 \ . \tag{8}$$

The proof of the convexity of the powers of K_1 is straightforward, see [7]. Expressing the invariant K_1 in the form

$$K_1 = \mathrm{tr}\,[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M}] = \mathrm{Cof}[\boldsymbol{F}^T\boldsymbol{F}] : \boldsymbol{a} \otimes \boldsymbol{a} = ||\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}||^2 \ , \tag{9}$$

we can give a rather simple geometric interpretation of this polynomial invariant. $\sqrt{K_1} = ||\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}||$ controls the deformation of an area element with unit normal $\boldsymbol{a}$. With the same arguments we can construct the function

$$K_2 := \mathrm{tr}\,[\mathrm{Cof}[\boldsymbol{C}](\boldsymbol{1} - \boldsymbol{M})] = I_1\,I_4 - I_5 \ , \tag{10}$$

which is polyconvex. The proof is omitted here. K_2 is associated to the deformation of an area element with a normal lying in the isotropy plane. For the polyconvex functions (8) and (10) we can give a simple geometric interpretation; further, more abstract polyconvex functions are e.g.

$$\psi_1^{ti} = \alpha_1\,K_1/I_3^{1/3}\ ; \quad \psi_2^{ti} = \alpha_2\,K_1^2/I_3^{1/3}\ ; \quad \psi_3^{ti} = \alpha_3\,K_2/I_3^{1/3}\ ; \quad \psi_4^{ti} = \alpha_4\,K_2^2/I_3^{1/3}\ , \tag{11}$$

with $\alpha_i \in \mathbb{R}^+$ for $i = 1, 2, 3, 4$. A spectrum of anisotropic polyconvex ansatz functions is presented in [7].

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