 CMC, vol.4, no.2, pp.55-62, 2006

Enforcing Boundary Conditions in Micro-Macro Transition for Second Order Continuum

Łukasz Kaczmarczyk[1]

Abstract: In recent years the multiscale computational homogenisation has been extensively developed. Such micro-macro modelling does not require any constitutive assumptions at the macro-level. The multi-scale computational homogenisation has also been extended for the second order continuum at the macro level Kouznetsova V.G., Geers M.G.D., and Brekelmans V.A.M (2004). The second-order framework is based on incorporation of the gradient of macroscopic deformation in micro to macro multiscale transition. The introduction of the second-order continuum at macro-scale takes into account the size effect and gives more accurate results in case of insufficient scale separation. The general framework of computational homogenisation has been presented in Kouznetsova V.G (2002).

keyword: computational homogenisation, second order continuum, intrinsic length scale

1 Introduction

In this paper the well-known framework of linking material properties at two levels of description is be presented. The materials are heterogeneous on one level (microscale), while the material is considered as homogeneous at macroscale level of observation. Typical examples of homogeneous material include metal alloys systems, porous media, policristaline materials and composites, i.e textile reinforced composites Haasemann G., Kästner M., and Ulbricht V. (2006), reinforced composite laminates Zhang Y. and Xia Z. (2005). Moreover, all materials, are heterogeneous at a certain scale, i.e nanoscale Shengping Shen S. and Atluri S. N. (2004). There are a number of strategies that are used in multiscale analysis, in this paper we consider a numerical approach, i.e. computational homogenisation (fig. 1). This micro-macro modelling does not led to closed form overall constitutive equations, insted it determines the stress-strain relation at every point of interest at macroscale by detailed modelling of microstructure attached to that point.

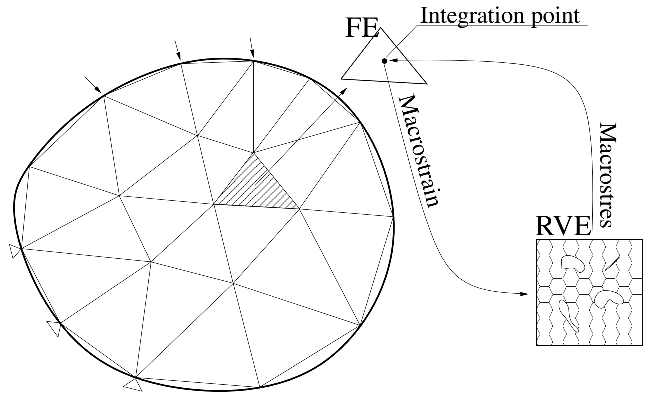

Figure 1 : Computational homogenisation

After Feyel F. (2003), multiscale models are constructed using three main ingredients (fig. 2):

1. a modelling of mechanical behaviour at microscale (the representative volume element RVE)
2. a localisation rule which determines the local solution inside the RVE, for given macroscopic deformation measures
3. a homogenisation rule giving the macroscopic stress measures, knowing the micromechanical stress state.

In Section 2 the boundary equations as well as macrostrain and macrostress expressed in terms displacements and traction forces on the boundary of RVE are given. In Section 3 after finite element discretisation and with deformation driven microstructures, the overall stresses and tangent moduli are exclusively defined in terms of discrete forces and stiffness properties of RVE. To enforce boundary conditions and to compute stresses and tangent moduli the projection matrices are used. Next the analytical solution of the stress-strain relation for a special case

[1] e-mail: *likask@twins.pk.edu.pl*, Institute of Computer Methods in Civil Engineering, Cracow University of Technology, Poland.

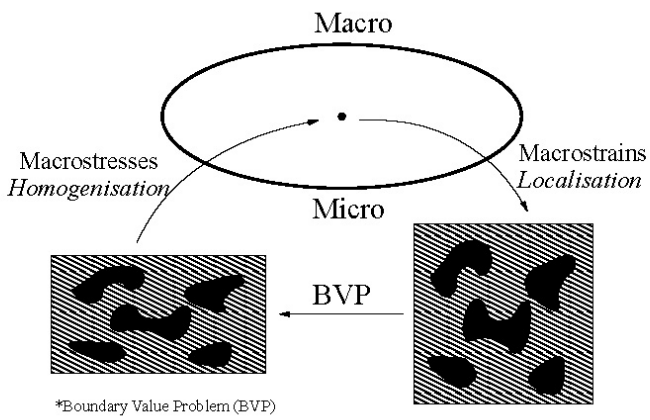

Figure 2 : Computing inhomogeneous material response

of homogeneous material with intrinsic length scale will be given. In Subsection 5 a numerical solution of a bending problem for a material with titanium matrix and silicon cabride fibres for (first-order and second-order homogenisation) will be presented. At the end conclusions are presented.

2 Macro to micro and micro to macro transitions

This paper concentrates on some issues of the fully coupled second order homogenisation scheme. Attention is focused on micro-macro transitions of the discretised microstructure. In the present paper a new approach is proposed which can handle any type of boundary conditions (i.e. displacement, periodic and static). The boundary conditions enforce the deformation of representative volume element (RVE) according to a given gradient and second gradient of displacements in average sense. We note that the method is used to couple two different continua: classical one at the microscale, and Mindlin's continuum Mindlin R.D (1965) at the macroscale. After expansion of the displacement vector at the geometric centre of RVE and truncation after second order term we obtain

$$\mathbf{u}(\mathbf{X},\mathbf{x}) = \mathbf{u}^0(\mathbf{X}) + \mathbf{x}\cdot\bar{\boldsymbol{\varepsilon}}(\mathbf{X}) + \frac{1}{2}\mathbf{x}\otimes\mathbf{x} : \bar{\boldsymbol{\eta}}(\mathbf{X}) + \mathbf{r}(\mathbf{X},\mathbf{x}), \quad (1)$$

where $\bar{\boldsymbol{\varepsilon}} = \mathrm{sym}[\mathrm{grad}[\mathbf{u}]]$ is macrostrain tensor, $\bar{\boldsymbol{\eta}} = \mathrm{grad}[\mathrm{grad}[\mathbf{u}]]$ is second-order macroscopic strain tensor, $\mathbf{r}$ is the microfluctuation of displacement added to fulfill equilibrium equation in RVE.

The boundary conditions can be written in a integral form as

$$\int_\Gamma \delta\mathbf{t}\cdot\mathbf{r}\,\mathrm{d}\Gamma = 0,\ \int_\Gamma \mathbf{n}\otimes\mathbf{r}\,\mathrm{d}\Gamma = \mathbf{0},\ \int_\Gamma \mathbf{n}\otimes\mathbf{x}\otimes\mathbf{r}\,\mathrm{d}\Gamma = \mathbf{0}, \quad (2)$$

where $\mathbf{n}$ is the normal vector field and $\delta\mathbf{t}$ is statically admissible variation of tractions on the boundary. If the first integral satisfies the Hill-Mandel theorem, the second and third integral enforce the deformation of RVE according to a given macrostrain tensor and given gradient of macrodeformation tensor in an average sense, correspondingly. For a further FE discretisation the boundary conditions can be expressed in terms of microscopic displacement tensor and macrostrains

$$\int_\Gamma \delta\mathbf{t}\cdot(\mathbf{u} - \mathbf{x}\cdot\bar{\boldsymbol{\varepsilon}} - \frac{1}{2}\mathbf{x}\otimes\mathbf{x} : \bar{\boldsymbol{\eta}})\,\mathrm{d}\Gamma = 0, \quad (3)$$

$$\int_\Gamma \mathbf{n}\otimes(\delta\mathbf{u} - \mathbf{x}\cdot\bar{\boldsymbol{\varepsilon}} - \frac{1}{2}\mathbf{x}\otimes\mathbf{x} : \bar{\boldsymbol{\eta}})\,\mathrm{d}\Gamma = \mathbf{0}, \quad (4)$$

$$\int_\Gamma \mathbf{n}\otimes\mathbf{x}\otimes(\delta\mathbf{u} - \mathbf{x}\cdot\bar{\boldsymbol{\varepsilon}} - \frac{1}{2}\mathbf{x}\otimes\mathbf{x} : \bar{\boldsymbol{\eta}})\,\mathrm{d}\Gamma = \mathbf{0}. \quad (5)$$

For completeness, the macroscopic strain and stress measures in terms of microquantities are given. For a statistically homogeneous body macroscopic quantities can be defined as averages microquantities over volume RVE Nemat-Nasser S. and Horoi M (1999), for simplicity for geometrically linear problem and quadratic RVE, we have

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{V}\int_\Gamma \mathbf{n}\otimes\mathbf{u}\,\mathrm{d}\Gamma, \quad \bar{\boldsymbol{\sigma}} = \frac{1}{V}\int_\Gamma \mathbf{x}\otimes\mathbf{t}\,\mathrm{d}\Gamma, \quad (6)$$

$$\frac{1}{2}\int_V (\mathbf{x}\otimes\mathbf{x}\otimes\mathbf{1} + \mathbf{x}\otimes\mathbf{1}\otimes\mathbf{x} + \mathbf{1}\otimes\mathbf{x}\otimes\mathbf{x})\,\mathrm{d}V : \bar{\boldsymbol{\eta}} = \int_\Gamma \mathbf{n}\otimes\mathbf{x}\otimes\mathbf{u}\,\mathrm{d}\Gamma, \quad (7)$$

$$\bar{\boldsymbol{\tau}} = \frac{1}{2V}\int_\Gamma \mathbf{x}\otimes\mathbf{x}\otimes\mathbf{t}\,\mathrm{d}\Gamma, \quad (8)$$

where $\bar{\boldsymbol{\sigma}}$ is second-order macrostress tensor work-conjugate to $\bar{\boldsymbol{\varepsilon}}$, $\bar{\boldsymbol{\tau}}$ is third-order macrostress tensor work-conjugate to $\bar{\boldsymbol{\eta}}$. It can be noted that macro quantities are given exclusively by displacements and traction forces on the boundary of RVE. According to Hill-Mandel theorem it can be shown that for the given equations the work of macrostrains on macrostresses is equal to the work of microstrains on microstresses in the RVE attached to a macroscopic point.

3 Finite element discretisation and enforcing boundary conditions for RVE

The application of boundary conditions and other constraints to the stiffness matrix and load vector is an integral part of finite element code. This process can present difficulties when certain combinations of boundary conditions for RVE occur. A general approach to the problem of enforcing constraints for any finite element code is shown in Ainsworth M (2001).

After FE discretisation of RVE for nodal displacement $\mathbf{u}$ is defined to be a solution of the constrained quadratic programming problem:

$$\begin{aligned} &\min_{\mathbf{u}} \quad Q = \frac{1}{2}\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} - \mathbf{u}^{\mathrm{T}}\mathbf{F}, \\ &\quad \text{subject to} \quad \mathbf{C}\mathbf{u} - \mathbf{g} = \mathbf{0}, \end{aligned} \tag{9}$$

where $\mathbf{K}$ is stiffness matrix, $\mathbf{F}$ is load vector, $\mathbf{C}$ is constraint matrix and $\mathbf{g}$ is displacement constraint vector. The common solution method is to introduce Lagrange multipliers $\boldsymbol{\lambda}$:

$$\mathcal{L} = \frac{1}{2}\mathbf{u}^{\mathrm{T}}\mathbf{K}\mathbf{u} - \mathbf{u}^{\mathrm{T}}\mathbf{F} + \boldsymbol{\lambda}^{\mathrm{T}}(\mathbf{C}\mathbf{u} - \mathbf{g}). \tag{10}$$

The Euler conditions for the stationary point of the Lagrangian are found to be

$$\mathbf{K}\mathbf{u} + \mathbf{C}^{\mathrm{T}}\boldsymbol{\lambda} = \mathbf{F},$$

$$\mathbf{C}\mathbf{u} = \mathbf{g}. \tag{11}$$

However, this solution approach increases the number of unknowns and the character of the matrix is altered (to an indefinite saddle point problem). The numerical solution of such problem is inefficient, so is not adequate for solving computationally complex multiscale problems where for each Gauss integration point the solution of the constrained quadratic problem has to be found.

In papers Miehe C. and Koch A (2002); Kouznetsova V.G., Geers M.G.D., and Brekelmans W.A.M (2004) the solution for micro-to-macro transition of discretised microstructure by the computation of condensed matrices associated with the boundary of RVE can be found. In this paper an alternative approach for solving such problems in case second order homogenisation is presented. Under the assumption that the problem is well-posed the following matrices are well defined

$$\mathbf{Q} = \mathbf{I} - \mathbf{R}\mathbf{C}, \tag{12}$$

$$\mathbf{R} = \mathbf{C}^{\mathrm{T}}(\mathbf{C}\mathbf{C}^{\mathrm{T}})^{-1}. \tag{13}$$

where $\mathbf{R}$ is auxiliary matrix and $\mathbf{Q}$ is projection matrix. If matrix $\widetilde{\mathbf{K}}$ and right hand vector $\widetilde{\mathbf{F}}$ are defined by expressions

$$\widetilde{\mathbf{K}} = \mathbf{C}^{\mathrm{T}}\mathbf{C} + \mathbf{Q}^{\mathrm{T}}\mathbf{K}\mathbf{Q}, \tag{14}$$

$$\widetilde{\mathbf{F}} = \mathbf{C}^{\mathrm{T}}\mathbf{g} + \mathbf{Q}^{\mathrm{T}}(\mathbf{F} - \mathbf{K}\mathbf{R}\mathbf{g}). \tag{15}$$

there exists a unique solution $\mathbf{u}$ of the problem (9)

$$\widetilde{\mathbf{K}}\mathbf{u} = \widetilde{\mathbf{F}}, \tag{16}$$

and the Lagrange multipliers are given by

$$\boldsymbol{\lambda} = \mathbf{R}^{\mathrm{T}}(\mathbf{F} - \mathbf{K}\mathbf{u}). \tag{17}$$

Matrix $\widetilde{\mathbf{K}}$ involves of computation the global stiffness matrix $\mathbf{K}$. However, in practical computations there is no obligation to preform global operations on matrices, or to assemble global matrix $\mathbf{K}$.Enforcing constraints can be performed element by element subassembly procedure.Ainsworth M (2001).

This approach enables one to apply any boundary condition, e.g. displacement, periodic or traction boundary conditions on the boundary of RVE. This method can also easily be applied to any shape of RVE.

3.1 Matrix form of boundary conditions

After FE discretisation of RVE the boundary conditions (3-5) can be written in a matrix form as:

$$\mathbf{C}\mathbf{u} = \mathbf{D}\bar{\boldsymbol{\varepsilon}} + \mathbf{E}\bar{\boldsymbol{\eta}} = \mathbf{g}, \tag{18}$$

matrices $\mathbf{C}$ is given by

$$\mathbf{C} = \int_{\Gamma} \mathbf{H}\mathbf{N}^{\mathrm{T}}\mathbf{N}\,\mathrm{d}\Gamma, \tag{19}$$

where matrix $\mathbf{D}$ and $\mathbf{E}$ are given by

$$\mathbf{D} = \int_{\Gamma} \mathbf{H}\mathbf{N}^{\mathrm{T}}\mathbf{X}\,\mathrm{d}\Gamma, \tag{20}$$

$$\mathbf{E} = \int_{\Gamma} \mathbf{H}\mathbf{N}^{\mathrm{T}}\mathbf{Z}\,\mathrm{d}\Gamma, \tag{21}$$

$\mathbf{N}$ is the matrix of shape functions and matrices $\mathbf{X}$ and $\mathbf{Z}$ are defined by

$$\mathbf{X} = \frac{1}{2}\begin{bmatrix} 2x & 0 & y \\ 0 & 2y & x \end{bmatrix}, \tag{22}$$

$$\mathbf{Z} = \frac{1}{4} \begin{bmatrix} 2x^2 & 0 & 2y^2 & 0 & xy & 0 \\ 0 & 2y^2 & 0 & 2x^2 & 0 & xy \end{bmatrix}. \tag{23}$$

In each row of matrix $\mathbf{H}$ there are nodal values of admissible distribution of traction forces on the boundary of RVE. For example in the case of first order homogenisation and periodic boundary conditions all antiperiodic and self-equilibred boundary conditions are admissible. Matrix $\mathbf{H}$ contains nodal values of all linearly independent antiperiodic self-equlibred distributions of traction on the boundary of RVE.

3.2 Computation stress and higher order stress

If the equilibrium equation is fullfield, the work of displacements on tractions is equal to the work of generalised displacements on Lagrange multipliers:

$$\mathbf{u}^{\mathrm{T}}\mathbf{t} = (\mathbf{D}\overline{\boldsymbol{\varepsilon}} + \mathbf{E}\overline{\boldsymbol{\eta}})^{\mathrm{T}}\boldsymbol{\lambda}, \tag{24}$$

After the solution of boundary value problem according to Hill-Mandel theorem, the first order macrostress vector is given in terms of the Lagrange multiplier vector and matrix $\mathbf{D}$:

$$\overline{\boldsymbol{\sigma}} = \frac{1}{V}\mathbf{D}^{\mathrm{T}}\boldsymbol{\lambda} \tag{25}$$

and the second order macrostress vector is given in terms of the Lagrange multiplier vector and matrix $\mathbf{E}$:

$$\overline{\boldsymbol{\tau}} = \frac{1}{V}\mathbf{E}^{\mathrm{T}}\boldsymbol{\lambda}. \tag{26}$$

3.3 Computation of tangent matrices

Close-form stress-strain relation is unknown at all stages of the computational homogenisation approach. For the finite element method at the macro level only the material tangent stiffness matrices and stress vectors or increments of strain vectors have to be determined at each Gauss integration point. The linearised relation between strain increments and stress increments stress for the second order continuum are given by

$$\Delta\overline{\boldsymbol{\sigma}} = \overline{\mathbf{C}}^1\Delta\overline{\boldsymbol{\varepsilon}} + \overline{\mathbf{C}}^2\Delta\overline{\boldsymbol{\eta}}, \tag{27}$$

$$\Delta\overline{\boldsymbol{\tau}} = \overline{\mathbf{C}}^3\Delta\overline{\boldsymbol{\varepsilon}} + \overline{\mathbf{C}}^4\Delta\overline{\boldsymbol{\eta}}. \tag{28}$$

To compute tangent stiffness matrices, $(3+6+3+6)$ linear equations at equilibrium for each RVE have to be solved. For example material tangent stiffness matrix $\overline{\mathbf{C}}^1$ is computed as the:

$$\overline{\mathbf{C}}^1 = [\delta\overline{\boldsymbol{\sigma}}^1, \delta\overline{\boldsymbol{\sigma}}^2, \delta\overline{\boldsymbol{\sigma}}^3]. \tag{29}$$

where columns $\delta\overline{\boldsymbol{\sigma}}^i$, $i = 1,2,3$ are computed for given increments of the strain vectors

$$\begin{array}{llll} \delta\overline{\boldsymbol{\sigma}}^1: & \text{for} & \delta\overline{\boldsymbol{\varepsilon}} = [1\,0\,0]^{\mathrm{T}}, & \delta\overline{\boldsymbol{\eta}} = [0\,0\,0\,0\,0\,0]^{\mathrm{T}}, \\ \delta\overline{\boldsymbol{\sigma}}^2: & \text{for} & \delta\overline{\boldsymbol{\varepsilon}} = [0\,1\,0]^{\mathrm{T}}, & \delta\overline{\boldsymbol{\eta}} = [0\,0\,0\,0\,0\,0]^{\mathrm{T}}, \\ \delta\overline{\boldsymbol{\sigma}}^3: & \text{for} & \delta\overline{\boldsymbol{\varepsilon}} = [0\,0\,1]^{\mathrm{T}}, & \delta\overline{\boldsymbol{\eta}} = [0\,0\,0\,0\,0\,0]^{\mathrm{T}}. \end{array} \tag{30}$$

We can that only the right hand side of the linear equations is different for each case, so after the decomposition of left hand side of linear equations the computation of tangent stiffness matrices can be made efficient.

4 Analitical solution for stress-strain relation

In this a special case of homogeneous Hooke's material with intrinsic length scale L section is considered. First and second order approach is elaborated in terms of finite element solution procedure. The approximation space of 9-node finite element contains the solution for the displacement field for quadratic RVE of size L. The stiffness matrix for 9-node FE and auxiliary matrices are computed analytically and after enforcing traction boundary conditions, from equations given in former sections tangent stiffens matrices were computed.

For tangent material matrix $\overline{\mathbf{C}}^1$ the Hooke's equations are recovered

$$\begin{bmatrix} \overline{\sigma}_{11} \\ \overline{\sigma}_{22} \\ \overline{\sigma}_{12} \end{bmatrix} = \begin{bmatrix} \lambda+2\mu & \lambda & 0 \\ \lambda & \lambda+2\mu & 0 \\ 0 & 0 & 2\mu \end{bmatrix} \begin{bmatrix} \overline{\varepsilon}_{11} \\ \overline{\varepsilon}_{22} \\ 2\overline{\varepsilon}_{12} \end{bmatrix}. \tag{31}$$

It can be noted that the solution does not depend on L, since for the first-order homogenisation approach we assume that the intrinsic length size is infinitesimally small comparing to the characteristic size of a structure at macroscale of observation. Higher order tangent matrix

$\overline{\mathbf{C}}^4$ is computed analytically as

$$[\overline{\tau}_{111},\overline{\tau}_{222},\overline{\tau}_{221},\overline{\tau}_{112},\overline{\tau}_{121},\overline{\tau}_{122}]^{\mathrm{T}}$$
$$= d\begin{bmatrix} a & 0 & -a & 0 & 0 & -b \\ 0 & a & 0 & -a & -b & 0 \\ -a & 0 & a & 0 & 0 & b \\ 0 & -a & 0 & a & b & 0 \\ 0 & -b & 0 & b & c & 0 \\ -b & 0 & b & 0 & 0 & c \end{bmatrix}\begin{bmatrix} \overline{\eta}_{111} \\ \overline{\eta}_{222} \\ \overline{\eta}_{221} \\ \overline{\eta}_{112} \\ 2\overline{\eta}_{121} \\ 2\overline{\eta}_{122} \end{bmatrix}, \tag{32}$$

where:

$$a = L^2(2\mu+\lambda)/2, \quad b = L^2\mu,$$

$$c = L^2(3\mu+\lambda), \quad d = \frac{\mu}{3(4\mu+\lambda)}. \tag{33}$$

The higher order tangents $\overline{\mathbf{C}}^2$ and $\overline{\mathbf{C}}^3$ are both zero for the problem considered. We note that higher order tangent matrix $\overline{\mathbf{C}}^4$ for the second-order continuum clearly depends on size L of the RVE considered, since higher-order homogenisation approach is able to take into account size effects.

The analytically derived stiffness matrices for periodic and traction boundary conditions are the same for the considered problem, since if material is homogeneous microfluctuation of displacement field is zero for each point in RVE.

In the case of displacement boundary conditions an analytical solution is difficult to obtain, since microfluctuation field of displacement contains higher order polynomials. Thus, for homogeneous material higher order macrostress $\overline{\boldsymbol{\tau}}$ is dependent on type the of boundary conditions. It can not be treated as inconsistency because it can be shown that for statically admissible strain $\overline{\boldsymbol{\varepsilon}}$ and higher order strain $\overline{\boldsymbol{\eta}}$ (at macro level of observation) the microfluctuation of displacements vanishes for the given problem.

It must be added that for a centrosymmetric material the Mindlin's model not can be recovered, because quadratic RVE exhibits only four symmetries.

5 Numerical example

An academic type example of this framework is discused in this section, following the results obtained by Feyel F. (2003) for Cosserat continuum. Let us consider the following plane strain problem: a long fibre square composite structure in fig. 3. The size of the structure is supposed to be 3mm whereas the unit cell is 0.5mm and radius of fibre is 0.15mm. The mechanical response of the structure is computed in three different ways, i.e. direct solution, the mesh has 41735 degrees of freedom (left mesh for the direct solution in fig. 3) and two multiscale approaches (right mesh for multiscale solution in fig. 3). In the case of computational homogenisation approach at macro scale classical and gradient continuum are considered. Classical displacement 9-node FE and mixed Q18G16L4 Shu J.Y., King W.E., and Fleck N.A

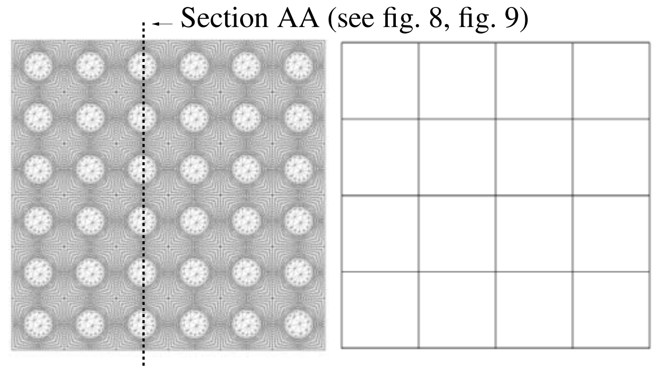

Figure 3 : Discretisation for direct computation and reference mesh (left), discretisation for multiscale model.

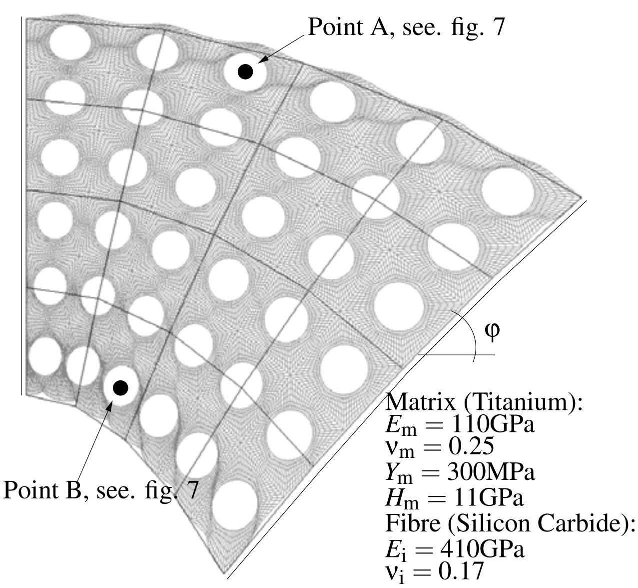

Figure 4 : Deformation for direct solution method and multiscale solution method.

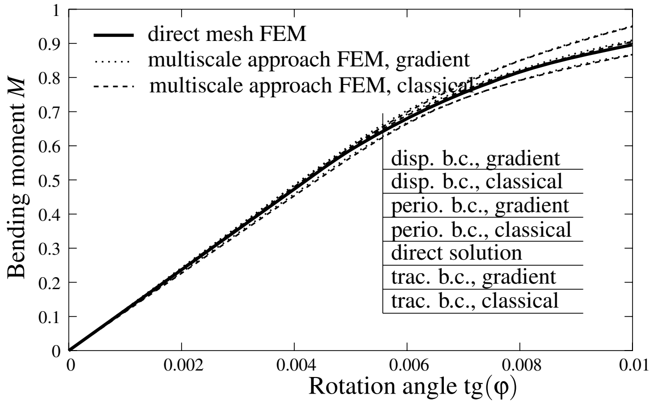

Figure 5 : Equilibrium paths for direct solution and classical, gradient continuum with displacement, periodic and traction boundary conditions

(1999) FE for classical continuum and Mindlin's continuum is used correspondingly.

We use a simple material model for titanium matrix of the microstructure - isotropic J2 plasticity with linear hardening. For both matrix and silicon carbide fibre the elastic response is described by Hooke's law, see fig. 4.

The structure is subjected to bending load. Deformation of reference (direct) solution and multiscale solution is presented in fig. 4. In the case of direct and first order computational homogenisation, the application of boundary conditions at macro level of observation is straightforward. On the left edge the nodal displacements in horizontal direction are blocked. On the right edge the horizontal displacements are applied according to given rotation angle φ. For second order continuum at the macro scale of observation the higher order boundary conditions on gradients of displacements have to be applied. On left the edge nonsymmetric part displacement of gradient is set to zero (micro rotation was blocked). On right hand side nonsymmetrical part displacement gradient was applied according to the to given rotation angle φ.

In fig. 5 the equilibrium paths for reference solution and two multiscale approaches, for tree types of boundary conditions each, are shown. A surprisingly good agreement between the reference diagram and the multiscale approach, even for first order homogenisation framework is noticed. The homogeneous displacement and stress boundary conditions provide the upper and lower bounds on the response. The solution for the periodic deformation lies between them.

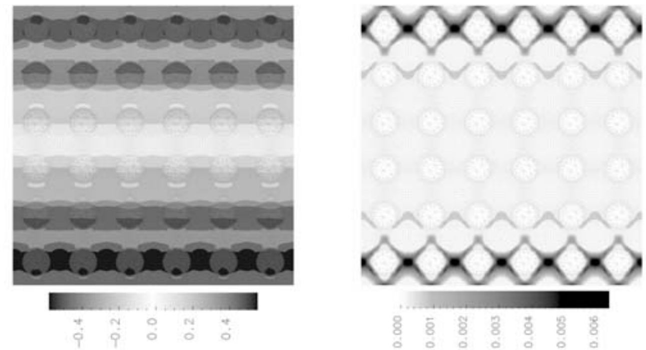

Figure 6 : Distribution of microstress σ_x (left) and distribution of equivalent plastic strain (right).

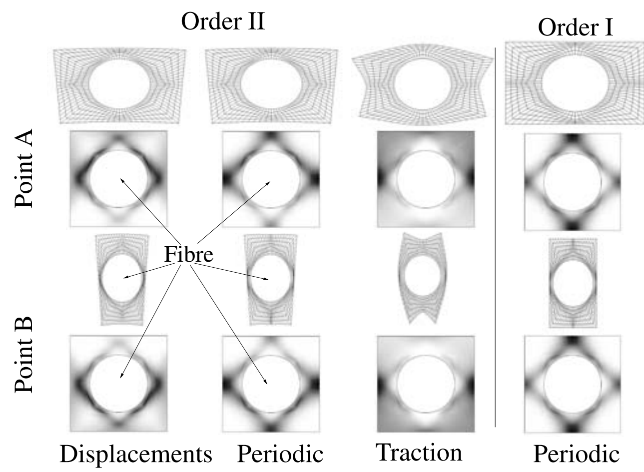

Figure 7 : Deformation of RVE and distribution of equivalent plastic strain in RVE. Position of macroscopic point A and point B in fig. 4

The distribution of stress component σ_x and of the equivalent plastic strain for the reference solution are presented in fig. 6. Deformation of RVE and distribution of microscopic equivalent plastic strain can be seen in fig. 7. First order homogenisation solution not can take into account the gradient of displacement so RVE does not bend. Second order homogenisation solution takes into account size effect since the RVE is bending. The distribution of equivalent plastic strain for given RVE is the same as for the reference solution in the case of displacement and periodic boundary conditions. It can be noted that the solution for traction boundary conditions gives inadequate RVE deformation and the distribution of equivalent plastic strain.

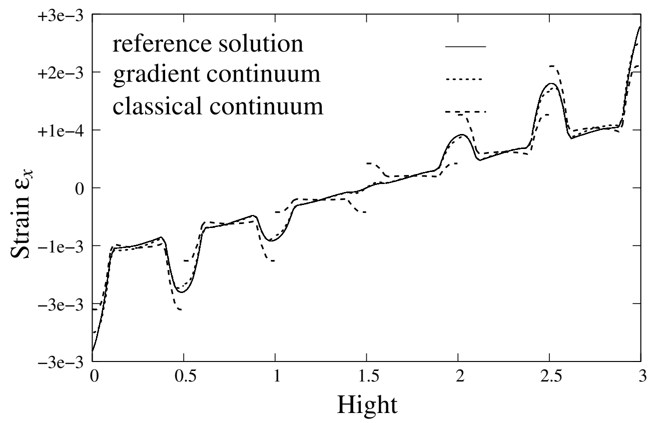

Figure 8 : Distribution of microstrain on along section AA for rotation angle $\text{tg}(\varphi) = 0.0005$.

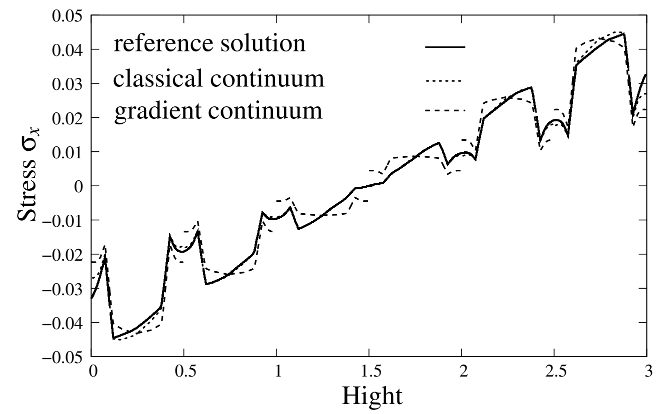

Figure 9 : Distribution of microstress along section AA for rotation angle $\text{tg}(\varphi) = 0.0005$.

Fig. 8 and 9 show the distribution of strain ε_x and stress σ_x along section AA (see fig. 3), correspondingly. The comparison of reference solution and displacement boundary conditions in the case of gradient continuum and classical continuum shows very good agreement except of boundary edges. In the case of first order homogenisation approach an inability to take in account the gradient of displacements can be observed.

6 Conclusions

Computational homogenisation can be used to couple two different continuum at macro scale, classical and gradient. The advantage of second order homogenisation framework is that is allows one to escape from the classical assumption of scale separation. Taking into account size effects enables us to use multiscale models when the size of RVE does not vanish. Moreover, when localisation takes place the results should be meaningful.

In the paper the method of enforcing boundary condition for micro-to-macro transitions has been proposed. This method enables us to enforce any type of boundary conditions consistent with Hill-Mandel theorem. Moreover, it cat be applied to any shape of RVE which enables us to model effective material with different number of symmetries.

7 Acknowledgements

Financial supports of the Polish Ministry of Scientific Research and Information Technology Society, grants: No. 4 T07E 060 29 "Coupling of FEM and ANNs in The Analysis of Solids with Microstructure and Structures of Unknown Constitutive Equations", is gratefully acknowledged.

References

Ainsworth M (2001): Essential boundary conditions and multi-point constraints in finite element analysis. *Comput. Methods, Appl. Mech. Engrg,*, vol. 190, no. 2001, pp. 6323–6339.

Feyel F. (2003): A multilevel finite element method (FE2) to describe the response of highly non-linear structures using generalized continua. *Comput. Methods Appl. Mech. Engrg.*, , no. 192, pp. 3233–3244.

Haasemann G.; Kästner M.; Ulbricht V. (2006): Multi-Scale Modelling and Simulation of Textile Reinforced Materials. *CMC: Computers, Material & Continua*, vol. 3, no. 3, pp. 131–146.

Kouznetsova V.G (2002): *Computational homogenization for the multi-scale analysis of multi-phase materials*. PhD thesis, Technishe Universiteit, Eindhoven, 2002.

Kouznetsova V.G.; Geers M.G.D.; Brekelmans V.A.M (2004): Multi-scale second-order computational homogenization of multi-phase materials: a nested finite element solution strategy. *Comput. Methods Appl. Mech. Engrg.*, vol. 194, no. 2004, pp. 5525–5550.

Kouznetsova V.G.; Geers M.G.D.; Brekelmans W.A.M (2004): Size of a representative volume element in a second-order computational homogenization framework. *International Journal for Multiscale Computational Engineering*, vol. 2, no. 4, pp. 575–598.

Miehe C.; Koch A (2002): Computational micro-to-macro transitions of discretized microstructures undergoing small strains. *Archive of Applied Mechanics*, vol. 72, no. 2002, pp. 300–317.

Mindlin R.D (1965): Second gradient of strain and surface-tension in linear elasticity. *International Journal of Solids and Structures*, vol. 1, pp. 417–438.

Nemat-Nasser S.; Horoi M (1999): *Micromechanics: overall properties of heterogeneous materials*. Elsevier.

Shengping Shen S.; Atluri S. N. (2004): Computational Nano-mechanics and Multi-scale Simulation. *CMC: Computers, Materials & Continua*, vol. 1, no. 1, pp. 59–90.

Shu J.Y.; King W.E.; Fleck N.A (1999): Finite element for materials with strain gradient effects. *International Journal For Numerical Methods in Engineering*, vol. 44, no. 1999, pp. 373–391.

Zhang Y.; Xia Z. (2005): Micromechanical Analysis of Interphase Damage for Fiber Reinforced Composite Laminates. *CMC: Computers, Materials & Continua*, vol. 2, no. 3, pp. 213–226.