

Application of the variational multiscale method to damage of composites

Andrea Hund¹, Ekkehard Ramm¹

¹ Institute of Structural Mechanics, University of Stuttgart, Pfaffenwaldring 7, 70569 Stuttgart, Germany

ABSTRACT

This paper is devoted to the mechanical and numerical modelling of fiber reinforced concrete structures, taking into account the nonlinear material behaviour of the components and their interaction on the microlevel. Formulations for simulating a structure's response with full resolution of the material heterogeneities, which may be called Direct Numerical Simulations (DNS), are prohibitive due to the problem size. This obstacle is overcome by applying the Variational Multiscale Method (VMM) to bridge the scales via a variational projection between the behaviour on the scale of the material heterogeneity and the macroscopic structural behaviour.

1 INTRODUCTION

Fiber reinforced concrete (cement) is a widely used material allowing to design very thin structures. A combination of brittle and low strength cement with brittle, but high strength and stiff fibers or fiber filaments e.g. carbon or glass, can nevertheless generate a ductile material with relative high ultimate strength. The structural ductility results from microscopic frictional processes between brittle matrix and brittle fibers, and within the fiber compound. The properties of the composite depend on the one hand on the material layout, e.g. the properties of its components, the fiber length, content, coating and orientation (length scale μm) and on the other hand on the structural layout, e.g. ply thickness (length scale cm). This gives an idea of the physically intrinsic scales appearing: A "microscale", the scale of material heterogeneity and a "macroscale" related to the structural dimensions. The post critical behaviour of such a composite is driven by the accumulation of the failure mechanisms on the "microscale". This can be fiber or matrix cracking, debonding between the fibers in a filament, or between fiber and matrix.

This paper presents a model for 2D structures of fiber reinforced concrete, taking into account the material behaviour of the material components and their interaction on the microlevel by applying the Variational Multiscale Method. This method provides the inclusion of the nonlinear material behaviour on the microlevel projected on the macroscopic analysis model.

2 OVERVIEW

Multiscale methods are required, if the structural size is much larger than the smallest component, to be incorporated for the desired accuracy, i.e. if it is impossible to use the local necessary resolution for the entire structure. Some multiscale methods are developed to embed physical fine-scale properties, e.g. microstructural material layout or localisation effects, for the purpose of "model adaptivity". Others are introduced to reduce the discretisation error and are therefore an alternative to h-/p-adaptive methods. A further application is to provide stabilisation to the formulation.

The VMM was introduced by Hughes et al. [8] as a general framework for a large variety of multiscale problems in solid and fluid mechanics. The approach utilizes a variational projection between different scales whereas small scale information is incorporated into the coarse scale solution. Garikipati and Hughes [6] applied the VMM to localisation phenomena; Hughes [9] and Gravemeier [7] adopted the VMM for laminar and turbulent incompressible flow simulation. Masud [10] presents an application of the method for developing stabilized finite element formulations for small strain inelasticity.

According to Fish [5], the VMM can be regarded as a "superposition based method". These methods are based on a decomposition of the solution function $\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$ into global $\bar{\mathbf{u}}$ and local fluctuating displacements \mathbf{u}' . Various assumptions are made, to reduce the problem size in comparison to a DNS. These assumptions are naturally accompanied by a loss of information. For most of the meth-

ods, an interface between the global and the local model is defined, where the displacements \mathbf{u}' are assumed to vanish, i.e. \mathbf{u}' is then defined locally, resulting in a partial decoupling of the global–local equation system. The "superposition based methods" differ in the approximation of $\bar{\mathbf{u}}$ and \mathbf{u}' , the global and local mechanical models, the transfer between the scales and the solution of the global–local equation system. Another representative of the superposition based methods is for example the s–version of FEM (Fish [4]), developed as an alternative to the h- and p-adaptive methods to reduce the discretisation error. Belytschko [1] developed the "spectral overlay method" to enhance the formulation for problems with high gradients, e.g. for localisation. Bridging the scales for strong discontinuity problems and stabilisation of the formulation by introducing the possibility of displacement jumps in the FE-formulations is performed in the "Strong Discontinuity Approach" (Simo et al. [12]) with local additional DOF's and with the "XFEM" (Belytschko et al. [11]), where the additional DOF's are global field parameters.

Another direction followed in multiscale modelling for heterogenous materials are mathematical and numerical homogenisation and expansion methods. These are based on the assumption of scale separation, i.e. the scale of material heterogeneity is so small compared to the structure's scale, that this scale is not resolved for a finite structural part, as it is done in a superposition based method, but the stress-strain behaviour of a structural point is described by a so-called Representative Volume Element (RVE). Fish [5] developed a multigrid method for problems with heterogeneous materials using mathematical homogenisation for the macro–response and high frequencies of the solution being resolved by relaxation methods using a special transfer operator.

3 CONCEPT OF VMM

The VMM was, according to Hughes et al. [8], motivated by the fact, that standard Galerkin methods are not robust in the presence of multiscale phenomena. The method utilizes an additive decomposition of the solution \mathbf{u} into coarse $\bar{\mathbf{u}}$ and fine \mathbf{u}' scale components $\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$. Likewise an additive split for the test functions $\delta\mathbf{u}$ is introduced, assuming linear independence of the coarse and fine solution and test function spaces: $\delta\mathbf{u} = \delta\bar{\mathbf{u}} + \delta\mathbf{u}'$. Starting from an abstract BVP,

$$\text{Find } \mathbf{u} \text{ such that} \quad \begin{aligned} \mathcal{L}\mathbf{u} &= \mathbf{f} && \text{in } \Omega \\ \mathbf{u} &= \hat{\mathbf{u}} && \text{on } \Gamma. \end{aligned} \quad (1)$$

\mathcal{L} being a differential operator, \mathbf{f} and $\hat{\mathbf{u}}$ given and Ω a bounded domain in \mathbb{R}^3 with smooth boundary Γ . The corresponding weak form reads

$$a(\delta\mathbf{u}, \mathbf{u}) = (\delta\mathbf{u}, \mathbf{f}). \quad (2)$$

two interacting nonlinear weak form expressions arise, denoted coarse and fine scale problem.

$$\begin{aligned} \text{coarse scale problem:} & \quad a(\delta\bar{\mathbf{u}}, \bar{\mathbf{u}}) + a(\delta\bar{\mathbf{u}}, \mathbf{u}') = (\delta\bar{\mathbf{u}}, \mathbf{f}) \\ \text{fine scale problem:} & \quad a(\delta\mathbf{u}', \bar{\mathbf{u}}) + a(\delta\mathbf{u}', \mathbf{u}') = (\delta\mathbf{u}', \mathbf{f}). \end{aligned} \quad (3)$$

(\cdot, \cdot) being the $L_2(\Omega)$ inner product, and $a(\delta\mathbf{u}, \mathbf{u}) = (\delta\mathbf{u}, \mathcal{L}\mathbf{u})$. Solving for $\mathbf{u}' = \mathbf{u}'(\bar{\mathbf{u}})$ as a function of $\bar{\mathbf{u}}$, and inserting this solution into the coarse scale equation results in a model, formulated exclusively in the coarse scale displacements, but including the effect of the fine scale solution onto the coarse one by an additional term, compared to a standard Galerkin formulation.

No matter whether \mathbf{u}' is defined locally or globally, the effect of \mathbf{u}' on $\bar{\mathbf{u}}$ is always nonlocal. Hughes et al. [8] showed the analogy of this methodology to stabilized methods for elementwise defined \mathbf{u}' .

4 APPLICATION OF THE VMM TO FIBROUS COMPOSITES

In the following the VMM is applied to a 2D-model of fiber reinforced cement under the assumption of small strains, taking into account nonlinear material behaviour of the components.

4.1. Subdivision of the domain

Following the policy "as accurate as necessary, but not more", the multiscale scale separation will be performed only in a part of the domain Ω . At every load level, Ω is cut into a part Ω^d , where a multiscale analysis is necessary for the desired accuracy of the model and the remaining part $\Omega^{el} = \Omega / \Omega^d$, as depicted in Fig. 1. This subdivision changes during the loading process. The stress-strain relation $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{\varepsilon}' + \bar{\boldsymbol{\varepsilon}}, \text{history})$ in Ω^d , called "micromaterial law", is specified by a damage law for the two components fiber and concrete. Possible crack evolution in the intermediate layer, the interface between concrete and fibers, is described by a regularized strong discontinuity approach. The traction-crack opening relationship will be defined by damage mechanics as well, according to Chaboche et al. [2] and Döbert [3]. In Ω^{el} a homogenised elastic material law, the "macromaterial law" $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\bar{\boldsymbol{\varepsilon}})$ is defined. At the boundary between Ω^d and Ω^{el} Dirichlet conditions $\mathbf{u}' = \mathbf{0}$ have to be fulfilled to ensure displacement continuity.

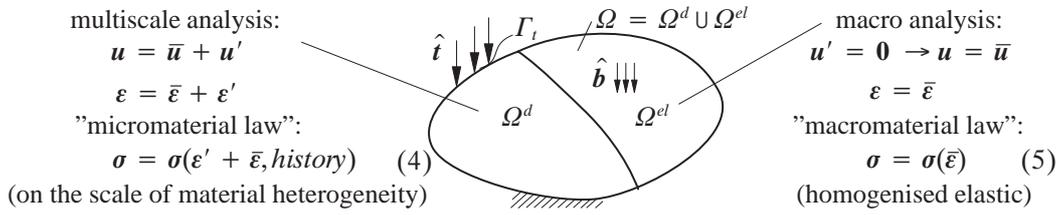


Figure 1: Subdivision of domain Ω at a certain load level

4.1.1. Micromaterial Law

In the domain Ω^d a classical isotropic strain based (1-d)-damage law serves as constitutive law for the fibers and the matrix material, respectively. The interfaces, a thin coating of the fibers, play an important role in the stress transfer of a composite. The displacement jump $[\mathbf{u}]$, appearing in this film, is regularised by a linear interpolation over the interface thickness t , see Fig. 2. The regularised strains $\boldsymbol{\varepsilon}$ in the interface are given by

$$\boldsymbol{\varepsilon} = \frac{1}{t} \text{sym}([\mathbf{u}] \otimes \mathbf{n}) \quad \text{for } \mathbf{x} \text{ in } \Omega^{IF}. \quad (6)$$

The constitutive equations, expressed as the relation between the traction $\mathbf{t} = [t_n \ t_t]^T$ and the displacement jump $[\mathbf{u}] = [[u_n] \ [u_t]]^T$ normal and tangential to the interface, distinguish the cases:

- normal tension or shear: softening behaviour described by damage model,
- normal compression: elastic behaviour,
- normal compression and shear: elastic in normal direction, damaging combined with contact friction behaviour, applying plasticity, in tangential direction

In the domain of the interface, the virtual internal energy can be transformed to

$$\delta W^{int} = \int_{\Omega^{IF}} \delta \boldsymbol{\varepsilon} : \boldsymbol{\sigma} \, dV = \int_{\Gamma^{IF}} [\delta \mathbf{u}] \cdot \mathbf{t} \, dA. \quad (7)$$

4.1.2. Macromaterial Law

In Ω^{el} it is assumed that the strains are small, that all composite components behave elastically. An averaged elastic material law for the composite, with material parameters extracted from a preceding "homogenisation" procedure, and the assumption $\mathbf{u}' = \mathbf{0}$ are sufficient.

4.1.3. Condition of Initialisation

An equivalent strain measure $\varepsilon_v(\boldsymbol{\varepsilon})$ is introduced to determine the region Ω^d . It is used, to decide for each Finite Element in a load step whether or not the macro-analysis with the macromaterial law

is sufficient in this Element. The definition of $\varepsilon_v(\boldsymbol{\varepsilon})$ depends on the special material layout of a composite and $\varepsilon_v(\boldsymbol{\varepsilon}) = \varepsilon_v^0$ determines the limit of elasticity.

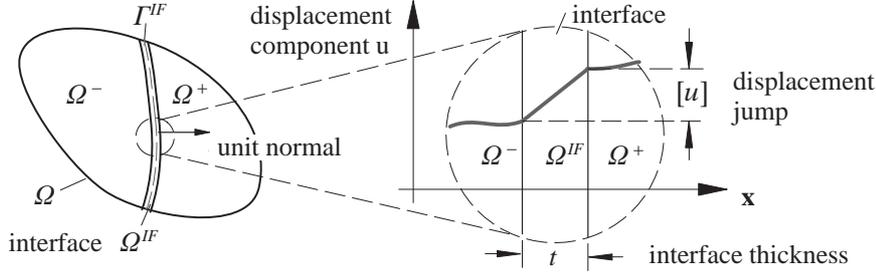


Figure 2: Kinematics in the interfaces

4.2. Weak form

Starting point is the weak form of the boundary value problem in micro resolution, the formulation for a DNS of the problem, analogous to (2)

$$\int_{\Omega} \delta \varepsilon_{ij} \sigma_{ij} dV = \int_{\Omega/\Gamma^{IF}} \delta \varepsilon_{ij} \sigma_{ij} dV + \int_{\Gamma^{IF}} [\delta u_i] t_i dA = \int_{\Omega} \delta u_i \hat{b}_i dV + \int_{\Gamma^t} \delta u_i \hat{t}_i dA. \quad (8)$$

Thereby \hat{b}_i denote components of the body forces and \hat{t}_i traction loads acting on the Neumann boundary Γ_t . The stresses are driven by the micromaterial law (4). For the kinematic quantities, the following decomposition into coarse and small scale variables holds

$$\mathbf{u} = \begin{cases} \bar{\mathbf{u}} + \mathbf{u}' & \text{in } \Omega^d \\ \bar{\mathbf{u}} & \text{in } \Omega^{el} \end{cases} \quad \boldsymbol{\varepsilon} = \begin{cases} \bar{\boldsymbol{\varepsilon}} + \boldsymbol{\varepsilon}' & \text{in } \Omega^d \\ \bar{\boldsymbol{\varepsilon}} & \text{in } \Omega^{el} \end{cases} \quad [\mathbf{u}] = \begin{cases} [\bar{\mathbf{u}}] + [\mathbf{u}'] & \text{in } \Omega^d \\ [\bar{\mathbf{u}}] & \text{in } \Omega^{el}. \end{cases} \quad (9)$$

The scale separation for the test functions reads

$$\delta \mathbf{u} = \begin{cases} \delta \bar{\mathbf{u}} + \delta \mathbf{u}' & \text{in } \Omega^d \\ \delta \bar{\mathbf{u}} & \text{in } \Omega^{el} \end{cases} \quad \delta \boldsymbol{\varepsilon} = \begin{cases} \delta \bar{\boldsymbol{\varepsilon}} + \delta \boldsymbol{\varepsilon}' & \text{in } \Omega^d \\ \delta \bar{\boldsymbol{\varepsilon}} & \text{in } \Omega^{el} \end{cases} \quad [\delta \mathbf{u}] = \begin{cases} [\delta \bar{\mathbf{u}}] + [\delta \mathbf{u}'] & \text{in } \Omega^d \\ [\delta \bar{\mathbf{u}}] & \text{in } \Omega^{el}. \end{cases} \quad (10)$$

Due to the assumed linear independence of the spaces for the coarse and fine scale functions, two interacting nonlinear weak form expressions on both scales arise by the split (9) and (10).

$$\begin{aligned} &\text{coarse scale} \\ &\text{problem on } \Omega^{el} \cup \Omega^d: \quad \int_{\Omega} \delta \bar{\varepsilon}_{ij} \sigma_{ij} dV = \int_{\Omega} \delta \bar{u}_i \hat{b}_i dV + \int_{\Gamma^t} \delta \bar{u}_i \hat{t}_i dA \end{aligned} \quad (11)$$

$$\begin{aligned} &\text{fine scale} \\ &\text{problem on } \Omega^d: \quad \int_{\Omega^d/\Gamma^{IF}} \delta \varepsilon'_{ij} \sigma_{ij} dV + \int_{\Gamma^{IF} \in \Omega^d} [\delta u'_i] t_i dA = \int_{\Omega^d} \delta u'_i \hat{b}_i dV + \int_{\Gamma^d} \delta u'_i \hat{t}_i dA \end{aligned}$$

$$\begin{aligned} \text{with:} \quad \sigma_{ij} &= \sigma_{ij} \text{ (macromaterial, } \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} \text{)} && \text{in } \Omega^{el} \\ \sigma_{ij} &= \sigma_{ij} \text{ (micromaterial, } \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} + \boldsymbol{\varepsilon}', \text{ history)} && \text{in } \Omega^d / \Gamma^{IF} \\ t_i &= t_i \text{ (micromaterial, } [\mathbf{u}] = [\bar{\mathbf{u}}] + [\mathbf{u}'], \text{ history)} && \text{in } \Gamma^{IF} \in \Omega^d \end{aligned}$$

4.3. Discretisation of the model

As an analytical solution of the "fine scale problem" can hardly be found, both equations are solved by the Finite Element Method. Due to physical evidence showing a local influence of damage the fine scale solution may be limited to small subdomains. From this, we assume as a first approximation, that \mathbf{u}' is restricted to the elements of the coarse scale problem so that the fine scale problem decouples elementwise. This assumption depends of course on the resolution of the coarse scale

problem and has to be verified by comparing the results to those of a DNS. For bilinear interpolation of $\bar{\mathbf{u}}$ and elementwise restriction of \mathbf{u}' , the spaces of the ansatzfunctions for \mathbf{u}' and $\bar{\mathbf{u}}$, resp. $\delta\mathbf{u}'$ and $\delta\bar{\mathbf{u}}$ are linearly independent. Coarse and fine scale displacements are discretised as follows

$$\begin{aligned}
\text{coarse scale} \quad & \bar{\mathbf{u}} = \bar{\mathbf{N}} \bar{\mathbf{d}} \quad \bar{\boldsymbol{\varepsilon}} = \bar{\mathbf{B}} \bar{\mathbf{d}} \quad \text{and} \quad \delta\bar{\mathbf{u}} = \bar{\mathbf{N}} \delta\bar{\mathbf{d}} \quad \delta\bar{\boldsymbol{\varepsilon}} = \bar{\mathbf{B}} \delta\bar{\mathbf{d}} \\
\text{variables:} \quad & [\bar{\mathbf{u}}] = \mathbf{A} \mathbf{N}' \mathbf{L} \mathbf{V} \bar{\mathbf{d}} \\
\text{fine scale} \quad & \mathbf{u}' = \mathbf{N}' \mathbf{d}' \quad \boldsymbol{\varepsilon}' = \mathbf{B}' \mathbf{d}' \quad \text{and} \quad \delta\mathbf{u}' = \mathbf{N}' \delta\mathbf{d}' \quad \delta\boldsymbol{\varepsilon}' = \mathbf{B}' \delta\mathbf{d}' \\
\text{variables:} \quad & [\mathbf{u}'] = \mathbf{A} \mathbf{N}' \mathbf{L} \mathbf{d}'.
\end{aligned} \tag{12}$$

The discrete fine scale variables are supported on submeshes, locally defined on the elements of the coarse scale discretisation (see Fig. 3). $\bar{\mathbf{d}}$ are the nodal coarse scale DOF's, $\bar{\mathbf{N}}$ are bilinear coarse scale shapefunctions, $\bar{\mathbf{B}}$ their derivatives with respect to \mathbf{x} . \mathbf{A} transforms the displacement jumps into normal and tangential directions to the appropriate interface. \mathbf{L} filters the degrees of freedom producing the displacement jump. \mathbf{V} contains the shapefunctions $\bar{\mathbf{N}}$ for the coarse scale displacements at the submesh nodes. \mathbf{d}' are the nodal fine scale DOF's, \mathbf{N}' the fine scale ansatzfunctions and \mathbf{B}' their derivatives with respect to \mathbf{x} .

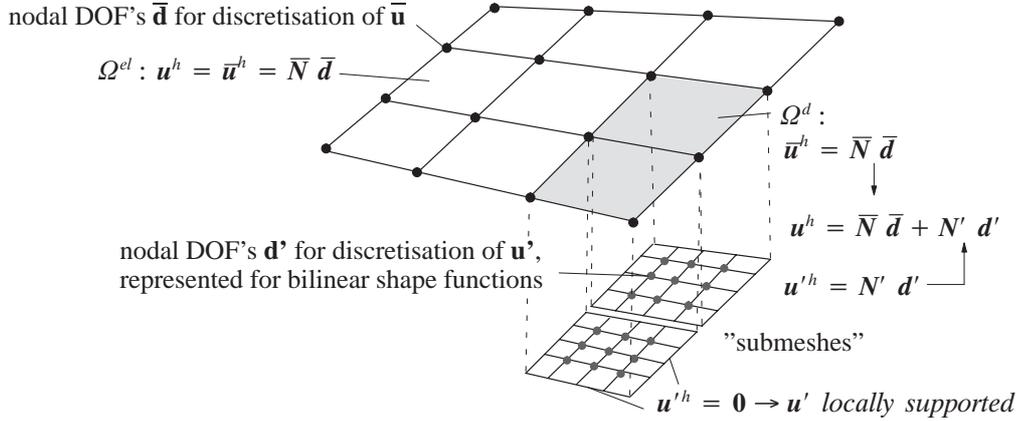


Figure 3: Discretisation

In the presented procedure the local "mesh refinement" is accompanied by a change in the model as a significant difference to hierarchical concepts.

4.4. Linearisation and Solution

The nonlinear coupled problems have to be linearised for a solution applying the Newton-Raphson method.

linearised coarse scale problem:

$$\begin{aligned}
& \left[\int_{\Omega^{el}} \bar{\boldsymbol{\varepsilon}}_{ij,\bar{d}_I} \frac{\partial \sigma_{ij}}{\partial \bar{\boldsymbol{\varepsilon}}_{kl}} \bar{\boldsymbol{\varepsilon}}_{kl,\bar{d}_J} dV + \int_{\Omega^{d'} \setminus \Gamma^{IF}} \bar{\boldsymbol{\varepsilon}}_{ij,\bar{d}_I} \frac{\partial \sigma_{ij}}{\partial \boldsymbol{\varepsilon}'_{kl}} \bar{\boldsymbol{\varepsilon}}_{kl,\bar{d}_J} dV + \int_{\Gamma^{IF} \in \Omega^{d'}} [\bar{u}_i]_{,\bar{d}_I} \frac{\partial t_i}{\partial [u_j]} [u_j]_{,\bar{d}_J} dA \right] \Delta \bar{\mathbf{d}}_J + \\
& + \left[\int_{\Omega^{d'} \setminus \Gamma^{IF}} \bar{\boldsymbol{\varepsilon}}_{ij,\bar{d}_I} \frac{\partial \sigma_{ij}}{\partial \boldsymbol{\varepsilon}'_{kl}} \boldsymbol{\varepsilon}'_{kl,d'_J} dV + \int_{\Gamma^{IF} \in \Omega^{d'}} [\bar{u}_i]_{,\bar{d}_I} \frac{\partial t_i}{\partial [u_j]} [u_j]_{,d'_J} dA \right] \Delta \mathbf{d}'_J \tag{13} \\
& = \int_{\Omega} \bar{u}_{i,\bar{d}_I} \hat{b}_i dV + \int_{\Gamma^t} \bar{u}_{i,\bar{d}_I} \hat{t}_i dA - \int_{\Omega^{el}} \bar{\boldsymbol{\varepsilon}}_{ij,\bar{d}_I} \sigma_{ij}^0 dV - \int_{\Omega^{d'} \setminus \Gamma^{IF}} \bar{\boldsymbol{\varepsilon}}_{ij,\bar{d}_I} \sigma_{ij}^0 dV + \int_{\Gamma^{IF} \in \Omega^{d'}} [\bar{u}_i]_{,\bar{d}_I} t_i^0 dA
\end{aligned}$$

linearised fine scale problem for *each* macroelement ℓ in Ω^d :

$$\begin{aligned}
& \left[\int_{\Omega_\ell^d / \Gamma_\ell^{IF}} \varepsilon'_{ij,d'\ell} \frac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}} \bar{\varepsilon}_{kl,d'\ell} dV + \int_{\Gamma_\ell^{IF}} [u'_i]_{,d'\ell} \frac{\partial t_i}{\partial [u_j]} [u_j]_{,d'\ell} dA \right] \Delta \bar{d}_J^\ell + \\
& + \left[\int_{\Omega_\ell^d / \Gamma_\ell^{IF}} \varepsilon'_{ij,d'\ell} \frac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}} \varepsilon'_{kl,d'\ell} dV + \int_{\Gamma_\ell^{IF}} [u'_i]_{,d'\ell} \frac{\partial t_i}{\partial [u_j]} [u_j]_{,d'\ell} dA \right] \Delta d_J'^\ell \quad (14) \\
& = \int_{\Omega_\ell^d} u'_{i,d'\ell} \hat{b}_i dV - \int_{\Omega_\ell^d / \Gamma_\ell^{IF}} \varepsilon'_{ij,d'\ell} \sigma_{ij}^0 dV - \int_{\Gamma_\ell^{IF}} [u'_i]_{,d'\ell} T_i^0 dA.
\end{aligned}$$

The linearised fine scale problems can be used to eliminate the small scale DOF's $\Delta \mathbf{d}'$ by static condensation than. The linearised coarse scale problem depends exclusively on the coarse scale DOF's $\Delta \bar{\mathbf{d}}$, enhanced by the solution of fine scales.

5 Perspectives

This study is still in progress. It is important to find a more efficient method to avoid the inversion of the small scale stiffness matrix for the static condensation of the small scale DOF's \mathbf{d}' . The size of this matrix depends on the radius of influence of the small scale solution onto the large scale. Other possibilities to solve the fine scale problem more accurate, see Gravemeier [7] have to be considered. In the presentation several numerical examples will be given.

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