International Journal for Multiscale Computational Engineering, 2(4)507-509(2004)

Preface to Special Issue on

Multiscale Computational Homogenization: From Microstructure to Properties

M.G.D. Geers, Guest Editor

Eindhoven University of Technology
Departement of Mechanical Engineering
P.O. Box 513
5600 MB, Eindhoven, The Netherlands

The past decade was marked by a substantial growth in the development of computational tools to reveal material properties through scale transitions. Whereas analytical, closed-form, and asymptotic homogenization schemes have been used with considerable success to predict average or apparent properties of engineering materials, new perspectives were opened through the integration and expansion of the acquired knowledge by making optimal use of numerical solution techniques. This topic is the main focus of this Special Issue, where several techniques are addressed to bridge scales from microstructure to properties.

Part of the work in numerical homogenization schemes has appeared as a natural extension of earlier work on elastic solids and composite materials. In here, homogenization techniques constituted an excellent tool to predict the effective or apparent linear elastic properties of heterogeneous materials. Several closed-form homogenization techniques were initially proposed in this context, e.g., the Voigt-Reuss-Hill bounds, the Hashin-Shtrikman variational principle, the self-consistent method, Mori-Tanaka approaches, etc. Asymptotic or mathematical homogenization schemes have been used frequently to assess effective properties of elastic heterogeneous materials, whereby extensions toward higher-order and nonlocal constitutive equations have been considered as well, e.g., the work of Drugan, Fleck, Forest, Smyshlyaev, Triantafyllidis, Willis, and many others. Whereas this works reasonably well for elastic materials, it becomes more and more complicated for highly heterogeneous and physically nonlinear materials. Physically nonlinear microstructures have been addressed by means of Taylor-Bishop-Hill estimates, several generalizations of self-consistent schemes, and asymptotic procedures (see, e.g., the work of Doghri, Fish, Ostoja-Starzewski, Ponte Castañeda, Suquet, and many others).

Extending this further to a geometrically and physically nonlinear regime is clearly more cumbersome. Even though some numerical homogenization frameworks have been proposed in this sense, a closed-form constitutive equation was generally assumed, which limits the applicability if one wishes to account for more

complex physics, geometrical nonlinearities, or damage and localization. These complexities are more easily dealt with by resorting to a full computational scheme, which enables the two-scale computational homogenization of complex multiphase solids. This category of techniques is essentially based on the solution of nested boundary value problems, one for each scale. If attention is focused on the nonlinear characteristics of the material behavior, this technique proves to be a valuable tool in retrieving the constitutive response. Computational homogenization schemes that fit entirely in a standard continuum mechanics framework (principle of local action) are now readily available in the literature (see, e.g., the work of Feyel, Ghosh, Kouznetsova, Miehe, Smit, Suquet, Terada, and others). The attractiveness of this approach lies in the fact that the constitutive response at the macroscale is *a priori* undetermined. No explicit assumptions are required at that level because the macroscopic constitutive behavior ensues from the solution of the microscale boundary value problem for which arbitrary nonlinear constitutive models can be used for each phase or interface. The solution of the macro- and microscale problem is a classical boundary value problem for which any appropriate solution strategy can be used (e.g., Finite Element (FE) Method, Element Free Galerkin), whereas the required macroscopic constitutive tangent operators can be obtained from the microscopic overall stiffness tensor. Recently, an extension toward a second-gradient continuum in the sense of Mindlin has been established as well.

Another well-known class of computational multiscale methods for the mechanics of materials are the variational multiscale methods. Based on a weak form of the governing equations, scales are separated whereby specific assumptions are needed on the fine-scale field. Elimination of the fine scale from the obtained formulation constitutes the upscaling step. Well-known fine-scale patterns (e.g., displacement discontinuities modeled by Heaviside functions) can be easily implemented, showing considerable similarities with solution methods based on the partition of unity concept.

Even though it is impossible to compose a Special Issue that covers all these recent trends, some selected articles clearly reflect the state of the art in some of these domains. The topics dealt with in this special issue on multiscale computational homogenization can be summarized as follows:

- Computational homogenization of geometrically and physically nonlinear solids by means of the numerical solution of nested boundary value problems
- The Voronoi cell method
- Combined homogenization in space and time
- Numerical solution of multiscale problems with embedded scales
- Multiscale analysis through transformation field analyses
- Solution and application of an extended version of the Hashin-Shtrikman variational principle
- Explicit computational determination of homogenized higher-order elastic constants through asymptotic methods
- Adaptivity in computational homogenization, where finer scales can be locally added if required by the desired accuracy

More details on each of the contributions are briefly provided below.

A frequently used numerical two-scale technique is probably the solution of an embedded multiple scale problem, driven by fracture.

A well-known example is the case were damage develops at a fine scale, leading to complete material degradation, which is captured by the embedding of a fine-scale discontinuous field in the coarse-scale solution. An example thereof is presented in the paper by Garikipati.

Resolving both spatial and temporal scales is another challenge for which various numerical techniques are, at present, being proposed. An illustration thereof is provided by Nouy and Ladevèze, where particular attention is given to a robust approximate solution of the many microproblems to be resolved, based on the concept of radial approximation.

As emphasized, physically and geometrically nonlinear and complex multiphase materials are best treated with a full computational nested multiscale solution scheme. In this special issue, two papers are devoted to this subject. Carrère, Feyel, and Kanouté propose a thorough comparison between such a two-scale nested FE solution framework and a transformation field analysis framework. Resolving the explicit role of the size of a microstructure is one of the great challenges in miniaturization. Standard, first-order homogenization methods do not allow one to take this particular influence into account in a well-defined manner. Kouznetsova, Geers and Brekelmans therefore concentrate on the second-order computational homogenization framework that they have developed recently, where the explicit role of an RVE (representative volume element) in such a second-order computational homogenization method is investigated and clarified.

A second illustration of the influence of size is given in the paper by Peerlings and Fleck, based on a natural extension of classical asymptotic homogenization theories. A rigorous link between two scales has been established for 3D linear elasticity, whereby a Mindlin-type strain-gradient continuum has been identified. All elasticity constants in this enriched continuum can be determined by means of the solution of a series of microstructural boundary value problems, as shown in the present paper.

Adaptivity is another aspect of great relevance in a computational multiscale model. An example thereof will be given for a composite material, where fiber-matrix debonding leads to engineering damage. A three-level approach with geometrically nested scales is here proposed by Ghosh and Raghavan, where each scale enters the solution algorithm in an adaptive manner. The combined and adaptive use of coarse-scale solution techniques (i.c., FEM) and a fine-scale algorithm (i.c., the Voronoi cell method) is thereby the key issue.

In some cases, the variational principles of Hashin and Shtrikman provide an interesting option to solve two-scale computational homogenization problems in an uncoupled manner. An illustration thereof is given in the paper of Šejnoha, Valenta, and Zeman, for statistically homogeneous composites, where an extension is presented in order to deal with eigenstress or eigenstrain distributions applied to a nonlinear viscoelastic composite.

In summary, this Special Issue offers a selected cross section of recent research activities that rely on a particular computational homogenization technique to upscale the mechanics of materials. This single issue does not aim to provide a complete overview, but it hopefully contributes to the future development of computational homogenization frameworks applied to engineering materials. I would like to thank all the authors for their valuable contributions, as well as all the reviewers for the considerable amount of time that they have spent on their task. The many critical remarks and comments provided have undoubtedly lead to a considerable increase in the quality of the papers. Finally, I would like to thank Professor Jacob Fish for inviting me to assemble this Special Issue and providing the necessary support with which to do so.