MULTI-SCALE SECOND-ORDER COMPUTATIONAL HOMOGENIZATION OF HETEROGENEOUS MATERIALS

V. Kouznetsova*,**, M.G.D. Geers**, W.A.M. Brekelmans**

* *Netherlands Institute for Metals Research, Rotterdamseweg 137, 2628 AL Delft, The Netherlands*

** *Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands*

Summary A novel second-order computational homogenization scheme suitable for a multi-scale modelling of macroscopic localization and size effects is proposed. The second-order scheme is an extension of the classical first-order computational homogenization framework and is based on a proper incorporation of the gradient of the macroscopic deformation gradient tensor and the associated higher-order stress measure into the macro-micro scale transition. The applicability of the approach is illustrated by several examples.

INTRODUCTION

Most of the materials produced and utilized in industry are heterogeneous on one or another spatial scale. Typical examples include metal alloy systems, porous media, polycrystalline materials and composites. The different phases present in such materials constitute a material microstructure. The (possibly evolving) size, shape, physical properties and spatial distribution of the microstructural constituents largely determine the macroscopic, overall behaviour of these multi-phase materials.

COMPUTATIONAL HOMOGENIZATION

To predict the macroscopic behaviour of heterogeneous materials various homogenization techniques are typically used. However, most of the existing homogenization methods are not suitable for large deformations and complex loading paths and cannot account for an evolving microstructure. To overcome these problems a computational homogenization approach has been developed, which is essentially based on the solution of two (nested) boundary value problems, one for the macroscopic and one for the microscopic scale. Techniques of this type (i) do not require any constitutive assumption with respect to the overall behaviour; (ii) enable the incorporation of large deformations and rotations on both the micro and macrolevel; (iii) are suitable for arbitrary material behaviour, including physically non-linear and time dependent behaviour; (iv) provide the possibility to introduce detailed microstructural information, including a physical and/or geometrical evolution of the microstructure, in the macroscopic analysis and (v) allow the use of any modelling technique at the microlevel. Existing *first-order computational homogenization* schemes [1, 2] fit entirely into a standard local continuum mechanics framework. The macroscopic deformation (gradient) tensor is calculated for every material point of the macrostructure and is next used to formulate kinematic boundary conditions for the associated microstructural representative volume element. After the solution of the microstructural boundary value problem, the macroscopic stress tensor is obtained by averaging the resulting microstructural stress field over the volume of the microstructural cell. As a result, the (numerical) stress-strain relationship at every macroscopic point is readily available. The first-order computational homogenization technique proves to be a valuable tool in retrieving the macroscopic mechanical response of non-linear multi-phase materials.

However, there are a few severe restrictions limiting the applicability of the first-order computational homogenization scheme (as well as conventional homogenization methods). Firstly, although the technique can account for the volume fraction, distribution and morphology of the constituents, it is insensitive to the absolute size of the microstructure. As a consequence, effects related to variations of this size cannot be predicted. Secondly, the approach is not applicable in critical regions of intense deformation, where the characteristic wave length of the macroscopic deformation field is in the order of the size of the microstructure. Moreover, if softening occurs at a macroscopic material point, the solution obtained from first-order computational homogenization leads to a mesh dependent macroscopic response due to ill-posedness of the macroscopic boundary value problem.

In order to overcome these limitations, a novel, *second-order computational homogenization* procedure is proposed [3, 4]. The second-order scheme is based on a proper incorporation of the gradient of the macroscopic deformation tensor into the kinematical micro-macro framework. The macroscopic stress tensor and a higher-order stress tensor are retrieved in a natural way based on an extended version of the Hill-Mandel energy balance. A full second-gradient continuum theory appears at the macroscale, which requires solving a higher-order equilibrium problem by a special finite element implementation.

RESULTS

Several microstructural analyses show that the second-order computational homogenization framework captures changes of the macroscopic response due to variations of the microstructural size as well as variations of macroscopic gradients of the deformation. If the microstructural size becomes negligible with respect to the length scale of the macroscopic deformation field, the results obtained by the second-order modelling coincide with those of the first-order approach. This important observation demonstrates that the second-order computational homogenization scheme is a natural extension of the first-order framework.

The most important feature of the second-order computational homogenization method is in fact that the relevant length scale of the microstructure is directly incorporated into the description on the macrolevel via the size of the representative cell. This size should reflect the scale at which the relevant microstructural deformation mechanisms occur. The concept of a representative volume element (RVE) has to be reconsidered in the second-order computational homogenization. Contrary to the classical definition of the RVE, it may not be taken arbitrarily large, since the RVE size sets the length scale of the macroscopic higher-order homogenized continuum. Therefore, the RVE size for a second-order computational homogenization analysis should generally be determined from physical and/or numerical experiments. On the other hand, introduction of the macroscopic length scale directly related to the size of the microstructure allows to describe certain phenomena that cannot be addressed by the first-order scheme, such as macroscopic localization and size effects, as will be illustrated in the following.

Tension of a voided plate (as a heterogeneous configuration), Figure 1a, with a material imperfection, which triggers the development of a localization band, is analyzed using the first-order and the second-order computational homogenization scheme. The first-order computational homogenization analysis results in a mesh dependent strain distribution, Figure 1b,c. The second-order scheme leads to a localization band, which is independent of the mesh size, Figure 1d,e.

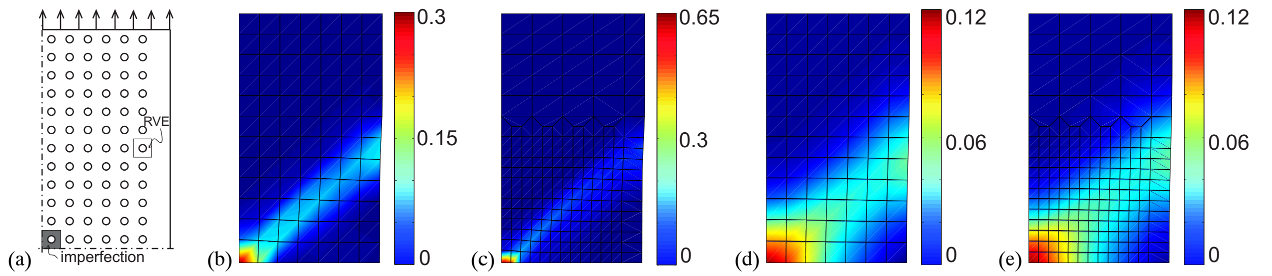

Figure 1. Homogenization analysis of a macroscopic localization problem. Geometry (a) and the strain distribution obtained by the first-order (b), (c) and second-order (d), (e) computational homogenization analysis using two finite element discretizations.

Furthermore, the second-order framework allows the modelling of surface layer effects via the incorporation of higher-order boundary conditions. Simple shear of a thin heterogeneous strip with several ratios of the strip thickness H to the microstructural length scale d is considered, Figure 2a. The constraints on the top and bottom surfaces are modelled using higher-order boundary conditions. Boundary layers with a vanishing shear are clearly observed, Figure 2b, giving rise to a size effect, Figure 2c. Figure 2d shows microstructural deformation patterns in three RVEs corresponding to different locations in the macrostructure.

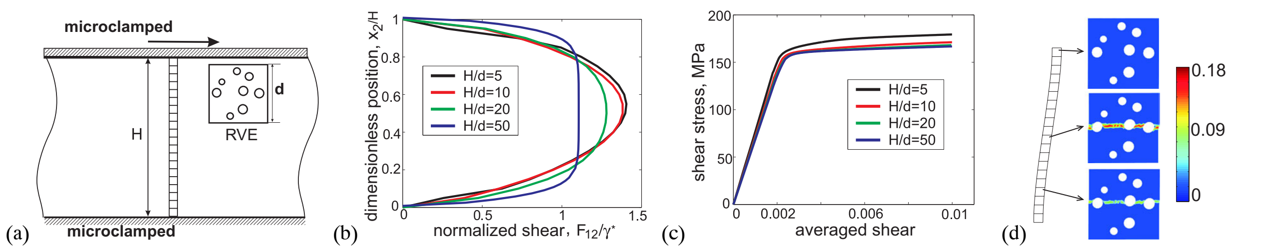

Figure 2. Homogenization analysis of the macroscopic boundary shear layer problem. Geometry (a), distribution of shear across the height of the macroscopic strip (b), shear stress-strain response (c) and microstructural deformation patterns in the sheared macroscopic layer for $H/d = 5$ (displacements are 10 times magnified).

CONCLUSIONS

Computational homogenization provides a versatile strategy to establish micro-macro structure-property relations based on the collective behaviour of the evolving, multi-phase microstructure. The novel second-order computational homogenization scheme allows to describe certain phenomena that cannot be addressed by the classical first-order scheme, such as (geometrical) size effects, macroscopic localization and surface layer effects.

References

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