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ON INTERPOLATION OF HOMOGENIZED COEFFICIENTS FOR ANALYSIS OF LARGE DEFORMATION

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Summary: *The paper deals with the method of interpolation of the homogenized effective material parameters which are computed by solving local microscopic boundary value problems. These coefficients constitute the tangent operator employed to linearize the problem of finite deformation. Due to finite deformations, the microscopic problems are only locally periodic and the effective coefficients as well. The proposed interpolation scheme enables to reduce wisely the number of microscopic problems that have to be solved to recover the macroscopic domain with relevant effective coefficients.*

1. Introduction

The topic of the paper is related to the problem of computing the finite deformation of hyperelastic media with locally periodic heterogeneous microstructure, cf. [1, 2, 6]; for applications see [4, 5]. The macroscopic problem is defined in terms of the homogenized coefficients constitute the tangent operator employed to linearize the problem of finite deformation; in our examples we use the updated Lagrangian configuration. Any reference configuration is associated with the local microstructures which determine values of the homogenized coefficients; these can be computed by solving the local microscopic boundary value problems with periodic boundary conditions. Any micro-structural periodicity is lost, when the material is subjected to a nonuniform finite deformation, so that an infinite number of the microscopic problems would have to be solved to recover the macroscopic domain.

In order to make the large deformation problem tractable numerically, we suggest to introduce an approximation scheme, so that we need to compute the homogenized coefficients right way at a selected points of the macrostructure. The deformation state of the microstructure is determined uniquely by the macroscopic deformation gradient $\boldsymbol{F}$. Therefore the approximation of the homogenized coefficients could be established in the space of the components F_{ij}, $i, j = 1, 2, (3)$, regardless the spatial position within the

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macroscopic domain. On the other hand, in two distant parts of the macroscopic domain the deformation can be quite different, so that it makes sense to relate the approximation also to the spatial position. These observations lead us to the concept of the *macro-elements*.

2. Concept of the macro-elements

We consider that the macroscopic domain Ω is decomposed into a finite number of *macroscopic subdomains* Ω_e, so that

$$\bar{\Omega} = \bigcup_e \bar{\Omega}_e \ . \tag{1}$$

In order to introduce a deformation-based interpolation scheme over each of the macroscopic subdomains, we shall assume that the variation of deformation tensors $\boldsymbol{F}(x)$, $x \in \Omega_e$ is only moderate. For $x' \in \Omega_e$ we define

$$h(x') \equiv \max\{\|\boldsymbol{F}(x) - \boldsymbol{F}(x')\| \,|\, x \in \Omega_e\}, \tag{2}$$

where $\|\cdot\|$ is the Frobenius norm. Further in each Ω_e we define the *central point* x^* for which

$$h(x^*) \leq h(x), \ \ \forall x \in \Omega_e \ . \tag{3}$$

Using the central point and the associated deformation ${}^*\boldsymbol{F} = \boldsymbol{F}(x^*)$ we decompose the deformation in Ω_e

$$\boldsymbol{F}(x) = \boldsymbol{f}(x) \ {}^*\boldsymbol{F} \ . \tag{4}$$

This decomposition is employed in the following definition of the macro-element $\mathcal{M}$:

$$\mathcal{M}({}^*\boldsymbol{F}, \{\boldsymbol{f}_j\}_{j=0}^m) = \{\boldsymbol{F} \mid \exists \boldsymbol{f} \in \mathrm{conv}\{\boldsymbol{f}_j\}_{j=0}^m \ : \ \boldsymbol{F} = \boldsymbol{f} \ {}^*\boldsymbol{F}\} \tag{5}$$

In (5) $\mathrm{conv}\{\boldsymbol{f}_j\}_{j=0}^m$ means the convex hull of a basis $\{\boldsymbol{f}_j\}_{j=0}^m$. The dimension $m+1$ of the basis will be specified later on. We recall that the macro-element is related to $m+1$ different microstructures; in the spirit of (4) they are obtained by deforming the "central microstructure" defined by ${}^*\boldsymbol{F}$. Therefore, it is natural to choose the identity mapping as $\boldsymbol{f}_0$.

Let us denote by $\mathcal{M}_e$ the macro-element, which is defined for the central point $x^* \in \Omega_e$, see (3). Desirably, the macro-element should recover deformation gradients in Ω_e, i.e. we want

$$\forall\, x \in \Omega_e \ : \ \boldsymbol{F}(x) \in \mathcal{M}_e \ . \tag{6}$$

This property is guaranteed, if we define the basis $\{\boldsymbol{f}_j\}_{j=1}^m$ in terms of the *box* in $\mathbb{R}^4$, or $\mathbb{R}^9$ for 2D, or 3D problems, respectively. Thus we obtain $m = 2^4$, or $m = 2^9$ tensors $\boldsymbol{f}_j$, respectively; the components of $\boldsymbol{f}_j$ are obtained combining the minimal and maximal values $\underline{a}_{\boldsymbol{i}}$, $\overline{a}_{\boldsymbol{i}}$ (the $\boldsymbol{i}$ is the multi-index):

$$\begin{array}{rcl} \underline{a}_{\boldsymbol{i}} & = & \min_x\{f_{ij}(x), ij \equiv \boldsymbol{i} \,|\, x \in \Omega_e\}, \ i,j = 1,2,(3) \ , \\ \overline{a}_{\boldsymbol{i}} & = & \max_x\{f_{ij}(x), ij \equiv \boldsymbol{i} \,|\, x \in \Omega_e\}, \ i,j = 1,2,(3) \ . \end{array} \tag{7}$$

The basis can get smaller, if the polar decomposition is applied. The deformation $\boldsymbol{f}$ in (4) determines[2], how the microstructure at x differs from that at x^*. Obviously, $\boldsymbol{f}$

[2]We use the abbreviated notation $\boldsymbol{F}(x) \equiv \boldsymbol{F}$, $x \in \Omega_e$, if not specified otherwise.

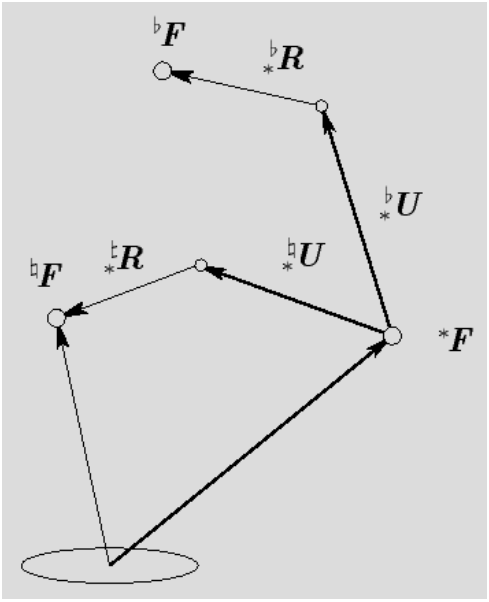

Figure 1: Polar decomposition of the macroscopic deformation gradients in Ω_e.

comprise also the rotation which, however, does not influence the deformation state of the microstructure.

Let us consider the deformation ${}^{\flat}\boldsymbol{F}$ decomposed, as follows

$$\begin{aligned} {}^{\flat}\boldsymbol{F} &= {}^{\flat}_{*}\boldsymbol{F}\,{}^{*}\boldsymbol{F} \\ &= {}^{\flat}_{*}\boldsymbol{R}\,{}^{\flat}_{*}\boldsymbol{U}\,{}^{*}\boldsymbol{F} \ . \end{aligned} \tag{8}$$

Thus, the polar decomposition of $\boldsymbol{f} \equiv {}^{\flat}_{*}\boldsymbol{F}$ yields the rotation tensor ${}^{\flat}_{*}\boldsymbol{R}$ and the right stretch tensor ${}^{\flat}_{*}\boldsymbol{U}$, which is symmetric. Due to this nice property we can reduce the number of the microstructural problems that have to be solved. Now the requirement, which is equivalent to that of (6), reads as

$$\forall\, x \in \Omega_e \,|\, \exists \boldsymbol{R}, \exists \boldsymbol{F} \in \mathcal{M}_e \,:\, \boldsymbol{F}(x) = \boldsymbol{R}\boldsymbol{F} \ , \tag{9}$$

where $\boldsymbol{R}^T = \boldsymbol{R}^{-1}$ is the orthogonal tensor of rotation which follows from (8) for $\boldsymbol{F}(x) \equiv {}^{\flat}\boldsymbol{F}$. The (reduced) basis for the macro-element which preserves (9) can be defined using the right stretch tensors $\boldsymbol{U} = {}^{\flat}_{*}\boldsymbol{U}$ employed in (8). Thus, each $\boldsymbol{f}_j$ is defined by 3, or 6 components in 2D, or 3D, respectively, attaining the values $\underline{b}_{\boldsymbol{i}}$, $\overline{b}_{\boldsymbol{i}}$:

$$\begin{aligned} \underline{b}_{\boldsymbol{i}} &= \min_x\{U_{ij}(x), ij \equiv \boldsymbol{i} \,|\, x \in \Omega_e\},\ i,j = 1,2,(3) \ , \\ \overline{b}_{\boldsymbol{i}} &= \max_x\{U_{ij}(x), ij \equiv \boldsymbol{i} \,|\, x \in \Omega_e\},\ i,j = 1,2,(3) \ . \end{aligned} \tag{10}$$

In this case the dimension of the basis is $m+1 = 2^3+1$ and $m+1 = 2^6+1$ for 2D and 3D, respectively.

3. Simplexes on the macro-element

The interpolation scheme on simplexes in $\mathbb{R}^d$ is described in details in [2]; it is based on sequential curve interpolation using the Hermit cubic polynomials. For 2D problems the

corresponding simplex is the tetrahedron with vertexes $\mathbf{x}^k$, $k = 1, 2, 3, 4$. The interpolation function $\tilde{\psi}$ is defined in terms of $\psi(\mathbf{x}^k)$ and $\nabla_{\mathbf{x}}\psi(\mathbf{x}^k)$ computed at each vertex, $k = 1, \ldots, 4$. Then, for a given $\mathbf{x}^\circ$, any point in the simplex, the interpolated function value is determined by the mapping

$$\left.\begin{array}{r} \mathbf{x}^\circ \\ \{\psi(\mathbf{x}^k),\ \nabla_{\mathbf{x}}\psi(\mathbf{x}^k)\}_{k=1,\ldots,4} \end{array}\right\} \longrightarrow \tilde{\psi}(\mathbf{x}^\circ)\ . \tag{11}$$

Here we explain, how to employ this scheme to define approximation of the homogenized coefficients on the macro-elements.

The properties (6), or (9) guarantee, that a deformation $\boldsymbol{F}(x)$ for $x \in \Omega_e$ belongs to the macro-element $\mathcal{M}_e$ (up to a rotation in the case of (9)). The vertexes of $\mathcal{M}_e$, the elements of $\mathbb{R}^d$, are formed by the basis elements $\boldsymbol{f}_j$, $j = 1, \ldots, m$ plus $\boldsymbol{f}_0$, which is the identity mapping corresponding to the "central microstructure" of $\mathcal{M}_e$. In what follows we treat only the case (9), so that for 2D problems $d = 3$ and for 3D ones $d = 6$. We recall, that for this case $\boldsymbol{f}_j$ are defined using the right stretch tensors, so that $(f_{kl})_j = (f_{lk})_j$.

Let ${}^\circ\boldsymbol{F}$ be the deformation, for which we want to obtain an approximation of the homogenized coefficients. The polar decomposition (8) yields ${}^\circ\boldsymbol{F} = {}^\circ_*\boldsymbol{R}\,{}^\circ_*\boldsymbol{U}\,{}^*\boldsymbol{F}$. In order to apply the interpolation scheme described above, we shall have to identify also one of the simplexes embedded in $\mathcal{M}_e$ which contain the deformation ${}^\circ_*\boldsymbol{U}$; its components form the components of the point $\mathbf{x}^\circ$. Adhering to the notation introduced in the previous paragraph, for 2D problems we write

$$\mathbf{x}^\circ = \begin{bmatrix} {}^\circ_*U_{11} \\ {}^\circ_*U_{22} \\ {}^\circ_*U_{12} \end{bmatrix}\ , \quad \mathbf{x}^k = \begin{bmatrix} (f_{11})_{j_k} \\ (f_{22})_{j_k} \\ (f_{12})_{j_k} \end{bmatrix}\ ,\ k = 1, \ldots, 4\ , \tag{12}$$

where the components f_{rs} are defined by (10). The indices $j_k \in \{0, \ldots, m\}$ determine a selection among $m+1 = 9$ elements of the basis of $\mathcal{M}_e$, so that $\mathbf{x}^\circ$ is a convex combination. In order to establish the selection and thereby the simplex uniquely, we can use the following algorithms:

1. The box $\mathcal{M}_e$ in $\mathbb{R}^d$ constituted using $\boldsymbol{f}_j$ (symmetric), $j = 1, \ldots, m$ is subdivided into a collection of non-overlapping simplexes one vertex of which is defined by $\boldsymbol{f}_0$, see Fig. 2. For example, in 2D, thus, we have to "check" up to all 12 simplexes to find the correct one.

2. We compute the distances $\rho_j = \|{}^\circ_*\boldsymbol{U} - \boldsymbol{f}_j\|$ and select $n = 4$ smallest ones $\rho_{j_1}, \ldots, \rho_{j_n}$. This selection may provide a simplex which does not contain ${}^\circ_*\boldsymbol{U}$. Then we have to resort for the secure algorithm 1.

When approximating the homogenized coefficients, i.e. $\psi := \hat{\mathcal{Q}}_{ijkl}$, for $i, j, k, l = 1, 2, (3)$ we employ the sensitivity of $\hat{\mathcal{Q}}_{ijkl}$ w.r.t. the deformation gradient, see [1, 2]. Thus we obtain the gradient of the homogenized coefficients $\delta\hat{\mathcal{Q}}_{ijkl}({}^\flat\boldsymbol{F}; \cdot)$; the dot is to be replaced by the relevant "direction", which is defined below. We consider ${}^\flat\boldsymbol{F}$, ${}^\natural\boldsymbol{F}$ and apply the decomposition w.r.t. to some $\boldsymbol{F}$:

$${}^\flat\boldsymbol{F} = {}^\flat\boldsymbol{f}\,\boldsymbol{F}\ , \quad {}^\natural\boldsymbol{F} = {}^\natural\boldsymbol{f}\,\boldsymbol{F}\ .$$

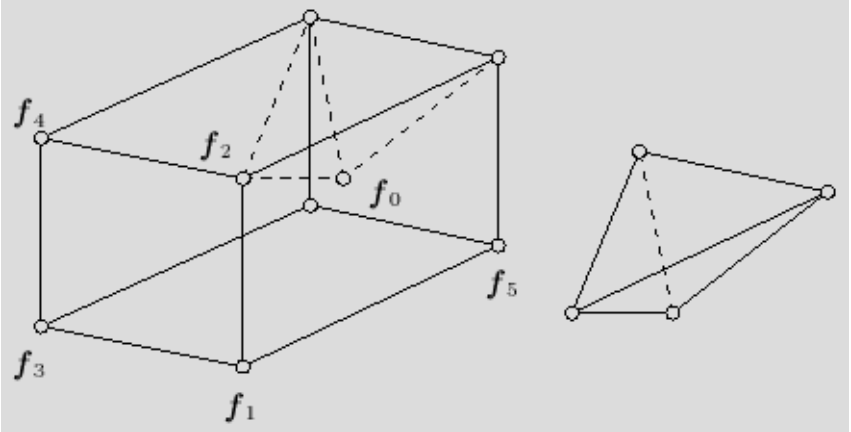

Figure 2: The macro-element in $\mathbb{R}^3$ for 2D problems. $\boldsymbol{f}_0$ is the central deformation (identity), $\boldsymbol{f}_j$, $j = 1, 2, \ldots, 8$ correspond to the right stretch tensors obtained using the polar decomposition. Right: one of the simplexes with vertexes $\mathbf{x}^k$, $k = 1, \ldots, 4$, which is embedded in the macro-element. The central point corresponds to the particular deformation in the macroscopic domain.

The following holds

$$ {}^{\natural}\boldsymbol{f} = {}^{\natural}_{\flat}\boldsymbol{f}\,{}^{\flat}\boldsymbol{f} = (\boldsymbol{I} + {}^{\natural}_{\flat}\boldsymbol{g})\,{}^{\flat}\boldsymbol{f} \ , \tag{13} $$

where $\boldsymbol{I}$ is the identity, so that we can express

$$ {}^{\natural}_{\flat}\boldsymbol{g} = ({}^{\natural}\boldsymbol{f} - {}^{\flat}\boldsymbol{f})\,{}^{\flat}\boldsymbol{f}^{-1} \ . \tag{14} $$

When the deformations ${}^{\flat}\boldsymbol{F}$ and ${}^{\natural}\boldsymbol{F}$ are closed enough each other, we can write

$$ \hat{\mathcal{Q}}_{ijkl}({}^{\natural}\boldsymbol{F}) \approx \hat{\mathcal{Q}}_{ijkl}({}^{\flat}\boldsymbol{F}) + \delta\hat{\mathcal{Q}}_{ijkl}({}^{\flat}\boldsymbol{F}; {}^{\natural}_{\flat}\boldsymbol{g}), \tag{15} $$

whereas the straightforward expression $\hat{\mathcal{Q}}_{ijkl}({}^{\flat}\boldsymbol{F}) + \delta\hat{\mathcal{Q}}_{ijkl}({}^{\flat}\boldsymbol{F}; {}^{\natural}\boldsymbol{f} - {}^{\flat}\boldsymbol{f})$ is not correct.

We remark, that a quite similar method is applied for approximation of the averaged stress on the macro-element.

4. Numerical examples and conclusions

In this paragraph we illustrate approximation errors in homogenized coefficients evaluated over a simplex, for hyperelastic material with incompressible inclusions, cf. [2, 4]. The relative error is evaluated w.r.t. the values obtained by the direct computation. In Tab. 1 we introduce the deformation gradients which constitute vertexes of the simplex.

Table 1: Deformation gradients $\boldsymbol{f}_i$ spanning the simplex ($\boldsymbol{F}_i = \boldsymbol{f}_i\boldsymbol{F}_1$).

Vertex: $i =$	1	2	3	4
$\boldsymbol{f}_i$	1.0 0.0 0.0 1.0	1.2 0.0 0.0 1.0	1.0 0.0 0.0 1.2	1.0 0.1 0.1 1.0
$\boldsymbol{F}_i$	1.0192 0.0922 0.1372 1.0039	1.2230 0.1106 0.1372 1.0039	1.0192 0.0922 0.1647 1.2047	1.0329 0.1925 0.2391 1.0131

Table 2: Relative error in the homogenized coefficients evaluated for different deformations: $\boldsymbol{F}_{\#} = \boldsymbol{f}_{\#}\boldsymbol{F}_1$.

Example #	1	2	3	4	5
f_{11}	1.0889	1.0300	1.0500	1.0400	1.1
f_{22}	1.0444	1.0700	1.0500	1.0100	1.1
f_{12}	0.0111	0.0350	0.0250	0.0050	0
error [%]	0.14	0.82	0.39	0.56	5.93

In our numerical tests, see Tab. 2, we observed that the maximum relative error in the (averaged) stress is less than that obtained for the homogenized coefficients. For these the relative error most often does not exceeds 1% (in the Example 5 the error is $\approx 6\%$).

The approximation scheme reported in the paper was employed in the coupled macro-micro analysis of large deforming hyperelastic continua with incompressible inclusions, cf. [2, 3] It has been observed that, approximating the "tangent stiffness" coefficients, convergence of the macroscopic iterations does not deteriorate, so that effectiveness of the coupled macro-micro algorithm increases. Thus, the coupled macro-micro analysis can be enhanced due to the approximation scheme suggested in this work. The approach suggested in the paper presents an alternative to the direct macro-micro analysis, which otherwise requires a massive parallel computational power.

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