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3D cellular automata finite element method with explicit microstructure: modeling quasi-brittle fracture using mesh-free damage propagation and multi-scale strain energy homogenization.

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Quasi-brittle fracture is an emergent characteristic, and this cannot be treated satisfactorily with numerical methods based on macromechanics. Because of their complex microstructure, the continuum approach can be too simple for these materials, and needs a finer discretization to obtain satisfactory results if the simulations are to be sensitive to the description of microstructural features. In numerical terms, this means that the computational cost of advanced methods, such as cohesive elements or embedded cracks, is often too high for engineering scale problems. Considering those arguments, in this paper we use the Cellular Automata integrated with Finite Element method to account for the effect of microstructure on quasi-brittle properties within the finite element simulation [1]. Here the microstructure is modeled explicitly by subdividing a finite element into small elements called cells. The heterogeneous microstructure is created from key cells, called seeds, from which particle-like regions may be grown with defined characteristics; by this topological approach we obtain sets of cells with variable properties to model the microstructure (rules are enforced during the selection of the seeds to avoid overlap between particles). As figure 1 shows, graded microstructures, textures and particle anisotropy can be readily simulated in microstructures with multiple phases. The influence of the initial finite element mesh is erased during the development of the microstructure.

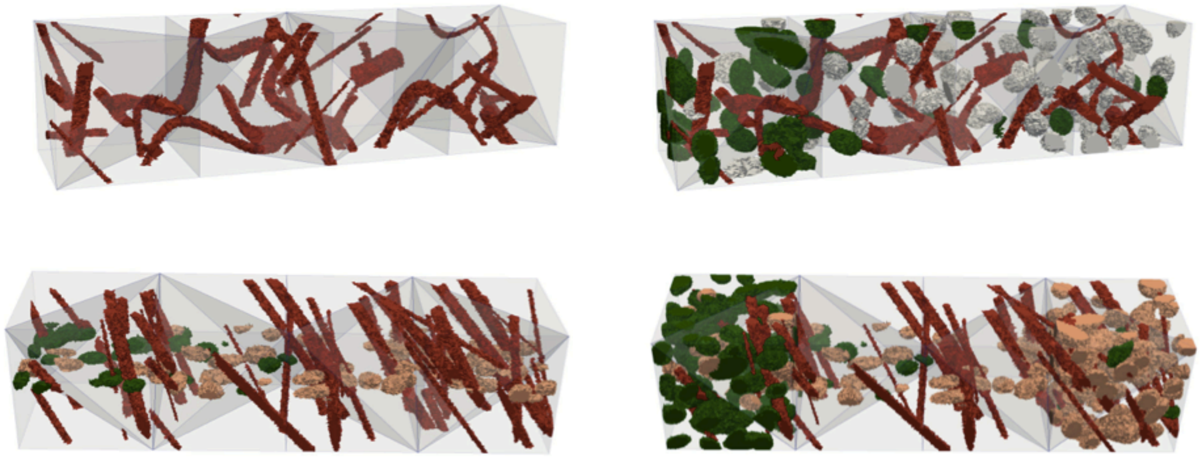

Figure 1: *Example of two microstructures created inside 20 tetrahedral elements with matrix, two different phases and fibres.*

We use a mesh-free approach for the damage development through the microstructure [2]. This uses the nodal displacements obtained in the FEM as boundary conditions, and computes the movement of the different phases of the microstructure. This is done through the adaptation of the mesh-free model to the microstructure and solving the equilibrium of strain energy. From this, the strains in the cells are computed and evaluated. A cell is removed when the damage criterion is satisfied (e.g. a critical strain is reached), updating the displacements of the microstructure afterwards. The damage of the cells alters the strain energy, leading to a homogenization that changes the material properties of the region represented in the mesh-free model and FEM. The fracture path is completely free with respect to the FE mesh.

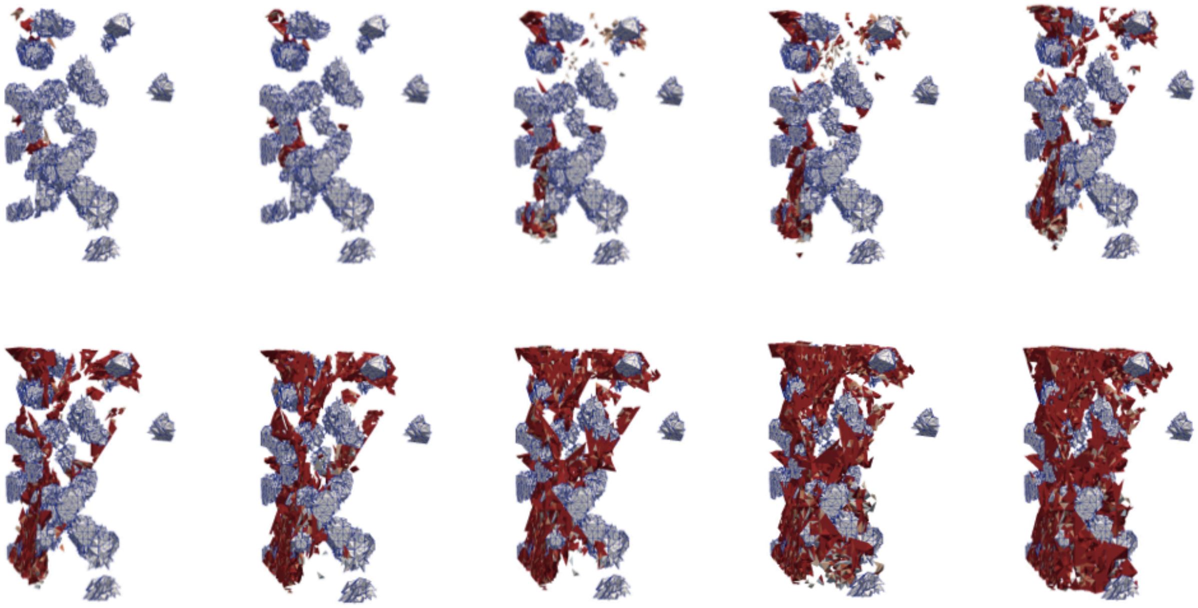

Figure 2: *Crack front formation. The damaged cells are plotted in red, and the pore cells in grey.*

In summary, by this method quasi-brittle fracture can develop freely through the microstructure (see figure 2), improving the accuracy and computational cost of the calculations at engineering length-scales in complex microstructures. This work is part of a larger project, which aims to experimentally validate the simulation of heterogeneous microstructures in structural integrity problems.

REFERENCES

[1] A. Shterenlikht and I. C. Howard. The CAFE model of fracture: application to a TMCR steel. *Fatig Fract Eng Mater Struct,* Vol. **29**, pp. 770-787, 2006.

[2] L. Saucedo and T.J. Marrow. 3D cellular automata finite element method to model quasi-brittle fracture. *Twelfth Intentional Conference on Engineering Structural Integrity Assessment Conference proceedings*, (ESIA12), May 2013, Manchester, UK.

[3] L. Saucedo Mora, M. Mostafavi, D. Khoshkhou, C. Reinhard, R. Atwood, S. Zhao, B. Connolly and T.J. Marrow, 3D cellular automata finite element (CAFE) modelling and experimental observation of damage in quasi-brittle nuclear materials: Indentation of a SiC-SiCfibre ceramic matrix composite, *3rd International Workshop on Structural Materials for Innovative Nuclear Systems (SMINS-3)*, October 2013, Idaho Falls, USA.