CONCURRENT MULTISCALE ANALYSIS OF HETEROGENEOUS MATERIALS

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Abstract. Concurrent multiscale analysis of quasi-brittle heterogeneous materials such as concrete and rock is conducted employing non-overlapping domain decomposition techniques. Initially, a coarse discretization with effective properties is considered at each domain. A zoom-in technique is performed at those domains in which non-linearities take place. The coarse mesh is replaced with a fine discretization which includes the lower scale constituents, e.g. aggregates or reinforcement. The present framework captures the interaction between the mesoscopic constituents and the strain/stress fields. The resulting crack path is in agreement with the one obtained with direct numerical simulations. It is shown that the interscale relations enforced at the interface between coarse and fine domains play an important role in the global response of the material.
1 INTRODUCTION

Multiscale analysis of materials used in engineering practice has recently become a leading research topic. Several phenomena such as cracking and failure are clearly multiscale and their simulation requires sophisticated computational techniques. This is the case for concrete material (Figure 1) where the mesoscopic constituents such as aggregates and reinforcement play a crucial role during fracture processes.

The main objective of a general multiscale analysis is to capture the origin and evolution of the targeted physical processes at a fine scale and their impact at a coarse scale of observation. This can be achieved by accounting for a refined representation of the material which eventually requires a different simulation strategy. Examples of such techniques can be found in [11] where fracture in concrete is simulated with the use of a lattice-particle model whereas standard finite elements (FE) are employed for the linear elastic region. The study of localization phenomena in granular frictional materials presented in [10] considers a particle model at the areas affected by large deformations and standard FEs at the rest of the sample. Other multiscale strategies are based on local material refinement and scale resolution without varying the computational approach—FEs are employed at both macro and mesoscopic scales in [13–15].

The approach adopted in this manuscript can be classified in this second group and processes both macro and mesoscopic scales in a concurrent manner. The focus is on the multiscale analysis of concrete-like samples and the influence of interscale links between macro and mesoscopic material resolutions.

2 CONCURRENT MULTISCALE ANALYSIS

In these techniques the effect of micro- and mesoscopic constituents is taken into account by increasing the resolution of the material scale at certain areas of interest. In this scenario, the whole fine scale region is considered in the computations as opposed to hierarchical methods where the behaviour of a reduced fine scale area is representative for the one at a larger scale. For this reason, concurrent techniques are recommended for multiscale analyses that require a moderate jump in scales due to the limit in computational resources. However, the interaction between fine scale heterogeneities and global stress and strain fields is accounted for with the same level of detail as in a direct numerical simulation (DNS).

Most of the concurrent multiscale methods consider a strong coupling between micro/meso and macro scales since displacement compatibility and global equilibrium are enforced across the whole structure [12, 13]. When large systems need to be resolved, the use of domain decomposition techniques is preferred. The present contribution falls in this group and shows some
similarities with the methods described in [14–16].

2.1 Multiscale domain decomposition modelling

Consider the equilibrium problem of the heterogeneous solid $\Omega$ with boundary conditions defined in Figure 2. The body $\Omega$ is split into $N_s$ non-overlapping domains $\Omega^{(s)}$ with $s \in [1, N_s]$. The interface between domains is denoted by $\Gamma_1$ (Figure 2). Continuity of the total displacement field $u$ at the interface $\Gamma_1$ between non-overlapping domains $s$ and $p$ implies

$$u^{(s)} = u^{(p)}$$

and is satisfied by means of linear multipoint constraints (LMPCs) as proposed in the Finite Element Tearing and Interconnecting (FETI) method [1].

In a general multiscale analysis, different resolutions, i.e. coarse, c, and fine, f, may co-exist in a decomposed sample (Figure 2). In this situation, the resulting interface $\Gamma_1 = \Gamma_1^{cc} \cup \Gamma_1^{ff} \cup \Gamma_1^{cf}$, where the superscripts $cc$, $ff$ and $cf$ denote coarse-to-coarse, fine-to-fine, and coarse-to-fine mesh connection, respectively. The interfaces $\Gamma_1^{cc}$ and $\Gamma_1^{ff}$ are conforming while the interface $\Gamma_1^{cf}$ is non-conforming. In this approach, the resulting boundary of a fine scale mesh is obtained by subdividing the boundary discretization of the initial matching mesh. In this manner, the non-conforming interface $\Gamma_1^{cf}$ contains a number of matching and non-matching nodes. All matching nodes in $\Gamma_1$ are referred to as independent while non-matching nodes are called dependent in the remaining of this text.

The continuity condition in (1) can be expressed using a signed Boolean matrix $B^{(s)}$ for all independent degrees of freedom (DOFs) and a constraint matrix $C^{(s)}$ for the dependent DOFs. The modified matrices $\tilde{B}^{(s)}$ are defined by row-wise concatenation of the Boolean matrices $B^{(s)}$.
and the constraint matrices $C^{(s)}$ as

$$
\begin{bmatrix}
\vec{B}^{(1)} & \ldots & \vec{B}^{(N_d)}
\end{bmatrix}
= 
\begin{bmatrix}
B^{(1)} & \ldots & B^{(N_d)}
C^{(1)} & \ldots & C^{(N_d)}
\end{bmatrix}.
$$

A field of Lagrange multipliers $\lambda$ is utilized to account for the LMPCs of the independent DOFs while the Lagrange multipliers $\mu$ are related with the LMPCs of the dependent DOFs (Figure 2 bottom). Hence the extended field of Lagrange multipliers

$$
\Lambda = \begin{bmatrix} \lambda \\ \mu \end{bmatrix}.
$$

After spatial discretization using standard finite element procedures, the discrete form of the equilibrium equations for each domain together with the interface compatibility condition, read

$$
K^{(s)}u^{(s)} + \sum_{\sigma=1}^{N_s} \vec{B}^{(s)}\Lambda = f^{(s)} \quad \forall s,
$$

where $K^{(s)}$, $f^{(s)}$, and $u^{(s)}$ denote domain stiffness matrix, force vector and displacement vector, respectively.

As described in [7] the main goal of the presented framework is the multiscale analysis of fracture processes in quasi-brittle materials. In this context, the fine scale domains are only utilized in those regions where the dominant non-linear processes, i.e. damage growth and coalescence, take place. The rest of the linear regions can be modeled with a coarse scale resolution with effective elastic properties. During an adaptive multiscale analysis, the number of fine domains is expected to increase and the structure of the modified matrices $B^{(s)}$ needs to be recomputed as soon as the spatial resolution of a domain is altered. A coarse scale domain is updated to its corresponding fine scale resolution with the use of a zoom-in technique and relaxation stages as described in detail in [7, 8]. The moment at which a zoom-in takes place is dictated by a prediction of an internal quantity (e.g., based on strain or stress tensors) as indicated in [6, 7].

### 2.2 Micro-to-macro connection

At a non-conforming interface $\Gamma_{1}^{cf}$ (top of Figure 3) an identity constraint is enforced by the signed Boolean matrices $B^{(s)}$ for all independent (ind) DOFs such that

$$
u^{f}_{\text{ind},i} = u^{c}_{\text{ind},i}, \quad i = 1, 2,
$$

where $u^{f}_{\text{ind},1}$ and $u^{f}_{\text{ind},2}$ represent the displacement vectors of two consecutive independent nodes along $\Gamma_{1}^{cf}$. However, different interscale links can be defined by constraining the dependent (dep) DOFs through the constraint matrices $C^{(s)}$. A master-slave relation is set between the displacements of dependent $u^{f}_{\text{dep},i}$ and independent $u^{f}_{\text{ind},i}$ nodes at the interface $\Gamma_{1}^{cf}$. The most common choice is to enforce strong compatibility between coarse and fine scale fields using full collocation (Figure 3) which can be expressed as

$$
u^{f,col}_{\text{dep},i} = u^{c}(x_i), \quad i = 1, nf,
$$
Non-conforming interface

Coarse mesh (c) Fine mesh (f)

Coarse side Fine side

$u^c_{\text{ind,2}}$ $u^f_{\text{ind,2}}$

$u^f_{\text{dep},n}$

$u^f_{\text{dep},l}$

$u^c_{\text{ind,1}}$

$u^f_{\text{ind,1}}$

Strong compatibility

Weak compatibility

Full collocation

$$[u^f_{\text{dep,j}}]^{\text{col}} = 0$$

Normal collocation

$$[u^f_{\text{dep,j}}]^{\text{col}} \cdot n = 0$$

Average compatibility

$$\int_{\Gamma^c_{\text{ef}}} (u^f(x) - u^c(x)) \, d\Gamma^c_{\text{ef}} = 0$$

Average compatibility with stiffness weighting

$$\int_{\Gamma^c_{\text{ef}}} (k_j f_j(x) u^f_j(x) - k_j f_j u^c_j(x)) \, d\Gamma^c_{\text{ef}} = 0,$$

$$j = 1, N_{\text{DOF}}$$

Figure 3: Strong and weak micro-macro connections.
$n_f$ being the number of dependent nodes between two consecutive independent nodes at $\Gamma_i^{cf}$.

Defining the deviation from the collocation constraint as

$$\left[ u^f_{\text{dep},i} \right]^{\text{col}} = u^f_{\text{dep},i} - u^f_{\text{dep},i}$$

full collocation is satisfied when

$$\left[ u^f_{\text{dep},i} \right]^{\text{col}} = 0, \quad i = 1,n_f. \quad (7)$$

A modified version of the collocation technique was recently introduced in [8] where strong compatibility is only enforced along the normal direction $n$ of the linear segment $\Gamma_i^{cf}$. In this view, normal collocation is satisfied when the normal component of the deviation is nullified. The corresponding constraint equation can therefore be written as

$$\left[ u^f_{\text{dep},i} \right]^{\text{col}} \cdot n = 0, \quad i = 1,n_f. \quad (8)$$

Physically, this is equivalent to state that the coarse and fine interfaces are conforming in terms of the resulting deformed geometry.

The compatibility condition at the interface between coarse and fine domains can be expressed in an average sense as

$$\int_{\Gamma_i^{cf}} (u^f(x) - u^c(x)) \, d\Gamma_i^{cf} = 0. \quad (10)$$

The corresponding $C^{(s)}$ matrices are found using the shape functions of the elements along the interface. The constraint in (10) essentially applies a constant force field $\Lambda(x)$ along the interface $\Gamma_i^{cf}$ delimited by two contiguous independent nodes in order to minimize the gap between the non-matching meshes (Figure 3).

As shown in [8], weighting functions based on nodal stiffness enforce a compatibility closer to the exact one for highly heterogeneous interfaces. Such a weak compatibility with stiffness weighting reads

$$\int_{\Gamma_i^{cf}} (k_j^f(x)u^f_j(x) - k_j^c u^c_j(x)) \, d\Gamma_i^{cf} = 0, \quad j = 1,N_{\text{DOF}}, \quad (11)$$

where $N_{\text{DOF}}$ is the number of DOFs per node and $k_j^f(x)$ represents a continuous function between two independent nodes along $\Gamma_i^{cf}$. The values of $k_j^f(x)$ are interpolated using the fine mesh shape functions at the interface and the diagonal stiffness coefficients $K_{ij}$ of the fine resolution domain—the index $l$ corresponds to node $i$ (located at $x$) and DOF $j$. Conversely, $k_j^c$ is taken as a constant stiffness coefficient which corresponds to the average value $k_j^f(x)$ along the fine side of the interface as

$$k_j^c = \int_{\Gamma_i^{cf}} k_j^f(x) \, d\Gamma_i^{cf} \Bigg/ \int_{\Gamma_i^{cf}} d\Gamma_i^{cf}. \quad (12)$$

The condition in (12) guarantees consistency in the sense that exact compatibility would also satisfy (11). Note that the force field tying two incompatible meshes increases at stiff interface segments (Figure 3).
3 NUMERICAL EXAMPLES

Several multiscale analyses of a concrete-like material are summarized in this section. They are designed to test the basic features of the multiscale approach introduced in Section 2.

3.1 Tensile test

A concrete sample is subjected to tensile loading as depicted in Figure 4. The body is decomposed into three non-overlapping domains. As shown in Figure 5, homogeneous coarse scale domains are represented by a single bilinear quadrilateral element whereas fine scale domains contain the mesoscale constituents and are meshed using linear triangular elements. Note that the mesoscopic structure is obtained by a two-dimensional translation of a material unit cell with periodic boundaries.

A gradient-enhanced damage model [2] is used in this study to model crack growth and coalescence in the material. A list of material parameters for each phase is given in Table 1. Initially, a set of coarse scale domains is considered with effective elastic properties considering periodic boundary conditions for a representative volume element (RVE). A representative quantity of the non-local equivalent strain $\varepsilon_{nl}$ is computed for each domain and serves as an indicator for the appearance of non-linearity (cf. [6]). The damage initiation threshold $K_0$ of the homogeneous bulk is taken as the minimum damage initiation threshold of the three concrete phases.

![Figure 4: Description of the tensile test for the concrete specimen.](image)

<table>
<thead>
<tr>
<th>Material parameters</th>
<th>Aggregates</th>
<th>Matrix</th>
<th>ITZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>Young’s modulus [GPa]</td>
<td>35.0</td>
<td>30.0</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson’s ratio [-]</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$\varepsilon_{nl}$</td>
<td>Non-local equivalent strain [-]</td>
<td>Mazars</td>
<td>Mazars</td>
</tr>
<tr>
<td>$K_0$</td>
<td>Damage initiation threshold [-]</td>
<td>dummy</td>
<td>$0.124 \times 10^{-4}$</td>
</tr>
<tr>
<td>$c$</td>
<td>Gradient parameter [mm$^2$]</td>
<td>0.75</td>
<td>0.75</td>
</tr>
<tr>
<td>$\omega(\kappa)$</td>
<td>Damage evolution law [-]</td>
<td>Exponential</td>
<td>Exponential</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Residual stress parameter [-]</td>
<td>0.999</td>
<td>0.999</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Softening rate parameter [-]</td>
<td>500</td>
<td>500</td>
</tr>
</tbody>
</table>

Table 1: Material data for the concrete specimen.

Due to the initial constant strain and stress distribution in the homogeneous bulk, a zoom-in is performed simultaneously for all domains. Damage nucleates at the ITZ and propagates...
through the matrix giving rise to a series of damage bands perpendicular to the loading direction (Figure 6). Due to the non-symmetry of the mesoscale geometry and the applied boundary conditions strains localize at the leftmost section of the sample with the appearance of a dominant damage band.

The applied load against the displacement registered at the right edge of the sample is compared to the one obtained with a DNS (Figure 7). The differences between both simulations are hardly visible except from the stage in which zoom-in is applied and a load variation is registered.

### 3.2 Influence of the interscale link in bending test

In this example a bending test is performed on a concrete beam (Figure 8). The sample is decomposed into two non-overlapping domains with the same geometry (Figure 9). The idea is to test different micro-to-macro connections that glue the different scale resolutions shown at the top of Figure 10. In this case the multiscale analysis is “static” and the resolutions do not change during the test. A linear elastic model is used for the homogeneous bulk and the three concrete phases considering the same moduli as in the previous section (Table 1). Two different coarse resolutions (discretizations I and II) are considered. Effective elastic properties are retrieved from the same RVE used in Section 3.1. Note that for discretization II the area of
Figure 6: Damage evolution during the adaptive multiscale analysis of the tensile test. 25× displacement magnification.

Figure 7: Load-displacement curves for the tensile test DNS and multiscale analysis. The inset shows the close-up of the load-displacement curve around a zoom-in event.

the RVE is larger than the one of the coarse element integration points. However, the total area in which homogenization takes places is formed by the number of sub-areas with homogeneous properties. In this case the refinement is only employed to provide a higher flexibility to the coarse mesh and to avoid shear locking.

The bending stiffness of the system is calculated as the relation between the vertical components of the force and displacement at the right edge of the sample. Table 2 contains the
Figure 8: Boundary conditions for the bending test.

![Diagram with boundary conditions](image)

Figure 9: Domain decomposition and FE discretizations.

![Domain decomposition and FE discretizations](image)

In general, the use of discretization II provides the closest values to the reference stiffness $0.845 \times 10^3 \text{N/mm}$ obtained with a fine discretization at both domains. The full collocation constraint (8) turns out to perform better than the normal collocation constraint (9) when analyzing the deformation of the sample. In fact, the deformed configuration of the interface corresponding to the reference solution is a linear segment due to the small deformations assumption. In this view, the collocation constraints naturally provide an accurate deformation at the interface (Figure 10). Coincidently, normal collocation is able to provide a closer value to the reference one due to two counteracting effects: the too coarse domain (stiffening) and the loose compatibility (softening).

<table>
<thead>
<tr>
<th>Coarse mesh</th>
<th>Full col.</th>
<th>Normal col.</th>
<th>Av. comp.</th>
<th>Stiff. weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>0.906</td>
<td>0.832</td>
<td>0.697</td>
<td>0.697</td>
</tr>
<tr>
<td>II</td>
<td>0.846</td>
<td>0.845</td>
<td>0.846</td>
<td>0.847</td>
</tr>
</tbody>
</table>

Table 2: Global stiffness [$\times 10^3 \text{N/mm}$] for the static multiscale test with different interscale constraints. The reference stiffness of the DNS is $0.845 \times 10^3 \text{N/mm}$. 
The average compatibility constraint (10) and average compatibility with stiffness weighting (11) provide very similar results in this example. Only when using the coarse discretization II the stiffness weighting constraint turns out to be slightly stiffer than the standard average compatibility.

A mechanical characterization of the proposed interscale links for simpler heterogeneous
3.3 Wedge split test

A multiscale simulation of the wedge split test, sketched in Figure 11, is carried out. The concrete sample is decomposed into 34 non-overlapping domains and the notch $\Gamma^a$ is modeled by means of the traction free interface $\Gamma^f$. The fine scale discretization used for the different domains and the RVE sample are identical to the ones presented in the previous examples. The coarse discretization II employed in Section 3.2 is adopted here for the coarse scale domains. A gradient-enhanced damage model is adopted again and the material parameters for each phase are listed in Table 1. The adaptive multiscale strategy considered in Section 3.1 with a full collocation interscale link is adopted in this example.

![Figure 11: Boundary conditions (left) and domain decomposition (right) for the wedge split test.](image)

The damage evolution after zoom-in at domains affected by non-linearity is shown in Figure 12. Despite the symmetry in the boundary conditions and geometry of the sample the final crack path is not aligned with the notch. This is due to the heterogeneous mesostructure and its interaction with the stress and strain fields at the fine resolution.

As observed in Figure 13 the load-displacement curve is in agreement with the one of the DNS and differences are not visible after zooming at all domains involved in the non-linear processes. The overall cost of the multiscale analysis is clearly lower than the one of the DNS since during the computation domains remain coarse and linear unless needed to be refined.

4 CONCLUSIONS

The concurrent framework presented in this manuscript proves to be adequate for the multiscale analysis of failure phenomena of quasi-brittle materials such as concrete. The nucleation and evolution of fracture processes is well captured and the overall response turns out to be in agreement with the DNS. The computational cost of the analysis is essentially linked to the extension of the fracture process zone. In this scenario, the domain decomposition plays an important role since larger domains will trigger a larger refined area when zoom-in takes place.

interfaces is discussed in more detail in [8].
Different interscale relations can be supported by the current framework. It is observed that collocation techniques generally provide a stiffer link than average compatibility constraints.

Figure 12: Damage evolution during the adaptive multiscale analysis of the wedge split test. 100× displacement magnification.
Figure 13: Load-displacement curves for the wedge split test DNS and multiscale analysis. The inset shows the close-up of the load-displacement curve around a zoom-in event.

References


