DUAL DISCRETE AND CONTINUOUS MESO-SCALE MODELLING OF CONCRETE

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Abstract. *The present paper is devoted to the development of a software equipment that allows to model composite materials by both discrete and continuous modelling approaches. The aim is to create a geometrical and topological representation of a discrete lattice particle model as well as its 1:1 twin counterpart as modelled by a continuum FEM model. Both representations capture the heterogeneous composite structure at the meso-level. The presented results illustrate the ongoing initial phase of the efforts of the team in advanced modelling of damage propagation within concrete.*

Keywords

Discrete lattice modelling, continuum modelling, composite materials, damage propagation, FEM, DFEM

1. Introduction

The fracture process within concrete is a complex mechanism which is influenced by its highly heterogeneous inner structure. In general, the fracture propagation can be divided into several variants: (1) separation between aggregates and cement paste, (2) development of microcracks within the cement matrix, and (3) diffusion of microcracks through aggregates [1]. The interfacial transition zone (ITZ), i.e. the connecting bond of roughly 20μm between the cement matrix and the aggregates, is typically the weakest link within the composite structure. Frequently, it is the ITZ that initiates the specimen failure by reaching its tensile or shear strength.

The mentioned fracture processes take place at the tip of the notch of a specimen, at the tip of a developed crack, or in general within a region with high stress concentration, i.e. the fracture process zone (FPZ) [2,3]. The emergence of FPZ in front of the notch/crack tip is the main driver of the quasi-brittle response of composite materials after exceeding the peak load during a fracture experiment [4-7]. An intensive research of fracture properties of concrete has been ongoing for almost six decades [8]. The studies began based on the theory of linear elastic fracture mechanics (LEFM) [9] and later, the field developed into a distinctive research topic. Due to the aforementioned heterogeneity, the LEFM turns out as an insufficient tool for description of fracture processes within concrete. In its essence, LEFM considers only a single crack which is quite unlike the FPZ within concrete that contains many growing and interacting micro-cracks. To capture this phenomenon, improvements were made upon the classical LEFM to accommodate such a diffused character of damage: e.g. the two-parametric fracture model [10], the effective crack model [11], the double-*K* fracture model [12] or the notion of the size-effect [13].

In engineering practice, utilisation of such advanced material models enhances the reliability of designed structures and/or optimization of the amount of material used while increasing the service life of the construction. In the realm of the finite element method (FEM) software, frequently used are e.g. the concrete damage plasticity model [14], the plastic fracture model used in the ATENA software [15], and the microplane M7 model [16]. However, the mentioned models consider the material as homogeneous in the macro scale without a direct reference to the material heterogeneity on lower scales. In such cases, the inner heterogeneity is incorporated into the model through the constitutive law (eventually spatially variable). Nevertheless, it remains a challenge for these models to capture the transition between a diffused damage to a clear discontinuity (fracture). Remedies of this drawback were proposed such as the visco-plastic modification in general form [17] or using a non-local approach, either in integral form due to Pijaudier-Cabot [18] or the gradient formulation by Peerlings [19]. Possibilities are also the Phase-field model [20] or the XFEM formulation [21]. Still, an accurate modelling of anisotropy emerging during loading remains a challenge as does the independence of model response on the orientation and size of the finite element mesh.

A direct counterpart to the models based on the continuum mechanics are the discrete meso-scale models

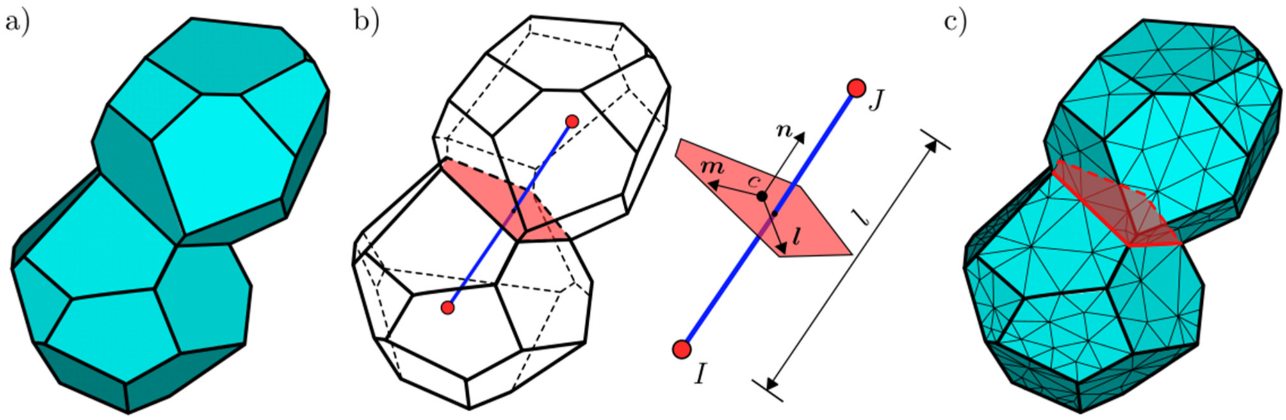

Fig. 1: Discrete and continuum modelling approaches: a) couple of aggregate volumes being modelled, b) discrete particle representation by a mechanical element, c) full continuum modelling of volumes with cohesive elements inserted on contact of aggregates.

that model the individual heterogeneous aggregates [22], prescribing constitutive laws at the meso-scale of the modelled inner material structure [23]. The meso-models allow a description of the damage and cracking evolution at the level of connection between the individual aggregates and the cement paste. This approach allows to capture the tensile softening of concrete after reaching peak load. Examples of meso-scale modelling approaches are the discrete finite element method (FEM) [24] and the lattice particle modelling (LDPM) [25]. The FEM models the individual aggregates as continuous and the interactions between aggregates and their surroundings are described through zero-thickness contact elements or by modelling cement paste with above-mentioned nonlinear material models. Typically, cohesive elements are inserted right between individual aggregates [26]. The high fidelity of such models comes at the expense of high computational demands of the solution as well as the assembly of the geometry and topology of the model itself.

With the ability of the meso-models to capture the inner heterogeneous structure comes the challenge of the actual generation of an accurate representation of such a structure. The representation of the inner structure is a parameter that critically influences the actual damage evolution and further crack propagation. It is reasonable to assume that the aggregates are distributed within a homogeneous cement paste. The positions of aggregates are affected by mixing and compacting of the concrete mixture. Furthermore, pores emerge during concrete congealing that might cause local stress concentrations, possibly initiating growth of micro-cracks. A number of approaches to meso-structure modelling was proposed during recent years. For further reading, see [27,28].

2. Dual discrete and continuous meso-scale modelling

The overarching aim of the research and development efforts is to create a framework that allows to generate: (i) the geometry and topology of a meso-scale discrete particle model of concrete and (ii) a corresponding 1:1 twin continuous FEM model of such a heterogeneous structure, see Fig. 1 and Fig. 2. For the solution of the discrete model, the Open Academic Solver (OAS) [29] project is used, given the experience of the team with its development. The continuous FEM model is to be executed within the ANSYS framework [30]. Both the modelling approaches are illustrated in Fig. 2. Given the experience of the authors with concrete damage and fatigue modelling using discrete models and continuum approaches, it is of great interest to have the possibility to create a continuous representation of a geometrically and topologically identical structure to the discrete particle model.

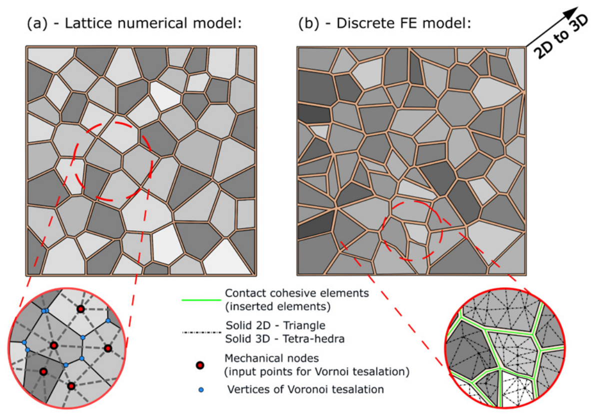

Fig. 2: Illustration of the meso-modelling approaches of a heterogeneous structure: (a) the discrete particle model, (b) the continuous model.

The discrete particle model assumes the interparticle contact, see Fig. 1a, to be represented by a single 2D mechanical element, see Fig. 1b. The aggregate volumes are created by Voronoi tessellation using randomly placed generator points according to a given minimum grain size, d_{min}. The mechanical elements connect the Voronoi generator points that are considered as centres of individual aggregates. In other words, the mechanical mesh corresponds with the

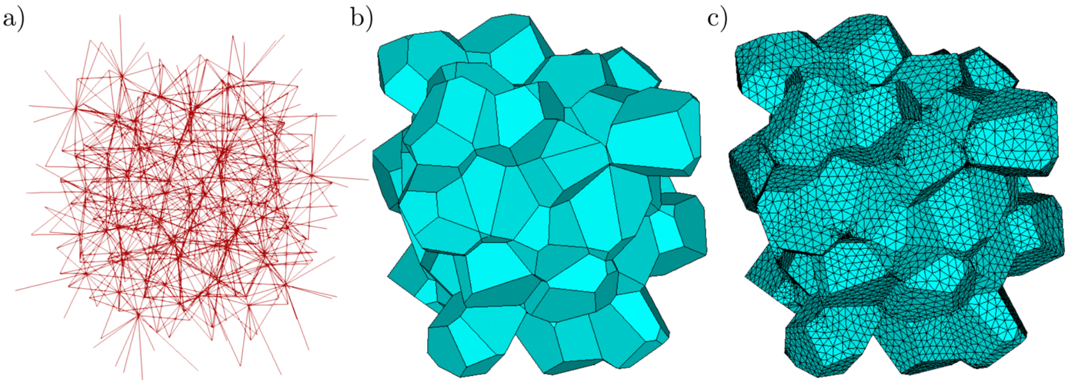

Fig. 3: Example of material volume modelled by: a) discrete mechanical elements, b,c) aggregate volumes and finite element mesh.

Delaunay triangulation. For an illustration, see Fig. 1b, where the contact area is A, the length of the mechanical element is l and the centroid of the contact facet is c. Thanks to Voronoi tessellation, the contact facets running along each aggregate form a convex polyhedron. It is ensured that the contact facets are perpendicular to the mechanical elements, intersecting them at the midpoint of the link. The contact area is considered as the cross-section of each mechanical element and the centroid of the contact as the mechanical element only integration point. A mechanical element is oriented by its local coordinate systems: in 3D by three vectors creating an orthonormal basis. The normal direction of the element, $\boldsymbol{n}$, is perpendicular to the contact facet. The directions of the two tangential components, $\boldsymbol{m}$ and $\boldsymbol{l}$, are selected randomly to complete the orthonormal basis.

The strain vector, $\boldsymbol{e}$, is computed as the mutual displacement vector rotated into the local coordinate system and divided by the length of a specific mechanical element, resulting in the normal strain component, e_N, and two tangential strains, e_M and e_L. The corresponding tractions read:

$$s_N = E_0 e_N,\ s_M = E_0 \alpha e_M,\ s_L = E_0 \alpha e_L \tag{1}$$

where E_0 is the effective Young modulus and α is the elastic parameter: the ratio between normal and tangential stiffness. In 3d, α reads [31]:

$$E_0 = \frac{E}{1-2\nu}, \quad \alpha = \frac{1-4\nu}{1+\nu} \tag{2}$$

where E is the Young modulus and ν is the Poisson ratio. For further reading on discrete lattice particle modelling, see e.g. [31]. The present paper is only concerned with modelling of an elastic material. Eventually, damage capabilities will be introduced to the constitutive model:

$$\begin{aligned} s_N &= (1-d) E_0 e_N, \\ s_M &= (1-d) E_0 \alpha e_M, \\ s_L &= (1-d) E_0 \alpha e_L, \end{aligned} \tag{3}$$

where d is the only increasing damage parameter that reaches between 0 (sound material) to 1 (fully damaged material).

The continuous FEM twin model is generated from the geometry and topology of the discrete particle model, see Fig. 2c. The continuous FEM model understands the regions of individual particles truly as volumes, therefore the structure directly follows the geometry of the generated Voronoi cells. First, keypoints are generated as the vertices of Voronoi cells. Knowing the mutual connectivity, lines are created, resulting in contact facet areas that enclose the volumes of individual aggregates. To correspond with the discrete model, the FEM model takes the input material parameters of the Young modulus, E, and the Poisson ratio, ν. To introduce the damage capability on the contact facets, cohesive elements are to be inserted, see Fig. 4.

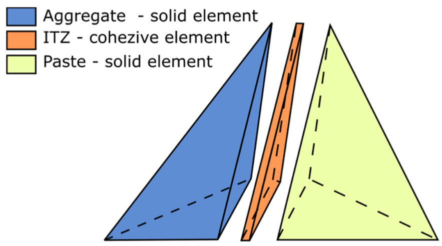

Fig. 4: Schematic illustration of FEM meso modelling using both solid elements and cohesive elements with zero thickness.

3. Modelling examples

In what follows, we provide the reader with examples illustrating the current capabilities of the modelling framework. In Fig. 3, displayed are models of an identical aggregate structure as captured by the developed modelling approaches. As an illustration of a 3D beam with a total length L = 252 mm, span L_S = 240 mm, width W = 80 mm and thickness B = 80 mm. see Fig. 5 for illustration. The minimum grain size is selected as $d_{\min}$ = 8 mm. The selected Young modulus value is E = 41 GPa.

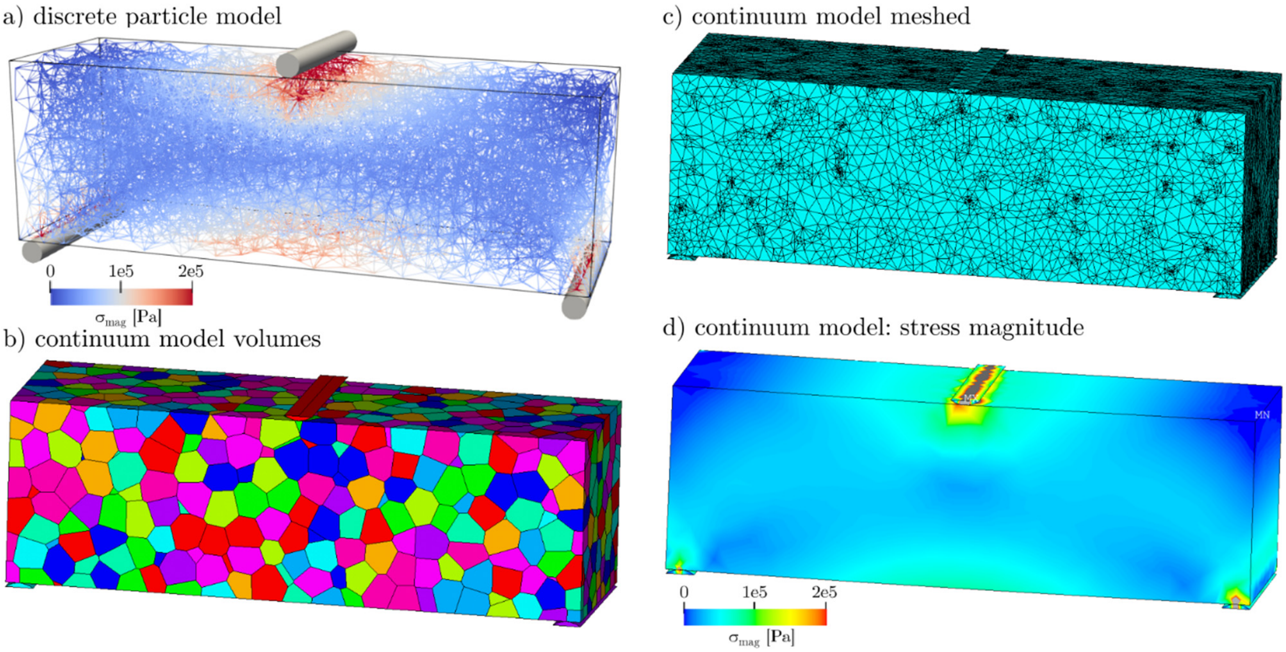

Fig. 6: A three point bending test specimen as modelled by: a) discrete mechanical elements, b, c, d) aggregate volumes, finite element mesh. In subplots a) and d), displayed is the stress magnitude as induced by vertical loading displacement of 0.001 mm.

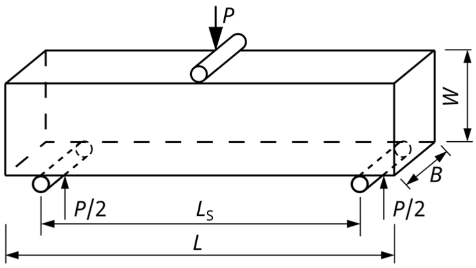

Fig. 5: Scheme of the three point bending test setup.

The test setup is modelled for purposes of demonstrating both the modelling approaches in the developed framework. In Fig. 6 is displayed the numerical model as captured by the structure of mechanical elements of the discrete meso-scale particle model and the continuum FEM model. For demonstration purposes, the stress magnitude, σ_{mag}, is computed by imposing a vertical loading displacement of 0.001 mm. The current implementation of the modelling framework is to be a subject of further long-term development.

The computational demands of the two modelling approaches differ significantly. This is to be expected, given the volume of additional information provided by the FEM model. For comparison, the discrete model displayed in Fig. 6 carries 15 626 degrees of freedom (DOF) which is a fraction of the 2 763 606 DOF of the FEM model displayed in Fig. 6c. The execution time grows accordingly, which is why the authors are thankful for the computational resources provided within the IT4I National Supercomputing Center (project OPEN-29-13).

4. Conclusion

The contribution presented the state of the ongoing development of dual discrete and continuous meso-scale modelling of concrete. The need for a framework that allows to assemble exact twin discrete-continuous mechanical models of heterogeneous materials is driven by the research interests of the authors. The inherent properties of the two approaches were discussed as well as the actual modelling procedures. Lastly, examples of modelled material structure and an actual concrete specimen were presented. The contribution presents a work-in-progress state of the developed modelling framework. The presented development continues, aiming for implementation of representation of pores and investigation of various damage material models. In the longer perspective, we intend to obtain supplementary experimental data to support and verify the numerical models.

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