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CHARACTERIZATION OF MATERIALS WITH MICROHETEROGENEOUS STRUCTURE

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Summary. *Computational methods for the determination of material properties of microheterogeneous materials including inelastic behaviour are discussed in this contribution. Applications related to this class of problems range over different length scales. These can cover up to six orders of magnitude, ranging from μm to m. Here homogenization concepts are employed to model the constitutive behaviour at macro scales based on results obtained at micro scales. Using the concept of representative volume elements (RVE), the theoretical background is discussed as well as the numerical treatment of the resulting complex, three-dimensional RVEs. Examples show applications within a range of materials used in engineering.*

1 Introduction

A description of the constitutive behaviour of heterogeneous materials such as concrete can be achieved by experimental investigations or by numerical simulations. While the

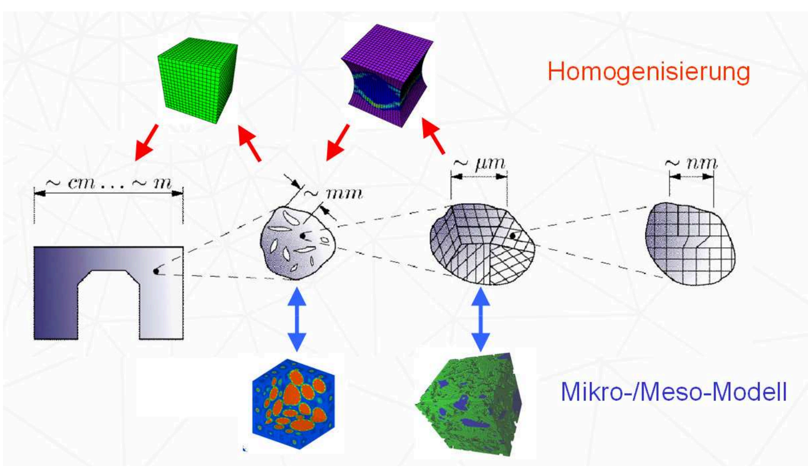

Figure 1: Multi scale description of a complex material like concrete

experimental techniques are applied successfully since several decades, the use of numerical simulation techniques is quite young. This is due to the fact that the underlying three-dimensional models are complex and need considerable computer power for reasonable computations.

Figure 1 depicts a special multi scale modelling process which can be used for many materials. Within this process different three-dimensional mechanical models are applied on each length scale in order to describe the constitutive behaviour on that scale. These are called *Representative Volume Elements* (RVE). Often the material on a specific length scale consists of different phases which have to be taken into account in order to characterize the material with sufficient accuracy. The RVE is then subjected to different loading conditions which lead to a material response. Based on these results a homogenization process can be initiated to describe the material behaviour averaged over the RVE. The resulting homogenized constitutive equation is then applied within the the next scale to model the constituents of the RVE belonging to that scale.

In this contribution an overview with regard to the theoretical and numerical treatment of multiscale modelling is presented. Due to lack of space only the basic ideas can be covered, details can be found in e.g. Torquato [6], Zohdi and Wriggers [7] and Löhnert [2].

2 Determination of the RVE

The representative volume element consists of different constituents or phases. Their distribution can be obtained either from actual CT-scans of the material or from statistical procedures.

For each constituent of the micro-structure constitutive equations have to be formulated based on experimental data and observations. If the material properties of the different phases in the RVE are not known, one can employ parameter identification processes to determine the missing constitutive data.

3 Homogenization

In order to obtain the the effective material properties for the next scale, homogenization is needed. The effective material tensor $\mathbf{C}^{eff}$ maps the volume average of strain on to the stress in case of linear elasticity

$$\langle \boldsymbol{\sigma} \rangle = \mathbf{C}^{eff} : \langle \boldsymbol{\epsilon} \rangle \, , \tag{1}$$

with $\langle \bullet \rangle = \frac{1}{V} \int_\Omega \bullet \, \mathrm{d}\Omega$. The volume of the RVE is denoted by V. Using three-dimensional finite element solution, the average stress and strain can be evaluated. In case of nonlinear material behaviour the effective material response $\langle \boldsymbol{\sigma} \rangle = \mathbf{f}^{eff}(\langle \boldsymbol{\epsilon} \rangle)$ is calculated in terms of the averaged quantities.

For a statistically representative analysis, the homogenization procedure is performed for many RVEs. The result of each calculation yields the effective constitutive parameters.

A probability density W of the effective Youngs-modulus E^{eff} of cement paste is shown in Figure 2 as an example for a computation with 4600 RVEs. The probability density of Youngs modulus is very close to a GAUSSian distribution.

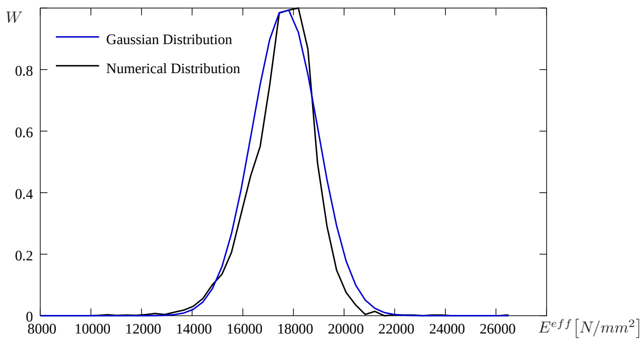

Figure 2: Probability density of Youngs modulus

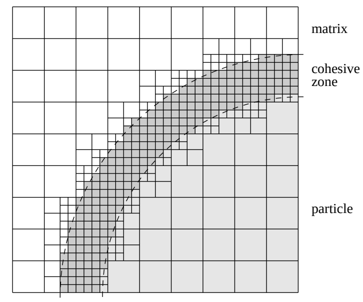

Figure 3: Discretization with hanging-nodes

4 Parameter identification

In case that the parameters of the material model on the micro-scale can not be determined through experimental results a parameter identification procedure is used to compute these. The idea of the identification is to determine the parameters such that the calculated result fits with experimental results f, while the displacements $\langle \boldsymbol{u}(\boldsymbol{\kappa})\rangle$ of the RVE depend on the material data $\boldsymbol{\kappa}$. This identification is obtained by solving an optimization problem where the data $\boldsymbol{\kappa}$ have to be calculated in a way, such that the objective function $A(\boldsymbol{\kappa})$ is minimized

$$A(\boldsymbol{\kappa}) := \sum_{i=1}^{n} \big(\langle \boldsymbol{u}(\boldsymbol{\kappa})\rangle_i - f_i\big)^2 \rightarrow \min \ . \tag{2}$$

The solution of (2) is obtained by a combination of a genetic algorithm and a gradient method. In a first step, the genetic algorithm yields a solution close to the global minimum. After that the optimization procedure switches to the more efficient LEVENBERG-MARQUARDT method.

5 Numerical Methods for Multiscale Analysis

Multi-scale analysis and homogenization involves multiple solutions of finite element models with over 1 Million unknowns. Hence efficient discretization schemes, algorithms and solvers have to be applied. In our approach the following methods were used.

1. **Discretization.** The discretization of the RVE is performed by using a meshing in which each element only consists of one phase. Since this does not model arbitrary shapes of particles in the microstructure correctly one has to use an adaptive

refinement, see Figure 3. A in depth discussion and comparison of this approach in comparison with an aligned mesh can be found in Löhnert [2].

2. **Finite elements.** Due to the special discretization the Cosserat point elements described in Löhnert et al. [3] is applied which is highly robust.

3. **Algorithms.** For the solution of the nonlinear response of the RVE which can include finite and inelastic deformations a Newton algorithm is used together with a standard load stepping procedure.

4. **Solvers.** The solution of the, in general, non-symmetric linear equation within each Newton step is performed by an iterative GMRES solver which can account for hanging nodes, see Löhnert [2]. Average solution times are about three minutes for one linear system with 400.000 unknowns.

5. **Parallel Solution.** In order to keep the overall computing time for homogenization and parameter identification within reasonable bounds, the calculations were distributed within a network environment using a client-server based system. A typical parameter identification, like described in section 3, requires on a stand alone standard computer system approximately one month CPU time. Within a network environment using 15 standard PCs the same identification was completed within 2.5 days.

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