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Reconstruction of a constitutive law for rubber from in silico experiments using Ogden's laws

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ABSTRACT

This article deals with the following data assimilation problem: construct an analytical approximation of a numerical constitutive law in three-dimensional nonlinear elasticity. More precisely we are concerned with a micro–macro model for rubber. Macroscopic quantities of interest such as the Piola–Kirchhoff stress tensor can be approximated for any value of the strain gradient by numerically solving a nonlinear PDE. This procedure is however computationally demanding. Hence, although conceptually satisfactory, this physically-based model is of no direct practical use. The aim of this article is to circumvent this difficulty by proposing a numerical strategy to reconstruct from in silico experiments an accurate analytical proxy for the micro–macro constitutive law.

1. Introduction

In this article we address a problem which exhibits at the same time very standard and rather unusual features: data assimilation in nonlinear elasticity for a micro–macro constitutive law.

Let us start with the features which make our problem a standard one in mechanical engineering: we wish to reconstruct an analytical constitutive law from a set of experiments. In particular, we aim at reconstructing a function (the energy density) from a set of samples (the experiments). Such problems are quite standard in elasticity. We refer the reader to the review paper Bonnet and Constantinescu (2005). Most of the constitutive laws used in rubber elasticity (or more generally in computational mechanics) are phenomenological (see for instance Ogden (1972), Ball (1977), Ogden (1986), Ciarlet (1988)): the law is supposed to have a specific analytical form characterized by some explicit parameters. For the constitutive law to be of any use, these parameters have to be fitted. This is where things get complicated. On the one hand, the more parameters the more accurate the phenomenological law. On the other hand, the more parameters the more difficult the data assimilation problem. There is a wide choice of measurements which can be used to estimate the parameters, see for instance Bonnet and Constantinescu (2005) and the references therein. For nonlinear materials, few theoretical results are available, and parameter identification methods are often based on direct measurements of the stress associated with a homogeneous strain and give satisfactory results only for a very small number of parameters. It is for instance rather well-admitted that Ogden's laws have the potential to model rubber elasticity quite well (Ogden, 1972; Ball, 1977; Ciarlet, 1988). Yet for reasonable sets of experimental data, there may be several possible sets of fitted parameters which give similar results on the set of data but which yield completely different behaviors in other regimes of interest, as shown in Ogden et al. (2004). Hence, although methods have been developed to fit parameters in Ogden's laws (Ogden, 1972; Twizell and Ogden, 1983; Gendy and Saleeb, 2000; Ogden et al., 2004), Ogden's laws are not so used in practice. The associated inverse problem is indeed often ill-posed: the observations obtained by mechanical experiments are too partial to characterize the constitutive law. Although this inverse problem is standard, there is up to now no fully satisfactory way to solve it in practice.

Let us turn now to the unusual features of this problem. Unlike purely phenomenological constitutive laws, the model under investigation here is based on some physical grounds at the scale of the polymer-chain network (Gloria et al., 2013). In particular

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the micro–macro constitutive law is obtained by a rigorous thermodynamic limit starting from a physically-based (without phenomenological parameters) model (Alicandro et al., 2011). As a by-product of the analysis, we learn that the associated micro–macro energy density satisfies some formula, which involves the solution of a nonlinear elasticity problem on a sequence of domains of increasing size (see Theorem 1 in Section 2). This is the so-called cell-problem in stochastic homogenization. Although this energy density is not analytical, it can be numerically approximated at any deformation gradient, as shown in Gloria et al. (2013). Hence it seems there is no need for data assimilation. Things are unfortunately not that simple and the solution method used to approximate the energy density is computationally very demanding. One cannot afford to include it into a nonlinear elasticity software. This is where data assimilation comes into the picture again: given a set of data generated by solving numerically the cell-problem we wish to construct an analytical approximation of the micro–macro constitutive law.

In this article we shall show that the specific features of our problem make the "standard inverse problem" recalled above much nicer. Data assimilation in rubber elasticity may be an ill-posed problem because the sets of data which are available are often too partial (engineering stress for uniaxial and biaxial tractions for instance). In particular all the regimes cannot be tested by mechanical experiments. On the contrary, for the micro–macro model and the numerical approximation method of the associated energy density we are dealing with here, any strain gradient can be considered: we have at our disposal an arbitrary amount of data at arbitrary values of the strain gradient. This opens the door to the use of reliable and efficient data assimilation methods. In addition, the analysis of the model and of its thermodynamic limit performed in Alicandro et al. (2011) is a very good guide to restrict the class of admissible energy densities in which to solve the inverse problem — which is the aim of our study.

The article is organized as follows. In Section 2 we briefly recall the micro–macro model for rubber, its structural properties and the link with analytical constitutive laws. In the following section, we describe the inverse problem to be solved and the numerical solution method used (an evolutionary algorithm). Section 4 is dedicated to the calibration and test of the method, for different analytical energy densities and with exact and noisy data. In the last section, we apply the method to the micro–macro model of interest. The numerical results are very good, both qualitatively and quantitatively. In particular they draw the link between a physical model based on "first principles" (the micro–macro model) and phenomenological constitutive laws for rubber.

2. Model and parametrization

2.1. Homogenization of a discrete model for rubber

In this subsection we recall the discrete stochastic homogenization results of Alicandro et al. (2011) which have allowed us to study the thermodynamic limit of a discrete model for rubber in Gloria et al. (2013). To this aim, we have to make precise the model for the polymer-chain network, and for the associated energy functional. The polymer-chain network is modeled by a stochastic lattice.

Definition 1. We say that a stochastic point process $\mathcal{L}$ in $\mathbb{R}^3$ (that is a sequence of random points in $\mathbb{R}^3$) is admissible if:

- (regularity) There exist $\mathbf{r} \geqslant r > 0$ such that almost surely:
  - any two points of $\mathcal{L}$ cannot be closer than r (hard-core property),
  - any ball of radius $\mathbf{r}$ contains at least one point of $\mathcal{L}$ (non-empty space property);
- (stationarity) $\mathcal{L}$ and $x + \mathcal{L}$ have the same statistics for all $x \in \mathbb{R}^3$;
- (ergodicity) $\mathcal{L}$ is ergodic.

We further assume that the Delaunay tessellation $\mathcal{T}$ of $\mathbb{R}^3$ into tetrahedra associated with $\mathcal{L}$ (that is, the vertices of $\mathcal{T}$ are given by $\mathcal{L}$) is almost surely unique (see Delone et al. (1976)).

In particular the edges of the Delaunay tessellation represent the end-to-end vectors of the polymer-chains. For rigorous definitions of admissible stochastic lattices and their Delaunay tessellations, we refer the reader to Alicandro et al. (2008) and Gloria and Penrose (2013), and to the references therein. Let us also introduce a rescaling of $\mathcal{L}$ and $\mathcal{T}$. For all $\varepsilon > 0$, we set $\mathcal{L}_\varepsilon := \varepsilon\mathcal{L}$, which satisfies Definition 1 with εr and $\varepsilon\mathbf{r}$ in place of r and $\mathbf{r}$, and with $\mathcal{T}_\varepsilon := \varepsilon\mathcal{T}$ in place of $\mathcal{T}$.

Given a tessellation $\mathcal{T}_\varepsilon$ of $\mathbb{R}^3$, one may define the space $\mathcal{S}(\mathcal{T}_\varepsilon)$ of continuous and piecewise affine deformations u_ε on $\mathcal{T}_\varepsilon$. Such deformations u_ε are such that their gradients ∇u_ε are piecewise constant on $\mathcal{T}_\varepsilon$. In particular, for every element T_ε (tetraedron) of the tessellation $\mathcal{T}_\varepsilon, \det \nabla u_{\varepsilon|T_\varepsilon}$ measures the ratio of volume between $u_\varepsilon(T_\varepsilon)$ and T_ε.

We are now in position to associate an energy with any deformation field $u_\varepsilon \in \mathcal{S}(\mathcal{T}_\varepsilon)$, on an open bounded domain D of $\mathbb{R}^3$. We consider two contributions: an energy associated with the changes of length of the edges of the tessellation, and an energy associated with the changes of volume of the elements of the tessellation. More precisely, denoting by $\mathcal{E}_d$ the set of edges of $\mathcal{T}$, we define the energy of $u_\varepsilon \in \mathcal{S}(\mathcal{T}_\varepsilon)$ on D by

$$F_\varepsilon(u_\varepsilon, D) = \varepsilon^3 \sum_{e\in\mathcal{E}_d, e\subset D/\varepsilon} W_{nn}\left(|e_1 - e_2|, \frac{|u_\varepsilon(\varepsilon e_1) - u_\varepsilon(\varepsilon e_2)|}{\varepsilon|e_1 - e_2|}\right) + \sum_{T\in\mathcal{T}, T\subset D/\varepsilon} |\varepsilon T| W_{\mathrm{vol}}(\det \nabla u_{\varepsilon|T_\varepsilon}), \tag{1}$$

where $e = (e_1, e_2)$ (e_1 and e_2 are the two vertices of the edge e), $W_{nn} : \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^+$ is the energy of the deformed edges, and $W_{\mathrm{vol}} : \mathbb{R} \to \mathbb{R}^+$ is the volumetric energy. Denote by $\mathbb{M}^3(\mathbb{R})$ the set of 3×3-real matrices. We make the following assumptions on W_{nn} and W_{vol}:

Hypothesis 1. There exist $p > 1$ and a positive constants C such that for all $r \leqslant \gamma \leqslant \mathbf{r}$, $\lambda \geqslant 0$, and $\Lambda \in \mathbb{M}^3(\mathbb{R})$,

$$\frac{1}{C}\lambda^p - C \leqslant W_{nn}(\gamma, \lambda) \leqslant C(\lambda^p + 1), \tag{2}$$

$$W_{\mathrm{vol}}(\det \Lambda) \leqslant C(|\Lambda|^p + 1). \tag{3}$$

In terms of mechanical properties these assumptions that have to be made for the analysis have two unphysical features: polymer-chains have infinite extensibility and the volumetric term does ensure the non-interpenetrability of matter. We then have the following convergence result (see Alicandro et al. (2008, Theorem 5)).

Theorem 1. *For all $\varepsilon > 0$, let $\mathcal{L}_\varepsilon$ and $\mathcal{T}_\varepsilon$ be the rescaled stochastic point process and the associated Delaunay tessellation of Definition 1. For every open bounded subset D of $\mathbb{R}^3$ with a Lipschitz-continuous boundary, we consider the energy $F_\varepsilon(u_\varepsilon, D)$ defined by (1) for $u_\varepsilon \in \mathcal{S}(\mathcal{T}_\varepsilon)$, and extended by $+\infty$ on $W^{1,p}(D) \setminus \mathcal{S}(\mathcal{T}_\varepsilon)$, for $p > 1$, W_{nn}, and W_{vol} as in Hypothesis 1. Then the functional $F_\varepsilon(\cdot, D)\Gamma(L^p(D))$-converges on $W^{1,p}(D)$ as $\varepsilon \to 0$ to the functional $F_V(\cdot, D)$ defined by*

$$F_V(u, D) = \int_D W_V(\nabla u(x))dx, \tag{4}$$