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Hexahedral Mesh Generation for Computational Materials Modeling

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Abstract

A parallel, adaptive overlay grid procedure is proposed for use in generating all-hex meshes for stochastic (SVE) and representative (RVE) volume elements in computational materials modeling. The mesh generation process is outlined including several new advancements such as data filtering to improve mesh quality from voxelated and 3D image sources, improvements to the primal contouring method for constructing material interfaces and pillowing to improve mesh quality at boundaries. We show specific examples in crystal plasticity and syntactic foam modeling that have benefitted from the proposed mesh generation procedure and illustrate results of the procedure with several practical mesh examples.

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Keywords: hexahedral mesh generation; overlay grid; computational materials modeling; crystal plasticity; syntactic foam;

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1. Introduction

Determining relationships between material behavior at different length scales is an active area of research and a key part of current integrated computational materials engineering initiatives [1][2]. Computational materials modeling efforts that explicitly resolve microstructure and/or meso-scale material features play an important role in understanding mechanical behavior, deformation and failure mechanisms that ultimately drive macroscale material behavior. However, most materials have features at this scale that are irregular geometry and present many challenges for mesh generation. Furthermore, it is often necessary to simulate the response of many unique realizations of the material microstructure to capture stochastic effects of variability in feature arrangement and to ensure that the predicted response is not unique to local features in any particular realization. This is particularly important when smaller stochastic volume elements (SVEs) are used to mitigate computational expense if the required size of a representative volume element (RVE) is large. In some cases, hex meshes may be necessary to enable certain features of the analysis or maintain compatibility with other meshed components. The meshing step can quickly become prohibitively expensive unless the complex microstructural features can be meshed in an automated way. Thus, a robust meshing algorithm that can quickly generate meshes on hundreds of material volume elements (RVE or SVE) is an enabling feature to perform comprehensive computational studies of material microstructure behavior.

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Current methods for automatic hexahedral mesh generation can be classified as *geometry-first*, or *mesh-first*. Where an explicit geometry representation such as a CAD design model is used, geometry-first approaches can be used to generate high quality, crafted meshes using block-structuring [3] [4] and pave and sweep [5] procedures. These methods begin with reference geometry that must be interactively cleaned-up and decomposed to admit a limited set of topologic meshing primitives. Geometry-first methods are impractical for computational materials modeling where methods must be completely automated and where the input can come from 3D image based data with highly complex material interactions. Instead, we utilize a mesh-first approach that begins with an overlay grid that is locally modified to incorporate microstructural features that will result in a conformal hexahedral mesh of the RVE.

A limited set of literature is available describing conformal hexahedral meshing procedures for computational materials modeling. Qian [10] and Zhang [12] propose procedures that build complex microstructures based upon the dual contouring approach introduced in [13]. Both hexahedral and tetrahedral approaches are described where meshes are generated for multiple material grain structures. Procedures for identifying and resolving complex topological interactions as well as the ability to produce smooth interfaces using geometric flow-based smoothing. These works illuminate important aspects peculiar to microstructures, however reported mesh quality [10] can be marginal at grain interfaces and do not appear to provide for distributed algorithms for scalable applications.

For our purposes we seek an all-hex meshing procedure for application to computational materials modeling that is fully automatic. Methods that require any user interaction to clean or decompose the geometry are impractical for this application. The ability to control the execution of the meshing tool via scripting is also desirable to facilitate rapid execution of hundreds of stochastic simulations. We note that the target analysis codes require computable quality hex elements with smooth conformal interfaces between materials. The hex method should also support multiple input sources including voxelated, volume fraction and analytic geometry. Topologic complexity with hundreds or even thousands of separate grain structures are also necessary for this application. Finally, the ability to rapidly run hundreds of stochastic models with meshes exceeding tens of millions of elements make distributed computing a vital requirement.

This work proposes an overlay grid procedure that builds on Sandia National Laboratories' Sculpt [6] meshing tool and later extended in [7][8][9]. In [6] we first introduced a parallel overlay grid procedure based on volume fractions for arbitrary geometry and later describe the smoothing procedures for this method in [7]. In [8] we provide a validation of meshes produced from Sculpt in application with computational mechanics codes and in [9], the method is extended to incorporate a new adaptive 2-refinement technique. In this work we extend the Sculpt application to address the specific problems encountered in computational materials modeling. New procedures are introduced to ensure the preceding requirements are met and that the resulting meshing tool can be used for practical, robust and efficient computational materials modeling.

2. Algorithm

2.1. Overview

The proposed methodology is based upon an overlay grid method where a Cartesian grid is used as the basis for the finite element mesh. The proposed procedure works directly from a volume fraction representation where $\sum_{j=0}^{k} vf(i,j) = 1$, with i a cell index and j a material index. With no explicit geometric or topology representation from which to work, the procedure extracts a boundary representation (B-Rep) topology and recovers approximated geometric interfaces from the volume fraction data.

2.1.1. Hex Meshing Procedure

In this work we propose a series of procedures that have proven effective in building hexahedral meshes for computational materials modeling on stochastic or representative volume elements. The following is an outline of the procedure used for generating hexahedral meshes with their corresponding section or external reference:

1. ***Process input data:*** Convert input data to Cartesian volume fractions if not already. (sec. 2.2)
2. ***Distribute data for parallelism:*** Distribute Cartesian volume fraction data to multiple processors via MPI. [6][9]
3. ***Refine or coarsen:*** Adaptively refine or coarsen the Cartesian grid to build a conformal unstructured base grid on which to build the geometry and mesh. (sec. 2.3)
4. ***Filter input data:*** Assign each cell of the base grid to its dominant material. Modify the assignment to eliminate non-manifold conditions and reduce potential mesh quality issues.(sec. 2.4)