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An adaptive relaxation algorithm for multiscale problems and application to nematic elastomers☆

Sergio Conti[a,*], Georg Dolzmann[b]

[a] Institut für Angewandte Mathematik, Universität Bonn, Bonn, 53115, Germany
[b] Fakultät für Mathematik, Universität Regensburg, Regensburg, 93040, Germany

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ABSTRACT

The relaxation of nonconvex variational problems involving free energy densities W which depend on the deformation gradient is frequently characterized by a hierarchy of structures at different and well-separated length scales. A wide range of these structures can be characterized as the superposition of one-dimensional oscillations on different length scales which are referred to as laminates of finite order. During a finite element simulation, the relaxed energy W^{qc} needs to be evaluated in each time step in each Gauss point in the triangulation. In this paper, an algorithmic scheme is presented that allows for the efficient computation of an approximation of the relaxed energy based on laminates of finite order in a large number of points. As an application, the relaxed energy for thin sheets of anisotropic nematic elastomers is studied in detail.

1. Introduction

The development of the numerical analysis of microstructures in solids emerged some 30 years ago together with the evolution of a mathematical theory for fully nonlinear models for phase transformations in solids (Ball and James, 1987; 1992; Bhattacharya, 2003; Chipot and Kinderlehrer, 1988). In this context, the variational problem is given by an energy density $W : \mathbb{R}^{n\times n} \to [0,\infty]$ which depends on the deformation gradient $F \in \mathbb{R}^{n\times n}$ and satisfies the fundamental principle of material frame indifference, $W(QF) = W(F)$ for all $Q \in \mathrm{SO}(n)$, and consists of the minimization of the energy functional

$$I[u] = \int_\Omega W(Du)\mathrm{d}x$$

in a class $\mathcal{A}$ of admissible deformations which is typically given by an affine subset of Sobolev functions satisfying prescribed Dirichlet boundary conditions. As a consequence of the frame indifference, the energy density usually fails to be quasiconvex in the sense of Morrey and minimizing sequences tend to develop oscillations on fine scales. In order to obtain an effective description, one replaces the variational problem with its relaxation I^{qc} which is given by a variational integral with the relaxed energy density W^{qc},

$$I^{qc}[u] = \int_\Omega W^{qc}(Du)\mathrm{d}x,$$

☆ This paper is dedicated to the memory of Professor Dr.-Ing. Christian Miehe.

* Corresponding author.
E-mail address: sergio.conti@uni-bonn.de (S. Conti).

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if W itself satisfies suitable growth conditions, see (2.1) for the definition of W^{qc} and Dacorogna (2008), Müller (1999) and Bhattacharya (2003) for more information on relaxation and Conti and Dolzmann (2015) for more general situations. This approach requires an explicit computation of the quasiconvex envelope W^{qc}. However, due to the complexity of the calculations required to derive such an explicit formula, only few examples for quasiconvex envelopes with immediate applications to problems in solid mechanics are known, see, e.g., Le Dret and Raoult (1995), DeSimone and Dolzmann (2002) and Conti and Dolzmann (2014). Examples of a combination of an analytical approximation of the relaxed energy with a finite element simulation can be found in Conti et al. (2002b, 2007). Relaxation ideas have been successfully applied to a number of different mechanical problems, see for example Ortiz and Repetto (1999), Miehe et al. (2002), Carstensen et al. (2008, 2002), Lambrecht et al. (2003), Miehe and Lambrecht (2003), Miehe et al. (2004), Kochmann and K.Hackl (2011) and Mauthe and Miehe (2015).

In view of these difficulties, a fully discrete approach is required for the successful numerical solution of nonconvex minimization problems in solid mechanics. Such an approach has to be based on a numerical computation of the relaxed variational problem. First results in this direction have been obtained in Bartels (2004, 2005), Bartels et al. (2004) and Dolzmann (1999). In this contribution we present a new algorithmic approach which is based on the observation that the numerical computation of the relaxation is in general coupled to a finite element simulation of an elasticity problem which requires the computation of the relaxed energy in many points, typically in the deformation gradients at all Gauss points of the underlying finite element discretization. The values of the local deformation gradient at these points are typically strongly correlated. In this situation, two strategies can be followed. One approach is related to on-the-fly computations within the concurrent multiscale framework pioneered in Aubry and Ortiz (2003), the other approach is based on a systematic exploitation of continuity properties of minimizing laminates, which is frequently observed, as proposed in this article. We refer to Section 2 for a detailed discussion of this approach and its numerical realization. A summary of these results was presented in Conti and Dolzmann (2017).

We also illustrate the effectiveness of our algorithm via an application to two model cases of physical interest. The first one is the two-well problem, coming from the study of martensitic phase transitions (Ball and James, 1992; Chipot and Kinderlehrer, 1988). The application of our algorithm has permitted to identify the specific lamination directions and to obtain an explicit formula for the relaxation of the energy, given in (3.1) below. A rigorous proof of the validity of the explicit formula has meanwhile been obtained and was published elsewhere (Conti and Dolzmann, 2014). We then turn to nematic elastomers, a material whose peculiar properties generated a large interest in the physics and mechanics communities in the last decades (see the discussion of the literature in Section 4). We show that our algorithm is able to provide a detailed characterization of the (previously unknown) mesoscopic phase diagram. We also show, via the computation of a stress-strain diagram for a uniaxial tension experiment, how relaxation affects the macroscopic properties of the material (see Section 4 for details).

The paper is organized as follows. In Section 2 we recall the mathematical theory underlying our numerical approach and present the algorithm in detail. Aspects of its implementation and its validation are presented in Section 3. Finally Section 4 contains an in-depth analysis of an anisotropic model for sheets of nematic elastomers. The appendix contains the mathematical proof of Proposition 4.3, which states that for membrane problems we can deal with relaxation in 2×2 matrices.

Notation. We say that W is rank-one convex if W is convex along all rank-one lines, i.e., for all $F\in\mathbb{R}^{n\times n}$ and $R\in\mathbb{R}^{n\times n}$ with $\operatorname{rank} R=1$ the functions $t\mapsto W(F+tR)$ are convex. Moreover W is polyconvex, if there exists a convex function g which depends on the vector $M(F)$ of all minors of F such that $W(F)=g(M(F))$. For $n=2$ this requires the existence of a convex function $g:\mathbb{R}^5\to\mathbb{R}$ with $W(F)=g(F,\det F)$ and for $n=3$ the existence of a convex function $g:\mathbb{R}^{19}\to\mathbb{R}$ with $W(F)=g(F,\operatorname{cof}F,\det F)$ where $\operatorname{cof}F$ denotes the (3×3)-matrix of all quadratic subdeterminants of F.

2. Algorithm

As discussed in the introduction, the concept of a fully discrete approach to the numerical simulation of multi-scale problems requires an algorithmic approach to the computation of the relaxed energy W^{qc}. At the beginning of a numerical simulation for the relaxed variational problem, no information about the relaxed energy is available. Every evaluation of an approximation of $W^{qc}(F)$ requires computational work. Typically this is done reducing to a finite-dimensional minimization problem which is then solved by locally optimizing the parameters with some variant of a steepest descent procedure. These local optimization algorithms require initial conditions. If no information is available, the initial conditions can be deterministic, e.g., assuming that no microstructure is needed, or random, e.g., generating some microstructure based on a random number generator. One key ingredient in our algorithm is that every computation of the relaxed energy provides information about the relaxed energy and the corresponding microstructure, and that this information should be saved and accumulated during the execution of the full simulation. The approach proposed in this article is to store the microstructures that are computed in a data structure and to construct from this information well adapted initial conditions for later computations of the relaxed energy.

In the following we assume that the free energy density W is defined on $\mathbb{R}^{m\times n}$, the case $m=n$ being the relevant case for applications in elasticity.