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On statistical strain and stress energy bounds from homogenization and virtual testing

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ABSTRACT

Computational homogenization for quasistatic stress problems is considered, whereby the macroscale stress is obtained via averaging on Statistical Volume Elements (SVE:s). The variational "workhorse" for the subscale problem is derived from the presumption of weak micro-periodicity, which was proposed by Larsson et al. (2011). Continuum (visco)plasticity is adopted for the mesoscale constituents, whereby a pseudo-elastic, incremental strain energy serves as the potential for the updated stress in a given time-increment. Strict bounds on the incremental strain energy are derived from imposing Dirichlet and Neumann boundary conditions, which are defined as suitable restrictions of the proposed variational format. For this purpose, both the standard situation of complete macroscale strain control and the (less standard) situation of macroscale stress control are considered. Numerical results are obtained from "virtual testing" of SVE:s in terms of mean values and a given confidence interval, and it is shown how these properties converge with respect to the SVE-size for different prescribed macroscale deformation modes and different statistical properties of the random microstructure. In addition, the upper and lower bounds for a sequence of increasing strain levels, for a fixed SVE-size, are used as "data" for the calibration of a macroscopic elastic–plastic constitutive model.

1. Introduction

The standard approach to account for the effect of randomized material micro-heterogeneities in constitutive modeling is to employ fully "nested" macro-subscale modeling based on homogenization on a Statistical Volume Element[1] (SVE), (c.f. Michel et al., 1999; Miehe et al., 1999; Miehe and Koch, 2002; Torquato, 2002; Ostoja-Starzewski, 2006, 2008; Kouznetsova et al., 2002; Geers et al., 2010; Zohdi and Wriggers, 2001, 2005; Temizer and Wriggers, 2008; Roters et al., 2010; Schröder et al., 2011; Danielsson et al., 2007). Although the basic procedure is now quite well established, many issues are still unresolved, for example in relation to the model assumptions that are (implicitly and explicitly) made as part of the computation. Among the issues are (1) to formulate and analytically assess the effectiveness of different prolongation conditions to the subscale (within the SVE) and to (2) establish rigorous bounds on energetic measures based on "virtual testing" of randomly chosen "samples" of the microstructural arrangement.

As to the first issue, it is clear that different model assumptions are possible in terms of the imposed boundary conditions and the appropriate variational format of the SVE-problem. The classical conditions are those of zero displacement fluctuation field (Dirichlet), boundary tractions generated by a constant macroscale stress tensor (Neumann) and (strong) micro-periodicity, defined by periodic displacement fluctuations and anti-periodic tractions. There is ample numerical evidence that periodic boundary conditions are efficient even when the microstructure is non-periodic (which is the most common situation). By "efficient" we here denote the property that the results converge rapidly when the SVE-size is increased (while the length-scale of the subscale features is kept fixed). However, it can not be generally proved for an arbitrary type of nonlinear and dissipative subscale constitutive assumption that the choice of periodic boundary conditions give the "best" results for a given size of the subscale computational domain on which the SVE-problem is defined. In this paper, we use

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[1] We prefer the notion SVE rather than the commonly used Representative Volume Element (RVE) since the fact that SVE:s of finite size are not truly representative is the topic of this paper.

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a recently proposed weak form of micro-periodicity condition as a "work-horse" (Larsson et al., 2011). This format has a number of properties that are believed to be advantageous. For example, this format encompasses in a quite direct fashion (1) the classical "strong format" of micro-periodicity and (2) the Neumann boundary condition on tractions. As it turns out, the Neumann boundary condition is completely equivalent to the weakest possible form of displacement micro-periodicity. Moreover, (3) the Dirichlet boundary condition can also be obtained from this variational format by restricting the space of displacements in a suitable way. The resulting formulation is, however, "non-conventional" from an operational point of view (as discussed below).

As to the second issue (which is the main focus in this paper), it is first noted that a wealth of literature has been devoted to the issue of providing upper and lower bounds to the expected value of the effective stiffness in elasticity. Examples are Teply and Dvorak (1988), Huet (1990), Hazanov and Huet (1995), Suquet (1993), Suquet (1977), Zohdi and Wriggers (2001, 2005), Ostoja-Starzewski (2008), Salmi et al. (2012) and Brisard et al. (2013). However, the expected value is never computable in practice; only the mean values are. Therefore, the main contribution in this paper regards the procedure and strategy to achieve both upper and lower bounds with a given confidence based on computations for a given SVE-size. This task turns out to not be entirely trivial, particularly not for nonlinear and dissipative material models (such as elasto-plasticity).

The paper is organized as follows: After giving a summary of the essential assumptions and the variational framework for (first order) computational homogenization in Sections 2 and 3, we outline the SVE-problem pertinent to the proposed variational micro-periodicity condition for macroscale strain and stress control in Section 4. The main part is Section 5, which deals with energetic bounds based on statistical considerations. Finally, in Section 6 we illustrate the ideas with the aid of a few numerical examples on SVE-computations. The paper is concluded by final remarks and an outlook to future work.

2. Homogenization of quasistatic stress problem

2.1. Preliminaries

Consider the spatial domain Ω with boundary Γ. The usual continuum relations are assumed to apply on the subscale such that the equilibrium equation representing quasi-static response reads.

$$-\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}=\boldsymbol{f}\quad \text{in } \Omega, \tag{1}$$

where $\boldsymbol{\sigma}$ is the stress, $\boldsymbol{\nabla}$ is the spatial gradient with respect to coordinates $\boldsymbol{x}\in\Omega$, and $\boldsymbol{f}$ is the body force. As to the relevant boundary conditions on Γ, we have the usual Neumann condition $\boldsymbol{t}\overset{\text{def}}{=}\boldsymbol{\sigma}\cdot\boldsymbol{n}=\boldsymbol{t}_{\text{p}}$ on Γ_{N}, where $\boldsymbol{n}$ is a unit normal vector, and the Dirichlet condition $u=\boldsymbol{u}_{\text{p}}$ on Γ_{D}. In order to simplify the subsequent discussion on homogenized properties and avoid unnecessary technical details, we shall henceforth assume that $\boldsymbol{t}_{\text{p}}=\boldsymbol{0}$.

Constitutive relations are needed to determine $\boldsymbol{\sigma}$ in terms of the (subscale) strain $\boldsymbol{\varepsilon}[\boldsymbol{u}]\overset{\text{def}}{=}(\boldsymbol{u}\otimes\boldsymbol{\nabla})^{\text{sym}}$ and, possibly, a set of internal variables $\underline{k}$ expressing dissipative mechanisms such that $\boldsymbol{\sigma}(\boldsymbol{\varepsilon},\underline{k})$. Upon integrating the corresponding evolution equations in time and solving for $\underline{k}$ for given $\boldsymbol{\varepsilon}$, we obtain the *algorithmic* stress-deformation relation.$\boldsymbol{\sigma}_{\text{a}}(\boldsymbol{\varepsilon})\overset{\text{def}}{=}\boldsymbol{\sigma}(\boldsymbol{\varepsilon},\underline{k}_{\text{a}}(\boldsymbol{\varepsilon}))$[2] Note that any algorithmic variable is an implicit function of its argument; however, this fact is not stressed further. The relation is explicit only if the material response is elastic.

Due to the excessive effort in resolving the fine scale representation, homogenization is introduced. The classical approach (which is adopted in this paper) is to introduce "model-based homogenization", whereby a local field y is replaced by the "running" volume average:

$$y(\overline{\boldsymbol{x}})\mapsto\langle y\rangle_{\square}(\overline{\boldsymbol{x}})\overset{\text{def}}{=}\frac{1}{|\Omega_{\square}(\overline{\boldsymbol{x}})|}\int_{\Omega_{\square}} y\,\mathrm{d}V,\quad \overline{\boldsymbol{x}}\in\Omega \tag{2}$$

representing a smoothing approximation on a Statistical Volume Element (SVE). In practice, the SVE:s are finite-sized and occupies the subscale region $\Omega_{\square}(\overline{\boldsymbol{x}})$ with boundary $\Gamma_{\square}$.[3] The typical dimension of an SVE is $L_{\square}=(|\Omega_{\square}|)^{1/n_{\text{dim}}}$, where $n_{\text{dim}}\in\{1,2,3\}$ is the spatial dimension. The SVE is centered at the macroscale position[4] $\overline{\boldsymbol{x}}\overset{\text{def}}{=}(1/|\Omega_{\square}|)\int\boldsymbol{x}\,\mathrm{d}S$ for any given $\overline{\boldsymbol{x}}\in\Omega$.

In order to establish the homogenized version of the weak format of equilibrium, we introduce the space-variational forms.

$$a(\boldsymbol{u};\delta\boldsymbol{u})\overset{\text{def}}{=}\int_{\Omega}\langle\boldsymbol{\sigma}(\boldsymbol{\varepsilon}[\boldsymbol{u}]):\boldsymbol{\varepsilon}[\delta\boldsymbol{u}]\rangle_{\square}\,\mathrm{d}V,\quad l(\delta\boldsymbol{u})\overset{\text{def}}{=}\int_{\Omega}\langle\boldsymbol{f}\cdot\delta\boldsymbol{u}\rangle_{\square}\,\mathrm{d}V \tag{3}$$

representing the internal and external virtual work, respectively, of the homogenized problem. The appropriate homogenized virtual work relation is thus given as: Find $\boldsymbol{u}\in\mathbb{U}$ s.t.

$$a(\boldsymbol{u};\delta\boldsymbol{u})=l(\delta\boldsymbol{u}),\quad \forall\,\delta\boldsymbol{u}\in\mathbb{U}^0 \tag{4}$$

Inside each SVE, the subscale displacement field is split into one smooth part, $\boldsymbol{u}^{\text{M}}$, and the subscale fluctuation, $\boldsymbol{u}^{\text{s}}$, i.e. $\boldsymbol{u}=\boldsymbol{u}^{\text{M}}+\boldsymbol{u}^{\text{s}}$. The scales are linked by expressing$\boldsymbol{u}^{\text{M}}(\overline{\boldsymbol{x}},\boldsymbol{x})$[5] for $\overline{\boldsymbol{x}}\in\Omega$ and $\boldsymbol{x}\in\Omega_{\square}(\overline{\boldsymbol{x}})$ in terms of the macroscale solution $\overline{\boldsymbol{u}}(\overline{\boldsymbol{x}})$ in an explicit fashion and defining the *approximate* solution$\boldsymbol{u}^{\text{s}}=\boldsymbol{u}^{\text{s}}\{\overline{\boldsymbol{u}}\}$[6] for given $\overline{\boldsymbol{u}}$. This (implicit) relation allows for computing the homogenized quantities in (3). Moreover, we introduce the standard assumption on (model-based) *first order homogenization*, according to which the macroscale field $\boldsymbol{u}^{\text{M}}$ varies *linearly* within each SVE. This means that we expand $\boldsymbol{u}^{\text{M}}$ as.

$$\boldsymbol{u}^{\text{M}}(\overline{\boldsymbol{x}},\boldsymbol{x})=\overline{\boldsymbol{u}}(\overline{\boldsymbol{x}})+\overline{\boldsymbol{\varepsilon}}(\overline{\boldsymbol{x}})\cdot[\boldsymbol{x}-\overline{\boldsymbol{x}}],\quad \overline{\boldsymbol{x}}\in\Omega,\quad \boldsymbol{x}\in\Omega_{\square}(\overline{\boldsymbol{x}}). \tag{5}$$

Here we introduced the (smooth) macroscopic displacement field $\overline{\boldsymbol{u}}$ and the corresponding strain field $\overline{\boldsymbol{\varepsilon}}\overset{\text{def}}{=}(\overline{\boldsymbol{u}}\otimes\boldsymbol{\nabla})^{\text{sym}}=\boldsymbol{\varepsilon}[\overline{\boldsymbol{u}}]$.

It is now tacitly used that the variation $\delta\boldsymbol{u}$ can be defined as the sensitivity[7] for a variation $\delta\overline{\boldsymbol{u}}$ and thus can be expressed as $\delta\boldsymbol{u}=\delta\boldsymbol{u}^{\text{M}}+(\boldsymbol{u}^{\text{s}})'\{\overline{\boldsymbol{u}};\delta\overline{\boldsymbol{u}}\}$, where

$$\delta\boldsymbol{u}^{\text{M}}=\delta\overline{\boldsymbol{u}}+\delta\overline{\boldsymbol{\varepsilon}}\cdot[\boldsymbol{x}-\overline{\boldsymbol{x}}] \tag{6}$$

Upon setting $\delta\boldsymbol{u}=\delta\boldsymbol{u}^{\text{M}}$ in (4), we obtain the macroscopic problem as that of finding $\overline{\boldsymbol{u}}\in\overline{\mathbb{U}}$ that solves the homogenized problem.

$$a(\boldsymbol{u}\{\overline{\boldsymbol{u}}\};\delta\boldsymbol{u}^{\text{M}}(\delta\overline{\boldsymbol{u}}))=l(\delta\boldsymbol{u}^{\text{M}}(\delta\overline{\boldsymbol{u}}))\quad \forall\,\delta\overline{\boldsymbol{u}}\in\overline{\mathbb{U}}^0. \tag{7}$$

[2] Henceforth, the subindex "a" is dropped without the risk of confusion.

[3] Henceforth, the argument $\overline{\boldsymbol{x}}$ is suppressed unless there is a risk of confusion.

[4] The choice is not unique: Another possibility is $\overline{\boldsymbol{x}}=\langle\boldsymbol{x}\rangle_{\square}$.

[5] Double arguments, e.g. $\boldsymbol{u}(\overline{\boldsymbol{x}},\boldsymbol{x})$, are used to explicitly point out the underlying scale separation.

[6] Curly brackets $\{(\bullet)\}$ indicate implicit and/or nonlocal functional dependence on $(\bullet)$.

[7] The sensitivity is defined as the Gateaux-derivative $(\boldsymbol{u}^{\text{s}})'\{\overline{\boldsymbol{u}};\delta\overline{\boldsymbol{u}}\}\overset{\text{def}}{=}(\partial/\partial\varepsilon)\,\boldsymbol{u}^{\text{s}}\{\overline{\boldsymbol{u}}+\varepsilon\delta\overline{\boldsymbol{u}}\}\big|_{\varepsilon=0}$.