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Generalized boundary conditions on representative volume elements and their use in determining the effective material properties

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ABSTRACT

When determining an effective stress–strain law by means of the representative volume element (RVE) method, one needs to subject the RVE to the effective strains by appropriate boundary conditions (BC). Usually, classical BC that prescribe a homogeneous stress or strain field at the boundary or a periodic unit cell are used. In this work, we discuss generalized BC, which involve the partitioning of the RVE boundary into *n* parts. It is demonstrated that the classical BC are contained as special cases, and that the Hill–Mandel-condition holds for all partitionings.

By a more or less fine surface partitioning, the generalized BC allow for a smooth scaling between the extremal cases of homogeneous stress or homogeneous strain BC. Further, by an irregular surface partitioning, one can obtain stochastic BC with an elastic stiffness close to the periodic/antipodal BC, but with a higher resistance against localization. This has been demonstrated by examining a softening example material. A test of plausibility for a RVE is to apply it to a homogeneous microstructure. Then, the microscale material law should be conducted directly to the macroscale. In case of softening microscale materials, this test works only for homogeneous strain BC. For homogeneous stress- and periodic/antipodal BC, localization occurs, accompanied by a drastic deviation from the expected stress–strain curve. From the generalization, one can derive stochastic BC that combine the moderate elastic stiffness of periodic BC with the high resistance against localization of homogeneous strain BC.

1. Introduction

The micro-scale structure of a material can have a considerable effect on the material properties as perceived on the macroscale. It may be the byproduct of a forming or solidification process, be an inseparable part of the material (e.g., fibers of wood), or it may be the result of a material design process (micro-structural reinforced or micro-architectured materials). In order to efficiently examine the micro–macro interaction, one needs fast, reliable and robust homogenization methods. These demands can be accounted for by the representative volume element method. The method consists basically in choosing a representative material sample (step 1), enforcing the average (macro) fields of the independent variable (e.g., the strains, step 2), solving the boundary value problem (step 3), and averaging the fields of the resulting dependent variable (e.g., the stresses, step 4). The method allows to obtain estimates of effective material properties when analytical homogenization is due to the geometric nonlinear setting or complicated interactions between the constituents hardly possible (e.g. [1]). Here, the term "representative" is used in an approximate sense as suggested in [15–17], compared to the strict interpretation of [18].

The present work is concerned with step 2, namely how the average macro-scale field may be imposed most efficiently. Since RVE are something artificial, there are no natural boundary conditions (BC), except for periodic microstructures. Then, the periodicity prescribes a specific self-interaction of the boundaries. Another possibility is to prescribe homogeneous fields on the boundary. Regarding the mechanical material behavior, one may prescribe either homogeneous deformations ($\boldsymbol{u} = \overline{\boldsymbol{H}} \cdot \boldsymbol{x}_0$) or homogeneous stresses ($\boldsymbol{t} = \overline{\boldsymbol{T}} \cdot \boldsymbol{n}_0$), see [14]. The latter BC are extremal in the sense that they result in the stiffest (homogeneous deformations) or softest (homogeneous stresses) possible RVE, while periodic BC lie between these extremes. Although the homogeneous deformation BC require, strictly speaking, a prescribed displacement gradient, we will refer to them in the remainder as homogeneous *strain* BC to emphasis the dual character of the pair stresses/strains and the resulting extremal BC.

Mostly, one of these three classical BC is employed. Due to a more complicated implementation and problems with RVE localization, the homogeneous stress BC are much less popular than the homogeneous strain BC and the periodic BC. Especially the periodic BC are commonly used, even for non-periodic structures, due to the absence of other popular BC that lie between the extremal BC. The reason is that it is not easy to give BC of moderate stiffness that comply with the Hill–Mandel-condition [5], which is a

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necessary condition for the RVE to converge to a macroscale material law as the RVE size is increased [14]. To the best knowledge of the author, only two other BC of non-extremal stiffness are known, namely the subspace decomposition of the boundary data, which consists of enforcing homogeneous displacements in one direction and homogeneous tractions perpendicular to this direction (or the other way around, [4]), and the gradual penalization of a deviation from the homogeneously deformed RVE by spring elements [3]. The aim of the present work is to give generalized BC that comply with the Hill–Mandel-condition, and enclose the classical BC (Section 2). From this generalization, one can construct BC that have yet unseen properties. The applicability of the generalized BC is examined for an elasto-plastic matrix inclusion material (Section 3). We demonstrate that elasto-plastic material homogenization can benefit from the properties of the generalization, especially when softening microscale materials are considered (Sections 4 and 5).

1.1. Notation

Throughout the work a direct tensor notation is preferred. Vectors are symbolized by lowercase bold letters, and second-order tensors by uppercase bold letters. The second-order identity tensor is denoted by $\boldsymbol{I}$. A dot represents a scalar contraction. If more than one scalar contraction is carried out, the number of dots corresponds to the number of contractions, e.g., $(\boldsymbol{a}\otimes\boldsymbol{b}\otimes\boldsymbol{c})\cdot\cdot(\boldsymbol{d}\otimes\boldsymbol{e}) = (\boldsymbol{b}\cdot\boldsymbol{d})(\boldsymbol{c}\cdot\boldsymbol{e})\boldsymbol{a}$, $\alpha = \boldsymbol{A}\cdot\cdot\boldsymbol{B}$.

The position vector of a material point is denoted by $\boldsymbol{x}(\boldsymbol{x}_0, t)$, where $\boldsymbol{x}_0$ indicates the position vector of the same material point in the reference placement. At $t = 0$, $\boldsymbol{x} = \boldsymbol{x}_0$ holds. The partial derivative of a function with respect to t with $\boldsymbol{x}_0$ kept constant is the material time derivative, indicated by a superimposed dot. The index "0" indicates that a function or derivative is to be evaluated in the reference placement or with respect to $\boldsymbol{x}_0$. Ω denotes the domain of the RVE under consideration. A bar denotes the unweighted volume average over Ω.

1.2. List of symbols

Ω	domain of the RVE
$\partial\Omega$	RVE boundary
$\partial\Omega_i$	part of $\partial\Omega$
k	number of surface partitions
n	number of discrete points contained in $\partial\Omega_i$, referred to as group size
n_{max}	number of discrete points contained in $\partial\Omega$
u_{abs}	absolute under-determinacy, u_{abs} = No. of vars. − No. of. eqs.
u_{rel}	relative under-determinacy, $u_{rel} = u_{abs}$/No. of vars.
$\boldsymbol{n}_0$	surface normal vector in the reference placement
$\boldsymbol{t}$	traction vector $\boldsymbol{t} = \boldsymbol{T}\cdot\boldsymbol{n}_0$
$\boldsymbol{u}$	displacement vector, $\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{x}_0$
$\boldsymbol{x}$	position vector
$\boldsymbol{H}$	displacement gradient
$\boldsymbol{T}$	first Piola–Kirchhoff stress tensor

2. Generalized boundary conditions

The generalized BC are given by.

- dividing the surface $\partial\Omega$ of the RVE into k parts $\partial\Omega_i$,
- and constraining $\boldsymbol{u}$ on each $\partial\Omega_i$ by

$$\underbrace{\overline{\boldsymbol{H}}\cdot\int_{\partial\Omega_i}\boldsymbol{x}_0\otimes \mathrm{d}\boldsymbol{A}_0}_{\overline{\boldsymbol{H}}_i} = \int_{\partial\Omega_i}\boldsymbol{u}\otimes \mathrm{d}\boldsymbol{A}_0. \tag{1}$$

In the latter equation, one can consider the left handside as the displacement gradient $\overline{\boldsymbol{H}}_i$ that is imposed on the surface part $\partial\Omega_i$. After fixing an average deformation $\overline{\boldsymbol{H}}$ and a surface partitioning, it can be calculated for each part $\partial\Omega_i$ of the surface.

One can show that the well known homogeneous strain-, homogeneous stress- and periodic BC are contained special cases, resulting from different surface partitionings:

- The **homogeneous strain BC** require an infinitely fine partitioning of the surface, i.e., Eq. (1) must hold pointwise on $\partial\Omega$ instead on average. Thus, we drop the integral,

$$(\overline{\boldsymbol{H}}\cdot\boldsymbol{x}_0)\otimes \mathrm{d}\boldsymbol{A}_0 = \boldsymbol{u}\otimes \mathrm{d}\boldsymbol{A}_0. \tag{2}$$

Comparing coefficients gives

$$\boldsymbol{u} = \overline{\boldsymbol{H}}\cdot\boldsymbol{x}_0, \tag{3}$$

which must hold everywhere on $\partial\Omega$. This corresponds to the well known homogeneous strain BC.

- For **periodic BC**, the partitioning is infinitely fine, but points are coupled pairwise such that

$$\mathrm{d}\boldsymbol{A}_0^+ = -\mathrm{d}\boldsymbol{A}_0^-, \tag{4}$$

holds, where the + and − sign index the two coupled points. Again, the integral is contracted at the two points,

$$(\overline{\boldsymbol{H}}\cdot\boldsymbol{x}_0^+)\otimes \mathrm{d}\boldsymbol{A}_0^+ + (\overline{\boldsymbol{H}}\cdot\boldsymbol{x}_0^-)\otimes \mathrm{d}\boldsymbol{A}_0^- = (\boldsymbol{u}^+\otimes \mathrm{d}\boldsymbol{A}_0^+) + (\boldsymbol{u}^-\otimes \mathrm{d}\boldsymbol{A}_0^-). \tag{5}$$

With Eq. (4) one can write

$$\overline{\boldsymbol{H}}\cdot(\boldsymbol{x}_0^+ - \boldsymbol{x}_0^-)\otimes \mathrm{d}\boldsymbol{A}_0^+ = (\boldsymbol{u}^+ - \boldsymbol{u}^-)\otimes \mathrm{d}\boldsymbol{A}_0^+, \tag{6}$$

where a comparison of coefficients gives the well known periodic BC,

$$\overline{\boldsymbol{H}}\cdot(\boldsymbol{x}_0^+ - \boldsymbol{x}_0^-) = \boldsymbol{u}^+ - \dot{\boldsymbol{u}}^-. \tag{7}$$

Further, periodicity requires an RVE shape that allows to fill the space entirely with instances of the RVE, and a corresponding coupling. However, one may as well apply Eqs. (6) and (4) to RVE that do not have such a shape, or employ a non-periodic node coupling.

- **Homogeneous stress BC** are obtained when there is no surface partitioning at all. Then Eq. (1) becomes with Gauss's theorem

$$\overline{\boldsymbol{H}} = \frac{1}{V_0}\int_{\partial\Omega}\boldsymbol{u}\otimes \mathrm{d}\boldsymbol{A}_0. \tag{8}$$

These, sometimes termed as *kinematic minimal BC*, correspond to the homogeneous stress BC. This has been demonstrated by Miehe [8] (Section 2.4.2), using Lagrangian multipliers to enforce the latter equation as a weak constraint. A proof of this statement that relies on the macroscopic stress power is contained in the Appendix.
It is noteworthy that Eq. (8) should always hold, since it is nothing else but the kinematic coupling between the micro- and macroscale [10]. One can see in fact that it holds independently of the surface partitioning. However, if Eq. (8) is the *only* constraint that is imposed on $\partial\Omega$, the resulting stresses on the RVE boundary are homogeneous.

2.1. The Hill–Mandel-condition

The Hill–Mandel condition demands the equivalence of the stress power as perceived on the macroscale to the integral of the stress-power over the RVE. For the large strain setting, it can be written as

$$\int_{\partial\Omega}\dot{\tilde{\boldsymbol{u}}}\cdot\boldsymbol{t}\,\mathrm{d}A_0 = 0, \tag{9}$$