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3D Cellular Automata Finite Element Method with explicit microstructure: modeling quasi-brittle fracture using Meshfree damage propagation

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Abstract

Quasi-brittle fracture is an emergent characteristic, and this cannot be treated satisfactorily with the 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. 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. 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. Here the microstructure is modeled explicitly by subdividing a finite element into small elements called cells. Graded microstructures, textures and particle anisotropy can be readily simulated in microstructures with multiple phases and the influence of the initial finite element mesh is erased during the development of the microstructure. This method provides two sets of elements representing the finite element model and the microstructure. The first is used to link the engineering scale problem with the microstructure, obtaining the stress and strain fields of the macro-mechanical problem. With those, we compute the micro-mechanical fields using the second set of elements, which describes explicitly the microstructure. We use the Meshfree approach for the damage development through the microstructure. The material properties of the finite elements are recomputed according to the microstructure damage and the fracture path is completely free with respect to the finite element mesh. By this method quasi-brittle fracture can develop freely through the microstructure, improving the accuracy and computational cost of the calculations at engineering length-scales in complex microstructures.

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1. Introduction.

Currently, one of the main problems in the numerical models is scale. If the microstructure is inserted in the model with a high fidelity, the computational cost grows making its application in an engineering scale difficult. Accordingly, if we model a full-scale component, in order to reduce the computational cost and make it feasible, a simplified model is used. One simplification is the use of a continuous material instead of a complex microstructure, and a coarse discretization compared with the microstructural scale, called a Representative Element Volume (REV). Consequently, the FEM needs to use a large mesh size to model the fracture of large-scale components.

In this paper we present an approach based on a Finite Element Model with a coarse mesh (REV), normalizing the energy release by the joint application of two models, a Meshfree Method and Cellular Automata. Applying this, the energy release of a coarse mesh (145 elements) is similar to that obtained with a fine mesh (27950 elements) in a conventional FEM. The Meshfree Model proposed is not developed inside a single Finite Element, instead a continuum Meshfree model is developed inside a set composed of the elements that may develop damage. Through the adaptation of the Meshfree Model to the microstructure, and also the cells that carry all the material properties and the damage information, a microstructure formed by matrix and phases of different properties can be modeled with high fidelity.

The paper is structured as follows: in section 2 a description of the model and the interaction between the different layers is provided; section 3 compares the strains obtained with our model and a high fidelity FEM in a complex microstructure; in section 4 we present an example of the energy release normalization, comparing our model against a FEM with cohesive elements.

2. Mechanical model

A general CAFE method is presented by Shterenlikht and Howards (2006), but in order to adapt this methodology to our requirements we insert variations in its discretization and the relationship between the CA and FE layers.

2.1. Subdivision algorithm and Cellular Automata

To ensure the versatility of our method we work with an irregular tetrahedral mesh, which increases the complexity of the subdivision process. To solve this, an iterative algorithm is developed, subdividing each tetrahedron in 4 through the use of a common vertex, and dividing the opposite face in 4 by the union of the midpoints of its edges. In order to create cells that are as regular as possible, the face of the tetrahedron chosen for division has the largest area. This process is iterated until the mean cell volume is representative of the microstructural size. The total number of cells inside an element is 4^n , n being the number of iterations. Once we have the set of cells, we identify those at center of the ellipsoids with various sizes and orientations that represent the different phases. In that way, the cells reproduce the volume and proportion of the different phases and matrix; it is also possible to insert straight and curved fibers, see Saucedo and Marrow (2013 a,b).

2.2. Finite Element model

The Finite Element part of the model is implemented within the software ABAQUS. For this we use a variation of the cohesive element, but instead of following a cohesive law, it receives from the microstructure information of the energy released in the fracture, which is used to update the mechanical response of the element.

2.3. Meshfree model

This layer is the link between the information of the Finite Element Method and the Cellular Automata. Once distributions the pores and particles (represented as ellipsoids in the model) are completely defined, we carry out a Delaunay triangularization to define the Inter Particle Domains (IPD); these are part of the discretization of the Meshfree model with the particles. Each ellipsoid is represented by 6 points (one at the end of each of its orthogonal

axes). Each IPD is composed of 4 ellipsoids and is defined by the 3 nodes of these that are closest to the IPD center. Consequently, in the Meshfree Model we have two different types of domains: the IPD that represent the matrix, and the particles where the domain is the interior of the ellipsoid with its 6 nodes. We consider a pore as an empty particle. The versatility of the Meshfree model allows us to have variable domains with different geometries and number of nodes. For this we enforce the maximum entropy conditions described by Arroyo and Ortiz (2006) and the geometrical adaptive conditions of Saucedo (2012).

Inside every Finite Element there are IPD and particles that became active when the element reaches a state sufficient to generate damage. Currently, we apply a stress criterion, such that damage occurs when the stress has a value of $0.5f_t$, where f_t is the representative tensile stress of the material. Hence, within each IPD and particle there are cells that will determine the material properties as damage develops.

2.4. Boundary conditions

The boundary conditions play an important role in the model. The inputs of the Meshfree model from the FE are the nodal displacements of the FE mesh. These are inserted as forces in the IPD that encloses each node, computed as the product of the IPD's local stiffness matrix and the displacements of the FE node. Once the Meshfree model is computed, the displacements of the Meshfree nodes are mapped into the nodes of the CA model to compute the cell's strain. The displacements of the CA model are interpolated using the shape functions of each IPD or Particle.

2.5. Erosion (i.e. Damage)

After the update of the displacements in the CA layer, the strain of every cell is computed and evaluated against its critical strain, this is used instead of the tensile strength in order to introduce the information of the cohesive law. If this is reached, the cell is removed (i.e. eroded), and the displacements of the nodes of that cell are updated. In order to reproduce the strain intensity caused by a fracture, the nodal displacements are updated by considering only the Meshfree nodes that are on the same side of the plane that is orthogonal to the principal eigenvector. This changes the strain of the cells in the neighborhood and allows the fracture to propagate.

2.6. Energy homogenization

This technique links the effects of the eroded cells and the FE behavior. For this, the strain energy of every IPD or Particle at the beginning of the step is corrected with the energy released by every cell eroded inside each Meshfree domain, thereby changing the material properties of the IPD or Particle accordingly. This is carried out similarly between the FE and Meshfree layer, changing the stiffness of the FE proportionally to the ratio between the sum of the strain energy of all the enclosed IPD and particles and the strain energy of the FE at the beginning of the step. Consequently, the damage is translated from the CA layer to the FEM in a consistent way.

3. Validation: strain distribution of a porous material

This validation example (a cube of $1 \times 1 \times 1 \text{ mm}$) shows how beginning from a coarse FE mesh (Fig. 1 left) and a microstructure (in this case 5 elements, 888 IPD, 70 pores and 132942 cells), the strains computed with a high fidelity FEM (40000 elements) can be reproduced with the CAFE model. The material properties used are a Poisson's ratio of 0.2 and a Young moduli of $E=12 \text{ GPa}$ for the matrix and $E=0 \text{ GPa}$ for the pores. The only variations in the constraints applied to the FEM and the CAFE calculation are that in the FEM a null displacement is applied to all of the bottom base, and a vertical displacement of 0.06 mm is applied in the top, whilst in the CAFE model those are only applied to the 8 nodes of the coarse FE mesh. This approximation has the effect of producing some higher deformations in the FEM than in the CAFE. The FEM is also stiffer than the Meshfree Model. The comparison between the strains obtained with both models in the same points of the domain is shown in Fig 2 (left). In this graph we can distinguish 3 different regions; *A*, *B* and *C*. *A* shows the general agreement between both methods, regions *B* and *C* are due to the localized difference strain concentrations between them. Fig. 2 (right) shows a comparison between the computational cost of both methods (in seconds) and its discretizations (i.e.

number of elements for the FEM and the number of cells for the CAFE); all the calculations were carried out with a serial code on the same work station.

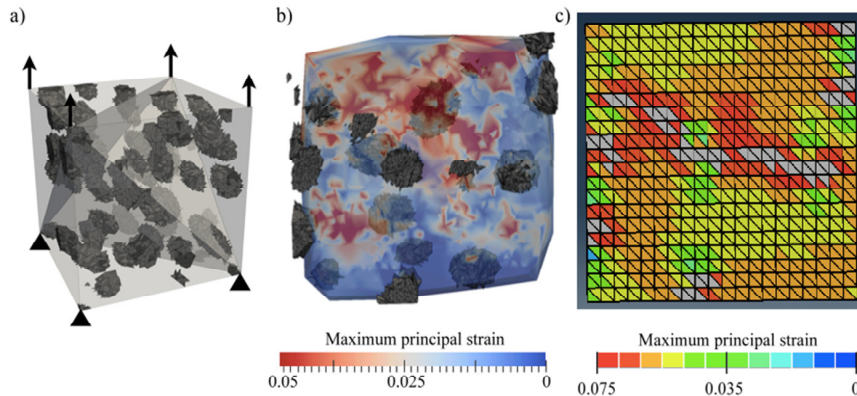


Fig. 1. Setup of the problem for the CAFE model (a), discretization and strain comparison between the FEM with 40000 elements (c) and the CAFE with 5 elements, 888 IPD, 70 Pores and 132942 cells (b)

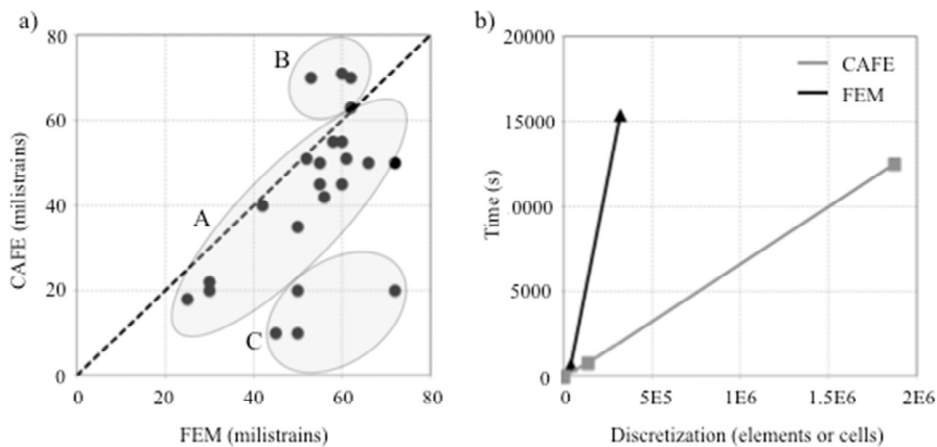


Fig. 2. Comparison of the strains (a) and computational cost (b) obtained with FEM and CAFE. The discretization plotted is the number of elements for the FEM and the number of cells for the CAFE model

4. Validation: Improvement of the energy release of a coarse discretization in FEM

In this example we compare FEM with cohesive elements against the CAFE model. The sample modeled is a $6 \times 6 \times 1$ mm rectangular prism with two opposite notches with 1 mm depth, each under a vertical tensile load. The fictitious material has a Young's modulus of $E=18$ Gpa, a Poisson's ratio of 0.2 and a tensile strength of 3.3 MPa. In the FE, a linear decreasing cohesive law was defined for the cohesive elements, with a critical strain (this is the ratio between the tensile strength and the Young's modulus) of 0.00018, reached at the tensile strength, and a final strain of 0.00055, which is a fix arbitrary value of the problem to represent the cohesive behavior. In the CAFE model, the failure strain of each of the cells is defined randomly between the critical and final strains of the FE cohesive law, assigned with a linear probability distribution. This reproduces the shape of the FE cohesive law.

The main result of this calculation is shown in Fig. 3 (left). This shows the difference between the FEM with meshes of 145 and 27950 elements, and also how the CAFE model (based on the mesh of 145 elements, with 4702 IPD and 212992 cells) homogenizes the energy release of the coarse mesh, reproducing the result obtained with the fine FE mesh. Fig. 4 (left) shows the relationship between the discretization of the Meshfree model (IPDs in blue and Pores in yellow) and two elements from the FE mesh with its nodes in red. In the Fig. 4 (right) the eroded cells are represented in black. Fig. 5 shows the fracture pattern of the FEMs with coarse and fine mesh and the CAFE model at 3 different points in the simulations; the onset of non linearity with damage initiation, the peak load and the final collapse.

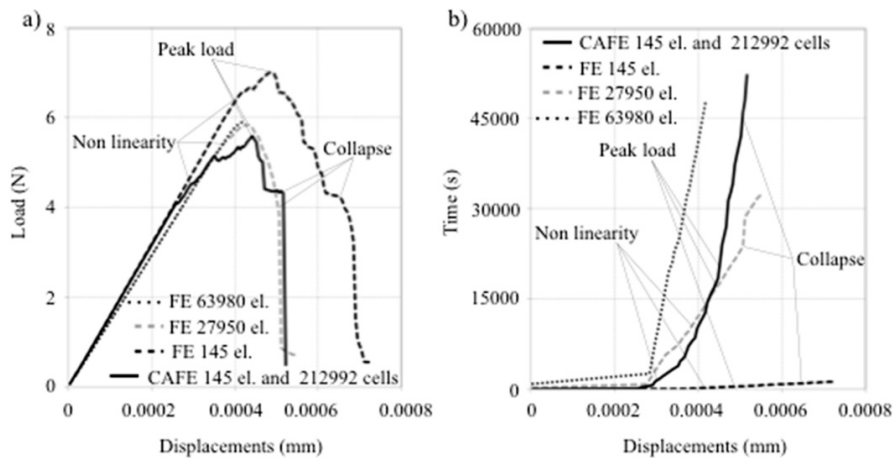


Fig. 3. Load displacement curves (a) and computational cost (b) of the different calculations

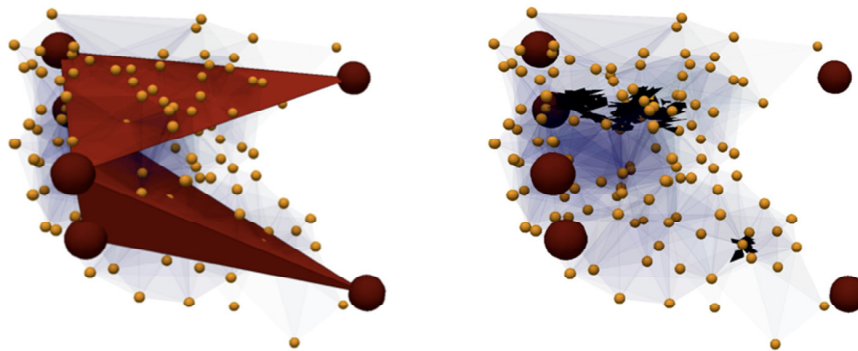


Fig. 4. View of the 3 scales, CA (eroded cells in black), Meshfree model (IPD in blue and Pores in yellow) and FE (element and nodes in red)

4. Conclusions

Through the multi-scale application of the Meshfree and a Cellular Automata models, we conduct a normalization of the energy release of a Finite Element Method calculation with a coarse mesh. This allows us to carry out efficiently FE calculations with a coarse mesh without losing accuracy in the solution. The goal is achieved through a high fidelity reproduction of the microstructure and the adaptation of the Meshfree Model to its geometry. Importantly, the computational cost of the CAFE method proposed is lower than a FEM with a similar discretization. This makes the CAFE model very promising for the fracture modeling of components at engineering scale, taking into account the microstructure of the material.

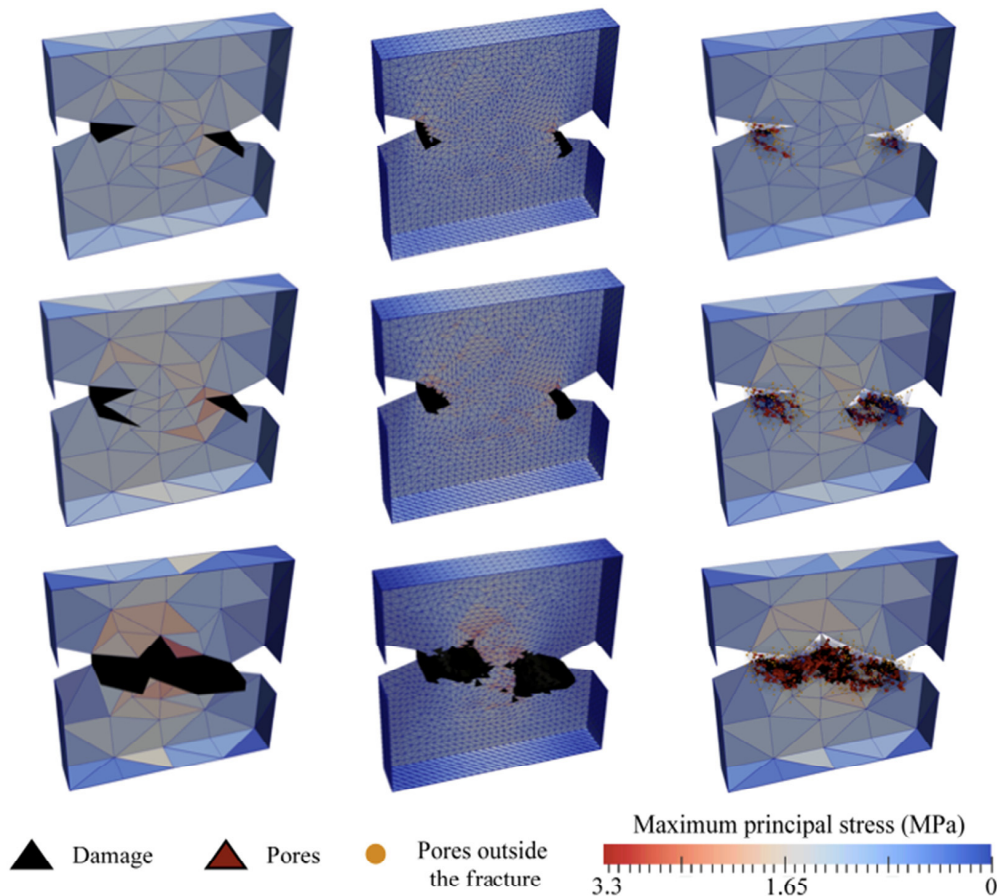


Fig. 5. From top to bottom the fracture pattern of the different models in the non linearity initiation, the peak load and the collapse. From left to right the FEM with 145 elements, FEM with 27950 elements and CAFE model with 5 elements, 4702 IPD and 212992 cells.

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