

## COMPUTATIONAL HOMOGENISATION OF MICROHETEROGENEOUS MATERIALS INCLUDING DECOHESION AT FINITE STRAINS

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**Summary** In this paper we present some aspects of computational homogenisation procedures of microheterogeneous materials which can show decohesion in a cohesive zone around the particles. Applications to this are e.g. polymer coatings stiffened with sand. Due to the decohesion we get finite deformations and finite strains within the RVE. The geometrical and material nonlinearities cause the main difficulties. The homogenisation procedure leads to an effective stress strain curve for the RVE. Here we set a special focus on the adaptive numerical model, the statistical testing procedure and the different boundary conditions (pure traction, pure displacement and natural boundary conditions) applied on the RVE.

### HOMOGENISATION AT FINITE STRAINS

The effective material data of a representative volume element (RVE) is obtained from the relation between the effective strains  $\varepsilon$  and the effective stresses  $\sigma$ . The effective material tensor  $\mathbb{E}^*$  maps the volume average of the strains on the volume average of the stresses

$$\langle \sigma \rangle_{\Omega} = \mathbb{E}^* : \langle \varepsilon \rangle_{\Omega} \quad (1)$$

with  $\langle \cdot \rangle_{\Omega} = \frac{1}{|\Omega|} \int_{\Omega} \cdot d\Omega$ .  $\Omega$  is the domain of the regarded RVE. Equation (1) also holds in the nonlinear range where  $\mathbb{E}^*$  depends on the deformation and maybe on the deformation path itself. A requirement for the strain measure in (1) is linearity in the displacements, also for the geometrically nonlinear theory.

The average strain theorem states that for a perfectly bonded RVE under uniform displacement boundary conditions the volume average of the deformation is the same as the given deformation on the boundary. Given a constant deformation gradient on the boundary  $\mathcal{F}$  it can be shown that

$$\langle \mathbf{F} \rangle_{\Omega_0} = \mathcal{F} + \frac{1}{|\Omega_0|} \int_{\partial\Omega_0^1 \cap \partial\Omega_0^2} \llbracket \mathbf{u} \rrbracket \otimes \mathbf{n}_0 d\partial\Omega_0^{1,2} \quad , \quad (2)$$

where  $\llbracket \mathbf{u} \rrbracket$  is the jump within the displacement field in case of a not perfectly bonded microstructure,  $\mathbf{n}_0$  is the unit normal vector, and  $\Omega_0^1$  and  $\Omega_0^2$  are the domains of the different materials in the RVE respectively. In case of a perfectly bonded microstructure the displacement jumps vanish. Then  $\langle \mathbf{F} \rangle_{\Omega_0} = \mathcal{F}$ , and similarly  $\langle \dot{\mathbf{F}} \rangle_{\Omega_0} = \dot{\mathcal{F}}$ .

The average stress theorem states that in the absence of body forces and under a uniform load on the boundary the volume average stress is the same as the given stress on the boundary. For finite deformations one has to distinguish between different configurations. Here we restrict ourselves to the mixed configuration. We assume a constant first Piola-Kirchhoff stress tensor  $\mathcal{P}$  on the boundary. Using Cauchy's theorem and applying the equations of motion one can show that

$$\langle \mathbf{P}^T \rangle_{\Omega_0} = \mathcal{P}^T + \frac{1}{|\Omega_0|} \int_{\Omega_0} \mathbf{X} \otimes \mathbf{f}_0 d\Omega_0 \quad (3)$$

which for zero body forces yields  $\langle \mathbf{P} \rangle_{\Omega_0} = \mathcal{P}$ .

A commonly accepted criterion for the choice of the size of the RVE is Hill's condition which states that for a perfectly bonded microstructure and no body forces the microenergy is equal to the macroenergy of the RVE. This leads to the fact that the RVE has to be small enough such that from the macroscopic point of view the strain and the stress of the macroscopic body can be assumed to be approximately constant at the location of the RVE. Due to that the RVE can be regarded as one point of the macroscopic structure. On the other hand the RVE has to be large enough such that the boundary field fluctuations are relatively small. For finite deformations one can show that in case of Dirichlet boundary conditions and a perfectly bonded microstructure as well as for pure Neumann boundary conditions and no body forces we have

$$\langle \mathbf{P} : \dot{\mathbf{F}} \rangle_{\Omega_0} = \langle \mathbf{P} \rangle_{\Omega_0} : \langle \dot{\mathbf{F}} \rangle_{\Omega_0} \quad . \quad (4)$$

### MATERIAL MODEL

The microstructure consists of randomly distributed spherical particles embedded in a binding matrix. The delamination process is restricted to a domain around the particles. This zone is also called "cohesive zone". Further details about the cohesive zone approach can be found for example in [6]. The material law chosen for the binding matrix and the inclusions is a simple compressible Neo-Hooke material with the Lamé parameters  $\mu^{(m)}$ ,  $\lambda^{(m)}$  and  $\mu^{(p)}$ ,  $\lambda^{(p)}$  respectively. The material model for the cohesive zone is a simple damage model following the suggestion of Zohdi [7]. The undamaged material is also a compressible Neo-Hooke material with the material parameters  $\mu_0^{(cz)}$  and  $\lambda_0^{(cz)}$ . The local degradation

is represented by a variable  $\alpha$  with  $0 < \alpha \leq 1$  which “weakens” the stiffness of the material. That means, the material constants become

$$\mu^{(cz)} = \alpha\mu_0^{(cz)} \quad \text{and} \quad \lambda^{(cz)} = \alpha\lambda_0^{(cz)} \quad . \quad (5)$$

The local constraint condition from which  $\alpha$  can be computed is  $\Psi(\alpha) = \mathcal{M}(\alpha) - \mathcal{K}(\alpha) \leq 0$  where  $\mathcal{M}(\alpha)$  is a scalar valued term representing the stress state of the material point

$$\mathcal{M}(\alpha) = \sqrt{\mathbf{g}(\boldsymbol{\sigma}_{\text{deg}}(\alpha)) : \mathbf{g}(\boldsymbol{\sigma}_{\text{deg}}(\alpha))} \quad \text{with} \quad \mathbf{g}(\boldsymbol{\sigma}_{\text{deg}}(\alpha)) = \eta_1 \frac{\text{tr}(\boldsymbol{\sigma}_{\text{deg}})}{3} \mathbf{1} + \eta_2 \left( \boldsymbol{\sigma}_{\text{deg}} - \frac{\text{tr}(\boldsymbol{\sigma}_{\text{deg}})}{3} \mathbf{1} \right) \quad (6)$$

and  $\eta_1$  and  $\eta_2$  are parameters scaling the isochoric and deviatoric parts of  $\mathbf{g}(\boldsymbol{\sigma}_{\text{deg}}(\alpha))$ .  $\mathcal{K}(\alpha)$  is a threshold value which depends on the damage variable  $\alpha$  itself.

$$\mathcal{K}(\alpha) = \Phi_{\text{lim}} + (\Phi_{\text{crit}} - \Phi_{\text{lim}}) \alpha^P \quad (7)$$

$\Phi_{\text{crit}}$  is the initial threshold value, and  $\Phi_{\text{lim}}$  is the threshold value in the limiting case when the material point has degraded completely ( $\alpha = 0$ ). Finally  $P$  is an exponent which controls the rate of degradation.

## NUMERICAL MODEL AND COMPUTATIONAL TESTING

The RVE is chosen to be a cube with a random distribution of inclusions. In three dimensions it is not easy to generate a mesh of only nicely shaped hexahedra elements for complex geometries. This motivates a different way of discretisation where we use only linear cube shaped elements which approximate the particle boundaries only roughly. In order to increase the accuracy of the discretisation we apply non-conforming elements close to the interfaces between the particles and the cohesive zone and the cohesive zone and the matrix material. An illustration of this discretisation can be seen in Figure 1. To get a representative material response one has to do statistical tests with different random distributions of inclusions. Of special interest is the number of particles needed for each test, the refinement of the mesh, the number of tests performed and of course the different boundary conditions. The tests done are performed with pure displacement boundary conditions, pure traction boundary conditions and natural boundary conditions. The necessary refinement of the mesh has been tested in a one particle test. The resulting strain energy as a function of the number of degrees of freedom is shown in Figure 2.

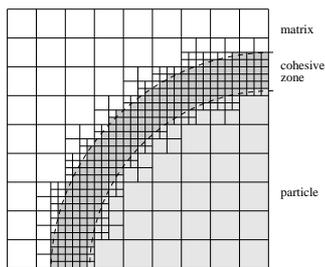


Figure 1: Discretisation with non-conforming cubic elements

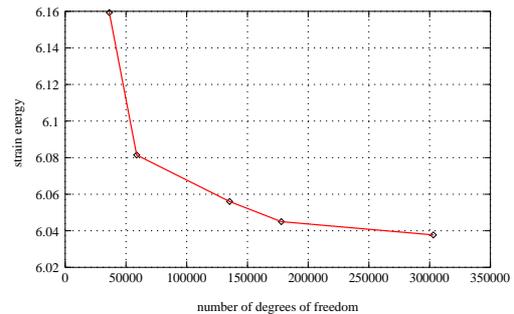


Figure 2: Convergence: overall energy

To figure out the required number of inclusions we look at the standard deviation of the stress response for multiple tests with the same number of inclusions. This value does not decrease with the number of tests performed. Only the number of inclusions in each test has an influence on it. However, to get a statistical representative response it is necessary to compute the same test many times with a different random distribution of the inclusions. In Figure 3 one can see that a relatively low number of inclusions is sufficient.

At last the number of tests which have to be computed to get a statistically representative result is important. It is not possible to increase the accuracy of the effective response by computing more tests. But at a higher number of tests performed, the collection of the effective results of each test form a more Gaussian distribution of the effective results. This is shown in the histograms in Figure 4 for 200 tests performed.

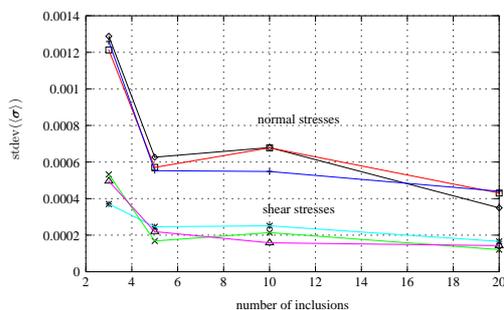


Figure 3: Standard deviation of the effective stresses

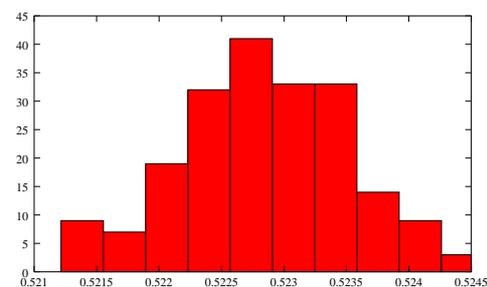


Figure 4: Histogram for effective Cauchy stress component  $\langle \sigma_{11} \rangle$

## References

- [1] Bishop, J.F.W. and Hill, R.: A Theory of the Plastic Distortion of a Polycrystalline Aggregate under Combined Stresses. *Phil. Mag.*, 42, (1951a), 414-427.
- [2] Bishop, J.F.W. and Hill, R.: A Theoretical Derivation of the Plastic Properties of a Polycrystalline Face-Centred Metal. *Phil. Mag.*, 42, (1951b), 1298-1307.
- [3] Hill, R.: The Elastic Behaviour of a Crystalline Aggregate. In: *Proc. Phys. Soc. (Lond.)*, A65, pages 349-354 (1952).
- [4] Reuss, A.: Berechnung der Fließgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle. *Z. angew. Math. Mech.*, 9, (1929), 49-58
- [5] Voigt, W.: Über die Beziehung zwischen den beiden Elastizitätskonstanten isotroper Körper. *Wied. Ann.*, 38, (1889), 573-587.
- [6] Needleman, A. et al: Matrix reinforcement, and interfacial failure. In: Suresh, S., Mortensen, A. and Needleman, A.: *Fundamentals of metal matrix composites*, Butterworth-Heinemann publishers (1993).
- [7] Zohdi, T; Wriggers, P.: Computational micro-macro material testing. *Archives of Computational Methods in Engineering.*, 8, 2, (2001), 131-228.