

INVESTIGATION OF CONSTRAINTS FOR SMALL SCALE SOLUTION WITHIN A MULTISCALE MODEL FOR COMPOSITES

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Summary. *This paper addresses the question of accurate and at the same time efficient conditions for the micro-macro-transition within multiscale models for the mechanical and numerical modeling of materials with microstructure in the nonlinear range. One intended application is the simulation of fiber reinforced concrete (cement), a material which allows to design very thin structures. The post critical behaviour is driven by the accumulation of the failure mechanisms on the microscale. Those failure mechanisms like matrix cracking, debonding between the fibers in a filament, or between fiber and matrix are incorporated in the macroscopic formulation using a strongly coupled multiscale method introduced as the variational multiscale method (VMM) by Hughes et al.⁵. A central point of the presented scheme for an efficient solution of the discrete problem is the locality constraint for the small scale part of the solution, leading to decoupled problems on the micro scale.*

1 OVERVIEW

According to Fish⁴, the VMM can be regarded as a "superposition based method". Those methods are based on a decomposition of the solution function $\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$ into global $\bar{\mathbf{u}}$ (large scale) and local fluctuating displacements \mathbf{u}' (small scale). For our applications \mathbf{u}' is induced by local stiffness variations due to microcracks in the composite. The underlying strategy is very close to domain decomposition methods, e.g. the multiscale method presented by Ladeveze⁷ and multigrid methods as shown by Bayreuther¹. Those methods provide iterative strategies for an efficient solution of large problems and may be classified as "solution methods". In contrast "local enrichment methods", a classification introduced by Fish et al.⁴ including the VMM, assume locality of the small scale part of the solution \mathbf{u}' ; this locality constraint is motivated by the underlying physics of the problem and reflects the decaying behaviour of the influence of microcracks on the solution \mathbf{u} . This assumption provides an improvement in the efficiency compared to solution methods: While domain decomposition methods iteratively search for the true coupling terms between substructures in the system matrix, the coupling terms are *assumed* based on the underlying physics in the presented scheme.

2 LOCALITY CONSTRAINTS

As already mentioned, the assumption of compactly supported small scale displacements within substructures, for our case within the Finite Elements of the large scale displacement discretization, is important for the efficiency. Several assumptions concerning the boundary-conditions for the small scale displacements are investigated in the presentation regarding accuracy, effort and application area. Displacement boundary conditions are the easiest and most efficient possibility, imposed by assuming the small scale displacements to vanish on the large scale element's edges Γ^B : $\mathbf{u}' = \mathbf{0}$ on Γ^B . These boundary conditions lead to accurate results for *local* failure and adequate proportions between the failure zone and the large scale discretization. For *expanding* failure these displacement constraints cause responses, which are too stiff, as can be seen in the example below, Figure 2. More accurate results for applications with expanding failure can be achieved by introducing additional constraints through Lagrange-multipliers in a weak sense. The Lagrange-multiplier can be interpreted as the boundary tractions, which leads to the name "stress boundary conditions". Marcovic⁸ introduced stress BC's by the weak constraint, that the mean value of \mathbf{u}' over the large scale element edges should vanish: $\int_{\Gamma^B} \lambda \cdot \mathbf{u}' dA = 0$, introducing Lagrange-multipliers as *local* variables, see³. The enforcement of the small scale displacements continuity on the large scale elements edges in a weak sense: $\int_{\Gamma^B} \lambda \cdot [\mathbf{u}'] dA = \mathbf{0}$, as shown by Farhat² can (depending on the discretization of λ) lead to very accurate results but on the cost of additional *global* degrees of freedom λ .

3 FORMULATION AND EXAMPLE

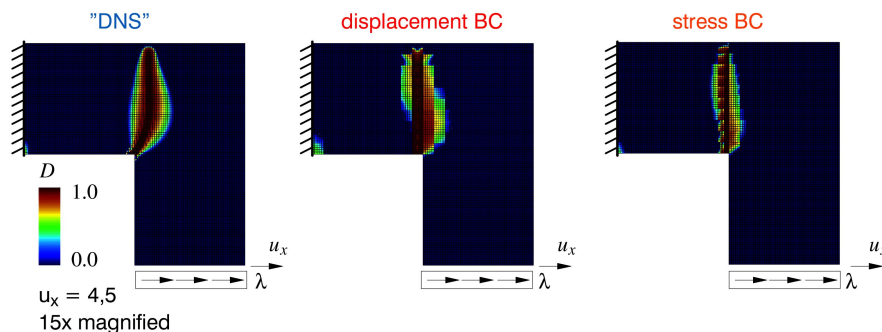


Figure 1: L-Shape: Deformed structures and damage distribution

Starting point is the boundary value problem including equilibrium of a 2-dim. structure, small strain kinematics and constitutive equations

$$\delta \Pi_{\mathbf{u}} = \int_{\Omega} \delta \varepsilon : \sigma dV - \int_{\Omega} \delta \mathbf{u} \cdot \hat{\mathbf{b}} dV - \int_{\Gamma^t} \delta \mathbf{u} \cdot \hat{\mathbf{t}} dA = 0. \quad (1)$$

The solution function and the test functions are decomposed into large and small scale part:

CPU–time for solution on 1 processor:

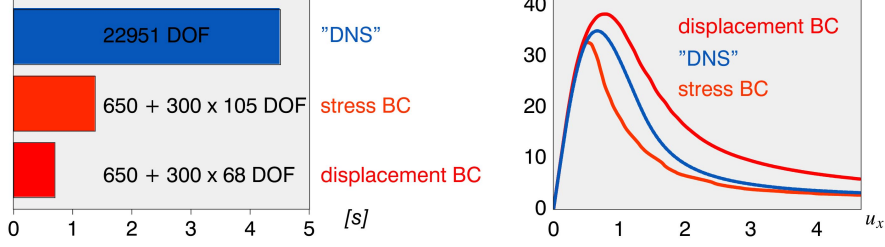


Figure 2: L-Shape: Solution time and load-displacement curves

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}' \quad \delta \mathbf{u} = \delta \bar{\mathbf{u}} + \delta \mathbf{u}'. \quad (2)$$

For a micro-material formulation with interfaces Γ^{IF} between fibers and matrix and gradient enhanced damage model for the concrete we get the following set of equations:

- large scale problem:

$$\delta \Pi_{\bar{\mathbf{u}}} = \int_{\Omega} \delta \bar{\boldsymbol{\varepsilon}} : \boldsymbol{\sigma}(\boldsymbol{\varepsilon}, D(\tilde{\boldsymbol{\varepsilon}}^v)) dV - \int_{\Omega} \delta \bar{\mathbf{u}} \cdot \hat{\mathbf{b}} dV - \int_{\Gamma^t} \delta \bar{\mathbf{u}} \cdot \hat{\mathbf{t}} dA = 0 \quad (3)$$

- small scale problem:

$$\delta \Pi_{\mathbf{u}'} = \int_{\Omega_l} \delta \boldsymbol{\varepsilon}' : \boldsymbol{\sigma}(\boldsymbol{\varepsilon}, D(\tilde{\boldsymbol{\varepsilon}}^v)) dV + \int_{\Gamma^{IF}} \delta[\mathbf{u}'] \cdot \mathbf{t} dA - \int_{\Omega_l} \delta \mathbf{u}' \cdot \hat{\mathbf{b}} dV - \int_{\Gamma_l^t} \delta \mathbf{u}' \cdot \hat{\mathbf{t}} dA = 0 \quad (4)$$

- nonlocal strains:

$$\delta \Pi_{\tilde{\boldsymbol{\varepsilon}}^v} = \int_{\Omega_l^{GE}} c \delta \nabla \tilde{\boldsymbol{\varepsilon}}^v \cdot \nabla \tilde{\boldsymbol{\varepsilon}}^v dV + \int_{\Omega_l^{GE}} \delta \tilde{\boldsymbol{\varepsilon}}^v \tilde{\boldsymbol{\varepsilon}}^v dV - \int_{\Omega_l^{GE}} \delta \tilde{\boldsymbol{\varepsilon}}^v \boldsymbol{\varepsilon}^v(\boldsymbol{\varepsilon}) dV = 0. \quad (5)$$

The small scale displacements \mathbf{u}' are assumed to be *locally supported* within every large scale element Ω_l , leading to *decoupling* of the small scale problem and of the equation of nonlocal strains. Additional constraint conditions introduce assumptions concerning the behaviour of the small scale displacements \mathbf{u}' on the large scale elements edges Γ_l^B . For example the assumption of vanishing mean value of \mathbf{u}' over Γ_l^B ,⁸ is expressed by

- locality constraint:

$$\delta \Pi_{\lambda} = \int_{\Gamma_l^B} \delta \lambda^{\mathbf{B}} \cdot \mathbf{u}' dA = 0. \quad (6)$$

λ can be identified as the (local) traction vector on the large scale element's edges. We are using FE-discretization for both the large and the small scale displacements, leading to a coupled set of nonlinear equations, iteratively solved by a Newton-Raphson scheme.

As a first example, the damage evolution of an L-Shape with gradient enhanced damage is investigated. The results of a DNS calculation, i.e. a calculation with "microresolution" used as reference solution are compared to calculations with the VMM using 300 large scale elements and displacement boundary conditions on the one hand and stress boundary conditions on the other hand, see Figures 1 and 2. As the failure zone expands over the large scale elements boundaries, the kinematic restrictions of the displacement boundary conditions lead to a too stiff load-displacement behaviour while the stress boundary conditions tend to be too weak but closer to the reference solution. The solving time is reduced to 1/5.5 and 1/3.75 respectively through the multicale model for this example. Further examples will be given in the presentation.

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