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Image-based finite element mesh construction for material microstructures

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Abstract

One way of computing the macroscopic behavior of a material sample with complex microstructure is to construct a finite element model based on a micrograph of a representative slice of the material. The quality of the results produced with such a model obviously depends on the quality of the constructed mesh. In this article, we describe a set of routines that modify and improve the quality of a 2D mesh. Most of the routines are guided by an effective element "energy" functional, which takes into account the shape quality of the elements and the homogeneity of the elements as determined from an underlying segmented image. The interfaces and boundaries in the image arise naturally from the segmentation process. From these routines, we construct a close-to-automatic mesh generator that requires only a few inputs, such as the linear sizes of the largest and smallest features in the micrograph.

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1. Introduction

Finite element modeling is a technique which is at its best where analytical models are inapplicable because of the complex spatial geometry of the modeling domain. Even so, most finite element packages require as input a numerical representation of the model geometry in terms of simple building blocks. The boundaries of the domain are described by points, straight lines, planes, and simple curves. In materials science, the starting point for the modeling effort is often a micrograph or other "analog" representation of the structure. An example is shown in Fig. 1. For these types of images, converting the boundaries to a simple numerical representation by hand is a tedious task. In this paper, we will describe how the software package OOF2 (named for "Object Oriented Finite-Elements", version 2) [1–4] circumvents this difficulty by creating meshes directly from images, simultaneously identifying boundaries in the image and bringing the finite element mesh into correspondence with these boundaries. With a unique, image-based, adaptive meshing technique, OOF2 is capable of parsing experimental data relating to polyphase, polydomain materials with complex geometries into a representation that is appropriate for use in a finite element simulation. Using this method, an explicit mathematical description of the image boundaries is not required, and is not explicitly constructed.

The OOF tool (in its original version, OOF1, and the current OOF2) has been used successfully in a wide variety

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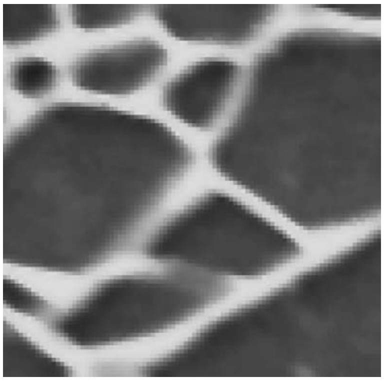

Fig. 1. *Microstructure image example*: A micrometer scale SEM image of plasma-etched Si_3N_4, provided by Chun-Hway Hsueh at Oak Ridge National Laboratory [5].

of applications, including studying the relationship between thermal properties and the structure of plasma-sprayed zirconia coatings [6], the effects of microstructure on the macroscopic mechanical properties of glass-matrix composites [7], the role of texture in the macroscopic response of polycrystalline piezoelectric materials [8], and the modeling and design of electrode microstructures in rechargeable lithium-ion batteries [9].

One option for forming a finite element mesh from an image is to do so directly, defining a square element for each pixel [10,11]. This has two major pitfalls. First, it usually creates too many elements – homogeneous regions can adequately be described by larger elements. Second, it introduces jagged edges where the boundary in the real material is smooth, which can lead to artificial features such as stress concentrations at pixel corners. It is useful to distinguish between the process of making a mesh of the image itself, which this direct approach does, and the process of making a mesh which approximates the underlying microstructure, using the image as necessarily approximate source data. The latter process gives higher quality meshes and is not encumbered by the discretization process that created the image [1].

The OOF2 meshing scheme begins with a coarse, regular, well-formed, space-filling mesh on the image, and then brings that mesh into correspondence with the image by a series of mesh-modifying steps which preserve the space-filling and well-formed character of the mesh. Mesh-modifying steps may refine elements, replacing them with smaller elements, or may move nodes and boundaries around to align them with image features. The elements are generally at least several pixels in size, which promotes efficient use of computational resources, and avoids accidental modeling of image artifacts. User judgement may be employed in selecting mesh modification steps and their parameters to help ensure that it is the underlying physical structure which drives this process. Because the well-formed, space-filling character of the mesh is preserved, unmeshable voids cannot arise, and illegal (inverted or concave) elements can be avoided.

2. Image-based meshing

The starting point for the OOF2 meshing scheme is an image which has been segmented, that is, broken up into distinct sets of pixels, each of which corresponds to a homogeneous part of the image. These image parts presumably are microstructural features such as grains or inclusions for which the bulk material properties are known (or can be assigned.) Image segmentation is a rich topic beyond the scope of this paper. For our purposes here, we will assume that a segmentation of the image exists, and also treat "pixel group", "pixel category", and "material" as synonyms, although they have slightly differing technical meanings within the OOF2 program.[1]

The goal of the meshing process is then to create a mesh whose element boundaries lie approximately along the pixel group boundaries, and for which the elements themselves are approximately regular in shape and homogeneous, enclosing pixels of exactly one pixel group. The technique used is to create an initial mesh that is a regular, space-filling grid of rectangles or triangles, with user-specified dimensions, and then optimize this mesh and align it with the boundaries of the microstructure using a variety of tools described below. Several methods move the nodes in order to improve homogeneity or shape quality. Other methods change the topology of the mesh by refining inhomogeneous elements, merging homogeneous elements, or correcting for badly shaped elements.

2.1. Quantifying the quality of the mesh

For an automated meshing procedure to work, a figure of merit, or a quantitative measure of the quality of the elements in the mesh, must be introduced that has as few components as possible. This quantitative measure must reflect the degree to which the mesh represents the microstructure, and must also reflect the degree to which the mesh will give rise to good convergence behavior in the finite element solution step.

To this end, we define two element functionals, which we call "energies". The shape energy quantifies the quality of the shapes of elements, and the homogeneity energy measures how well the mesh matches the pixel regions. We use the word "energy" because some of our mesh modification routines move the mesh nodes as if they were physical particles with potential energies given by the shape and homogeneity functionals. For example, the anneal routine (see Section 2.2.1) moves nodes randomly and accepts moves that lower the energy. A mesh is a good finite ele-

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[1] A "pixel group" is a set of pixels from the image. Each pixel may belong to many pixel groups simultaneously. A "material" defines the set of physical and crystallographic properties belonging to the microstructure at the location of a pixel. Each pixel can belong to at most one material. A "pixel category" is a label indicating the set of groups and materials to which a pixel belongs. All pixels with the same category have the same material and belong to the same groups.