Relaxed loading conditions for higher order homogenisation approaches

Ralf Jänicke[1*], **David Uribe**[1,2], **Oscar E. Ruiz**[2], and **Holger Steeb**[1]

[1] Mechanics – Continuum Mechanics, Ruhr-University Bochum, Germany
[2] CAD/CAM/CAE Laboratory, EAFIT University, Medellín, Colombia

The present paper deals with the formulation of minimal loading conditions for the application of numerical homogenisation techniques, namely the FE^2 methodology. Based on the set of volume averaging rules connecting the heterogeneous micro and the homogeneous macro scale, the minimal constraints on the deformation of a micro volume are derived for a classical Cauchy as well as for a micromorphic overall continuum theory. For both cases, numerical studies are included highlighting the main aspects of the proposed procedure.

Copyright line will be provided by the publisher

* Corresponding author: email ralf.jaenicke@rub.de, phone +49 234 32 22485, fax +49 234 32 14229

Copyright line will be provided by the publisher

1 Introduction

Heterogeneous materials are well known for their peculiar effective material properties which are driven by the underlying micro topology. Under quasi-static conditions, e. g. size dependent boundary layers (the smaller the stiffer) are to be observed [2, 17]. By contrast, a highly dispersive overall material behaviour of the compound can be found under high frequency loadings (sonic/ultrasonic) accounting for higher order wave modes due to micro structural degrees of freedom [1, 15].

In the following sections we will apply a mean-field-based homogenisation approach in order to describe the material properties of such materials on an effective scale. For this purpose, the heterogeneous medium on the micro scale has to be replaced by a homogeneous medium on the macro scale. The physical quantities of the macro scale will be interpreted in terms of volume averages of their microscopic counterparts. To this end, appropriate averaging rules have to be formulated defining a Dirichlet boundary value problem (BVP) on a micro volume which is considered to be representative for the entire mirco structure. Transferring the microscopic stress response back on the macroscopic level, the overall constitutive relations can be replaced by a Two-level calculation also stated as the FE^2 technique [4, 13] in the sequel.

Whilst the micro structure itself can be captured by a standard Cauchy continuum theory, different choices for the substitute medium are possible. Depending on the micro topological effects which are to be represented on the macro level different substitute media have to be considered. If the characteristic length scale of the micro structure is much smaller than the overall length scale (scale separation), a Cauchy substitute medium is sufficient to predict first order effects such as material or structural anisotropy [16]. However, higher order approaches are required if the characteristic length scales become comparable. Typical representatives of this class are e. g. the Mindlin's second gradient theory [14] or the micromorphic continuum theory proposed by Eringen [3].

In the sequel, the present contribution focuses on two cases. On the one hand, the Cauchy substitute medium will be considered. On the other hand the micromorphic continuum theory will be applied on the macro scale. For both, the formulation of microscopic BVP will be discussed, where usually polynomial Dirichlet boundary conditions are taken into account. By contrast, we propose the concept of the so-called *minimal boundary or loading conditions* [12], where the loading conditions are not prescribed explicitly as a Dirichlet BVP but in an integral sense constrained by the averaging rules.

All numerical examples are limited to 2D and to the range of small deformations in the context of quasi-static deformations. Linear elasticity is assumed. The discussion whcih micro volume size is necessary to end up with a representative volume element is omitted.

Copyright line will be provided by the publisher

2 First order homogenisation

Let us start our considerations with the substitution of a heterogeneous Cauchy medium by a homogeneous Cauchy medium. Moreover, let us assume an arbitrary shaped 2D micro volume of the size $V_m = l^2$. The micro volume is nested to a corresponding macroscopic material point via its volume centroid. Any position $\Delta\mathbf{x}$ inside the micro volume is expressed relative to the volume centroid. Taking into account the definition of the volume averaging procedure $\langle\Diamond\rangle = 1/V_m \int(\Diamond)\,\mathrm{d}v$, the averaging rules for the kinematic quantities read

$$\langle\Delta\mathbf{u}\rangle = \mathbf{0}, \qquad \mathrm{grad}_M^{\,\mathrm{sym}}\mathbf{u}_M = \langle\mathrm{grad}_m^{\,\mathrm{sym}}\Delta\mathbf{u}\rangle = \frac{1}{V_m}\int\limits_{\partial V_m}(\Delta\mathbf{u}\otimes\mathbf{n})^{\mathrm{sym}}\,\mathrm{d}a, \tag{1}$$

cf. [4, 13], where the subscript indices m and M refer to the micro and the macro scale, respectively and $\mathbf{n}$ refers to the outer normal vector on the boundary ∂V_m of the micro volume. From the physical point of view, eq. $(1)_1$ constrains the micro volume in a way that rigid body translation are omitted, whereas eq. $(1)_2$ states that the overall symmetric strain has to equal the volume average of the local strain or its boundary contribution, respectively. Usually, the kinematic averaging rules are evaluated applying a local Dirichlet BVP of the form

$$\Delta\mathbf{u} \quad = \quad \mathrm{grad}_M^{\,\mathrm{sym}}\mathbf{u}_M\cdot\Delta\mathbf{x} + \Delta\tilde{\mathbf{u}}. \tag{2}$$

For the additional fluctuation field $\Delta\tilde{\mathbf{u}}$, several cases can be considered:

a) $\Delta\tilde{\mathbf{u}} = \mathbf{0}\,\forall\,\Delta\mathbf{x} \in \partial V_m$. This special case represents the upper limit for the stress response of the micro volume and is commonly called Voigt limit. In general, the purely linear polynomial results in overestimated effective moduli due to clamping mechanisms at the boundary of the micro volume.

b) The fluctuation is considered to be periodic at homologous points of the micro volume surface whereas the surface traction vectors are anti-periodic. The periodic fluctuations allow the micro volume to overcome the clamping boundary conditions and to reduce the overestimated stress response of the micro volume. However, this special case requires geometrically periodic micro volumina which can not be guaranteed in general.

However there is no need to introduce polynomial loading conditions on the boundary of the micro volume. In order to circumvent the above limitations of the polynomial conditions we apply in the sequel the concept of *minimal loading conditions*, initially proposed in [12]. For this purpose, we consider eqs. (1) as integral constraints which control the deformation state of the micro volume without any further periodicity requirements. From the numerical point of view, these integral constraints can be easily implemented e. g. using a penalty formulation.

In order to circumvent too soft material response, we introduce an additional compatibility constraint. The need to do so can be easily motivated regarding Fig. 1 a), where a shear deformation mode is applied on an unit cell of a stiff grid structure (blue) embedded in a matrix (green, factor 0.0001 softer). The deformation only takes place in the soft phase, which obviously contradicts the real deformation behaviour of a periodic grid structure. However this effect can be corrected if one introduces the additional constraint that each phase has to contribute to the overall deformation according to its fraction of the boundary ∂V_m. The resulting deformation state is depicted in Fig. 1 b), c) and d) where the factor f decreases from 1 to 0.0001. For this special case, the result of the minimal loading conditions equals this one achieved applying periodic boundary conditions.

In the following we want to study the proposed minimal loading condition concept with additional compatibility constraint for an exemplary microstructure consisting of a soft matrix filled with stiff particles. The resulting deformation states under tensile and shear conditions are depicted in Figs. 2 and 3 in comparison to these ones of the Voigt (linear displacements, upper bound) and the Reuss limits (constant tractions, lower bound). In Fig. 4, the normalised strain energy of the three independent deformation modes for micro volumina with different sizes is given in relation to the upper and the lower bound.

As expected the application of the minimal constraints allow the microstructure to relax significantly compared to the Voigt limit. The observed strain energies are even closer to the Reuss than to the Voigt limit. However, this effect could be a consequence of the very special choice of the microstructure with stochastically distributed stiff particles. For more precise conclusions, a series of comparable structures should be explored which remains a task for future work.

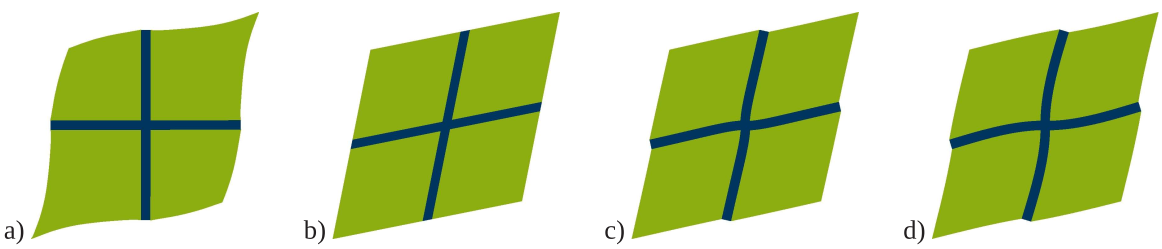

Fig. 1 Shear mode $1/2\,(u_{M1,2} + u_{M2,1})$ applied on an unit cell of a stiff grid structure (blue) in a matrix (green) which is factor f softer, a) $f = 0.0001$, no additional compatibility constraint, b) $f = 1$, c) $f = 0.01$, d) $f = 0.0001$

Copyright line will be provided by the publisher

Fig. 2 Stretch mode $u_{M1,1}$ of a micro volume ($l = 4\,\mathrm{mm}$) consisting of stiff particles (blue) in a matrix (green) which is factor $f = 0.1$ softer, a) Voigt limit (linear displacements), b) minimal boundary conditions and c) Reuss limit (constant tractions).

Fig. 3 Symmetric shear mode $1/2\,(u_{M1,2} + u_{M2,1})$ of a micro volume ($l = 4\,\mathrm{mm}$) consisting of stiff particles (blue) in a matrix (green) which is factor $f = 0.1$ softer, a) Voigt limit (linear displacements), b) minimal boundary conditions and c) Reuss limit (constant tractions).

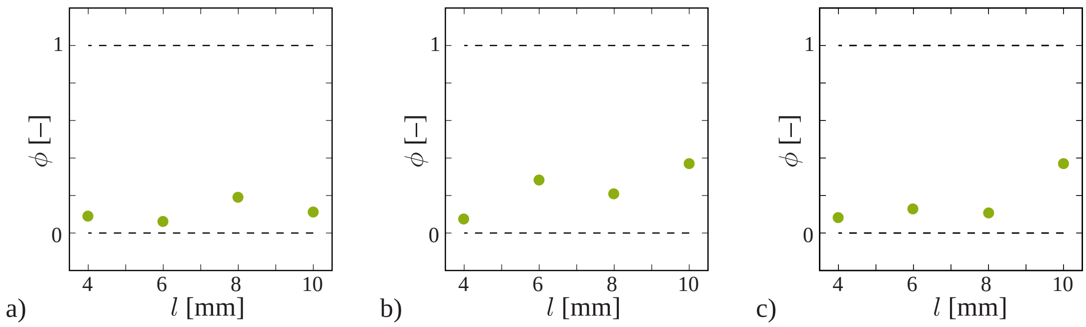

Fig. 4 Strain energy observed for different micro volumina of the size l^2 activated by the deformation modes a) $u_{M1,1}$, b) $1/2\,(u_{M1,2} + u_{M2,1})$ and c) $u_{M2,2}$. The strain energy is normalised with respect to the Voigt ($\phi = 1$) and the Reuss limit ($\phi = 0$) representing homogeneous strain (linear displacements) or constant traction boundary conditions, respectively.

3 Second order homogenisation

In the upcoming section we extend the concept of minimal loading conditions to a second order homogenisation scheme. For this reason, the kinematics of the substitute medium is enriched by additional degrees of freedom accounting for microscopic deformation mechanisms. Moreover, the second order extensions involve an internal length scale in an iherent way. In literature one can find basically two different approaches. The first one goes back to the seminal work of Mindlin [14] and introduces the second gradient of the overall displacement field as an additional and independent degree of freedom. The application of the second gradient continuum as a substitute medium for heterogeneous micro structures has been discussed in literature, e. g. [10, 11]. The second extension bases on the micromorphic continuum theory initially proposed by Eringen [3]. In contrast to the second gradient continuum, the so-called micro deformation tensor and its gradient, respectively, are introduced as independent degrees of freedom in addition to the usual displacement field. However, the micromorphic approach reduces to the second gradient concept, if the micro deformation is considered to equal the first displacement gradient. In the sequel, only the homogenisation rules for the micromorphic substitute medium will be discussed, which have been initially proposed by Forest et al. [5–9]. The kinematic averaging rules for a quadratic unit cell of the size $V_m = l^2$ read

$$\langle \Delta\mathbf{u} \rangle = \mathbf{0}, \ \mathrm{grad}_M \mathbf{u}_M = \langle \mathrm{grad}_m \Delta\mathbf{u} \rangle = \frac{1}{V_m} \int\limits_{\partial V_m} \Delta\mathbf{u} \otimes \mathbf{n} \, \mathrm{d}a, \tag{3}$$

$$\bar{\boldsymbol{\chi}}_M - \mathbf{I} = \frac{12}{l^2} \langle \Delta\mathbf{u} \otimes \Delta\mathbf{x} \rangle , \tag{4}$$

$$\mathbf{K}^3_M = \mathrm{grad}_M \bar{\boldsymbol{\chi}}_M = \frac{12}{l^2} \langle \mathrm{grad}_m (\Delta\mathbf{u} \otimes \Delta\mathbf{x}) \rangle = \frac{1}{V_m} \int\limits_{\partial V_m} \Delta\mathbf{u} \otimes \Delta\mathbf{x} \otimes \mathbf{n} \, \mathrm{d}a. \tag{5}$$

The crucial point of these relation can be observed regarding eq. (4), which can not be transformed into a surface integral. By consequence it is not possible to prescribe Dirichlet type conditions on the boundary ∂V_m [6]. In literature, several approaches are to be found [5, 7] dealing with a cubic polynomial for the microscopic displacement field. However, the displacement field has to be prescribed on the entire micro volume V_m. No reduction to its boundary ∂V_m is known, besides some special cases of regular grid structures [8, 9]. Thus, we propose to apply the concept of minimal loading condition for the second order homogenisation scheme. Besides the lacking periodic requirements this concept bears the advantage of circumventing a priori the formulation of any polynomial conditions. Eqs. (3–5) represent the minimal set of integral constraints enforcing the micro volume to undergo deformation modes driven by the overall kinematic quantities. Again, this concept can be easily implemented from a numerical point of view making use of a penalty formulation for instance.

In Fig. 5, several exemplary micromorphic deformation modes are given. The found results (Cosserat micro rotations of regular grid structures and bending mode of orthotropic unit cell) have been observed in literature [6, 8] applying polynomial loading conditions.

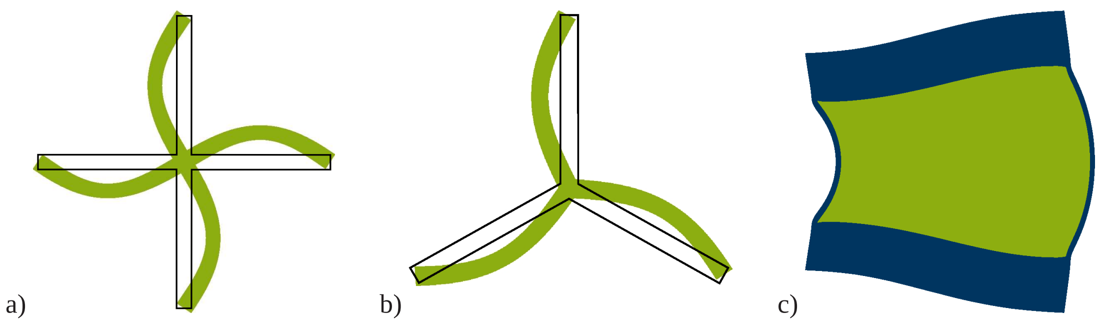

Fig. 5 The Cosserat type micro rotation $\bar{\varphi}_{M3} = \bar{\chi}_{M21} = -\bar{\chi}_{M12} = 1$, applied on the unit cells of a) the squared grid and b) the honeycomb structure. The Cosserat bending mode $\bar{\varphi}_{M3,2} = -K_{M122} = 2\,K_{M122} = 2\,K_{M121} = 1/\mathrm{mm}$, applied on the orthotropic unit cell c).

4 Conclusions

Finally, let us recall the basic findings of the present contribution addressing numerical homogenisation schemes. A general concept for the formulation of minimal loading conditions in terms of integral constraints on the micro volume has been introduced. In the case of first order homogenisation this procedure bears the advantage that no periodicity requirements exist on the geometry of the micro volume. In principle, even the shape of the micro volume can be chosen arbitrary and does not have to be necessarily chosen quadratic. Comparing the strain energy stored during unit deformations of heterogeneous micro volumina it has been found the minimal loading conditions, enriched with an additional compatibility constraint, to result in significantly softer material responses than the Voigt limit representing the upper bound on the homogenised strain energy.

In the very last section, the concept of minimal loading conditions has been extended to the second order homogenisation technique for micromorphic media substituting a heterogeneous Cauchy medium on the micro scale. Due to the extensions of the volume averaging concept it is no longer possible to formulate Dirichlet conditions on the boundary of the micro volume besides some special cases. For this reason, the averaging rules themselves have been used again as the minimal loading conditions for the micro volume. In comparison to the deformation behaviour of different structures, the resulting deformation modes can be validated qualitatively to examples given in literature.

In the future, further efforts have to be made in order to gain a deeper understanding of the proposed concept. Quantitative validations are planned. Finally, we intend to generalise the concept to 3D problems dealing with micro volumina resulting from CT analyses of real micro structures.

Copyright line will be provided by the publisher

References

[1] A. Aşkar and A. S. Çakmak, Int. J. Engng. Sci., **6**, 583 (1968).
[2] S. Diebels and H. Steeb, Proc. R. Soc. Lond. A, **458**, 2869 (2002).
[3] A. C. Eringen and E. S. Suhubi, Int. J. Engng. Sci., **2**, 189 (1964).
[4] F. Feyel and J. L. Chaboche, Comp. Meth. Appl. Mech. Eng., **183**, 309 (2000).
[5] S. Forest and K. Sab, Mech. Res. Commun. **25**, 449 (1998).
[6] S. Forest and D. K. Trinh, Z. Angew. Math. Mech. **90**, 90 (2011).
[7] R. Jänicke, S. Diebels, H. G. Sehlhorst and A. Düster, Continuum Mech. Therm., **21**, 297 (2009).
[8] R. Jänicke, Micromorphic media: Interpretation by homogenisation (Shaker, Aachen, 2010).
[9] R. Jänicke and H. Steeb, Comp. Mat. Science, DOI: 10.1016/j.commatsci.2011.04.011 (2011).
[10] L. Kaczmarczyk, C. J. Pearce and N. Bićanić, Int. J. Numer. Meth. Eng. **74**, 506 (2008).
[11] V. G. Kouznetsova and M. G. D. Geers and W. A. M. Brekelmans, Int. J. Numer. Meth. Eng. **54**, 1235 (2002).
[12] S. D. Mesarovic and J. Padbidri, Phil. Mag. **85**, 65 (2005).
[13] C. Miehe and A. Koch, Arch. Appl. Mech. **72**, 300 (2002).
[14] R. D. Mindlin, Arch. Rat. Mech. Anal. **16**, 51 (1964).
[15] A. S. Phani and J. Woodhouse and N. A. Fleck, J. Acoust. Soc. Am., **119**, 1995 (2006).
[16] H. G. Sehlhorst and R. Jänicke and A. Düster and E. Rank and H. Steeb and S. Diebels, Comp. Mech., **45**, 45 (2009).
[17] C. Tekoğlu and P. R. Onck, J. Mat. Sci. **40**, 5911 (2005).

Copyright line will be provided by the publisher