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Method for the explicit insertion of microstructure in Cellular Automata Finite Element (CAFE) models based on an irregular tetrahedral Finite Element mesh: Application in a multi-scale Finite Element Microstructure MEshfree framework (FEMME)

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ABSTRACT

Multiscale models are needed in simulations of mechanical and thermal properties that consider the microstructural heterogeneity of materials, in which a coupling is essential between the numerical models that deal with the different scales. In the class of cellular automata-finite element (CA-FE) or CAFE models, the use of a regular FE mesh restricts the model versatility due to the limited variety of engineering problems that can be simulated with such meshes. A novel methodology is proposed to create the homogeneous cells of the CA model from a mesh that is formed by irregular tetrahedrons. The result is more versatile and capable of modelling complex geometries, improving its applicability. The problem is solved through a subdivision algorithm that creates homogeneous tetrahedral cells, using a methodology to insert microstructures that can be described by particles, pores or fibres. Its use is demonstrated in a multi-scale Finite Element Microstructure MEshfree (FEMME) framework to calculate the elastic strains caused by microstructural features (pores); the method is shown to have a significantly lower computational cost than finite element simulations of equivalent levels of discretization.

1. Introduction

The importance of multi-scale models has grown in recent years, achieving increasing complexity in the problems addressed; these aim, for instance, to consider mechanical or thermal effects on the macrostructure that arise from the microstructural features. Prior to this, the effect of the microstructure has generally been neglected, or treated in a very limited manner, due to the high computational cost of introducing microstructure fidelity into large scale models; consequently, continuum material properties have been commonly used [1]. Multi-scale models address this problem by compensating for the use of a coarse discretization in the macrostructural model via the insertion of detailed microstructure only in those zones that require this refinement; for example, the damaged regions within fracture models. Various methods have been proposed, such as the stochastic multiscale model for fracture [2] that involves a statistical description of particles; the multiscale cohesive zone model [3], in which the bulk material is modelled as a quasi-continuum and the adaptive concurrent multiscale model [4], which utilizes an explicit description of microstructural features near the crack tip. Recently, a cellular automata (CA) finite element (FE) model with a microstructural adaptive meshfree framework [5] has inserted a high fidelity description of the microstructure into a Finite Element Microstructure MEshfree (FEMME) multiscale model of damage development, using the methodology that is explained here.

Cellular Automata Finite Element (CAFE) [6] models insert a detailed description of the microstructural material properties locally using CA within a larger scale FE model, coupling the macro and microstructural problems efficiently. The complexity of this approach lies in the achievement of continuity between the CA and FE layers, where the geometry of the cells in the CA model is embedded in the FE mesh. Traditionally, the solution to this problem is to split the regular three-dimensional finite elements into cubes of equal size representing the CA layer; this is very convenient for CA methods that are based on images [7–9]. Each cube of the discretization can be related to an image pixel, thus inserting the microstructure in the model from a description of the microstructure, which might be derived from a 2-dimensional or 3-dimensional image. The problem for CAFE is the limited versatility of regular FE meshes in the solution of engineering problems.

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In our case we use irregular tetrahedrons instead of regular elements in the FE mesh, which gives much greater versatility; such elements are optimal for the modelling of structures with a complex geometry. There are two problems to be addressed: the first is the homogenization of the two layers through their element geometries, because as the Finite Elements that host them, the cells of the CA layer should be based on irregular tetrahedrons; the second problem is the insertion of the microstructure, which can be done in the same way as the classical cubic-based CA (i.e. with high fidelity from an image or through a statistical description of the material) if the volumes of the different tetrahedral cells are of the same order. The method proposed here solves both of these problems and so allows insertion of the microstructure into CAFE models that are based on an irregular tetrahedral FE mesh.

The methodology described here allows one to describe, with computational efficiency, a complex graded microstructure with a generic Finite Element Model (FEM with irregular tetrahedrons) to simulate complex sample geometries [5]. A general CAFE method with hexahedron FE elements and a microstructure formed by one phase with variable material properties was first presented by Shterenlikht and Howards [6], achieving successful simulations of the fracture of steel. Following that methodology, in order to model fracture in materials with a complex microstructure, we insert variations in its discretization and the relationship between the CA and FE layers through the introduction of a Meshfree framework as another layer between them.

The paper is structured as follows: the subdivision algorithm to create tetrahedral cells with a homogeneous size from an irregular tetrahedral mesh is first presented, then the insertion of the microstructure through ellipsoids with different dimensions and orientations is explained. Some examples of its application are then described, creating graded microstructures with different phases and distributions, and also combining elliptical particles with straight and curve fibres. Its application is described in a simulation of the stress distribution within a porous body; in this Finite Element Microstructure MEshfree (FEMME) multiscale approach, FE are used to model the engineering scale problem, the microstructural adaptive meshfree (MAM) framework computes the displacements of the microstructural features from the displacements of the FE nodes, and the CA layer uses the displacements of the MAM layer to compute the strains in the cells, which typically have a size that is 2 orders of magnitude smaller than the FE mesh size. Here microstructural features are used as the discretization of the MAM framework to compute the internal displacements. A comparison is made, in terms of strain field and computational cost, at different levels of discretization against standard FE models that describes the same microstructure.

2. Subdivision

The first step is the subdivision of the irregular tetrahedron Finite Elements into smaller cells. The problem associated with this element geometry is that the cells also must be irregular tetrahedrons with homogeneous volumes. This homogeneity is essential to have a uniform distribution of the strain energy in the cells, since it depends on the cell volume. The subdivision algorithm is applied iteratively, subdividing each tetrahedron in 4. It starts with an irregular tetrahedron of the Finite Element mesh, dividing it in 4 tetrahedrons that will be subdivided as well in the next iteration of the algorithm. The number of tetrahedrons produced is 4^n, where n is the iteration number. This process is independent for each tetrahedron, and can be parallelized, perhaps it's computational cost is low, growing linearly as $(10^{-5}N_{tet}+0.908)$ seconds, being N_{tet} the number of tetrahedrons at the end of the process. It means that the subdivision of a tetrahedron in 1024 tetrahedrons takes 1 s, and in 4,194,304 tetrahedrons 43 s running as a serial code in a MacBook Air (2 GHz Intel Core i7). The main algorithm is applied to each tetrahedron (1–2–3–4 in Fig. 1) independently, and can be divided in 4 steps:

- *Step 1*: Evaluate the area of each face and choose the largest one (i.e. 2–3–4 in Fig. 1).
- *Step 2*: Take the vertex located opposite to the selected face and use it as a reference vertex (i.e. 1 in Fig. 1).
- *Step 3*: Subdivide the selected face (i.e. 2–3–4 in Fig. 1) in 4 triangles (i.e. 2–5–7, 5–6–7, 3–6–7 and 4–5–6 in Fig. 1), inserting nodes at the middle of each edge of the face as an average of the vertex associated with this edge (i.e. $\mathbf{x}_{node7}=0.5(\mathbf{x}_{node3}+\mathbf{x}_{node2})$, $\mathbf{x}_{node6}=0.5(\mathbf{x}_{node3}+\mathbf{x}_{node4})$, $\mathbf{x}_{node5}=0.5(\mathbf{x}_{node4}+\mathbf{x}_{node2})$ in Fig. 1)

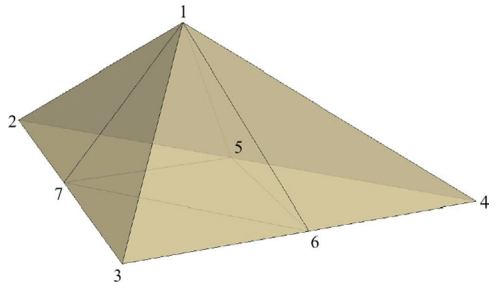

Fig. 1. Scheme of the subdivision algorithm.

This is applied iteratively to each tetrahedron separately, replacing the reference tetrahedral set by a new one with all the tetrahedrons produced in the subdivision. It was entirely implemented in Python 3.3, without the use of any other software. This is continued iteratively on each tetrahedron until all the tetrahedrons are smaller than a predefined critical size (see Fig. 2a); this might be the resolution of the experimental characterization of the microstructure, such as the pixel size in an image.

The application of the algorithm to a single tetrahedron over several iterations is shown in Fig. 2a; each iteration decreases the cell size and increases the number of tetrahedrons by a factor of 4^n, where n is the number of iterations. The subdivision algorithm results in a quite homogeneous cell size distribution with a standard deviation of the 8.5% after 5 iterations; the data in Fig. 2a are sorted in order of size of the longest edge of each cell. The cells are visualized in Fig. 2b, in which the body centre of each cell is marked. After the subdivision of a FEM mesh it remains structured, respecting exactly the same nodal coordinates and connectivity.

3. Insertion of the microstructure

The cells can then be used to provide a discretized description of the microstructure within the finite element by assigning to each cell the properties of its material phase. Each material phase is treated as a particle, simplified as a 3D ellipsoid with an assigned orientation and dimensions; a pore is simply an empty particle, or one with negligible properties. To insert each particle, a seed cell is chosen that is at its centre.

Each ellipsoid i is defined by Eq. (3).

$$\left[A^i\right]=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos(\alpha_1^i) & \sin(\alpha_1^i)\\ 0 & -\sin(\alpha_1^i) & \cos(\alpha_1^i)\end{pmatrix}\begin{pmatrix}\cos(\alpha_2^i) & 0 & -\sin(\alpha_2^i)\\ 0 & 1 & 0\\ \sin(\alpha_2^i) & 0 & \cos(\alpha_2^i)\end{pmatrix}$$