MATDAT18: Materials and Data Science Hackathon

Team Composition (2 people max.)

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Project Title

Image-based microstructural meshing in OOF

Project Synopsis (approx. 100 words)

The OOF project is a very general and extensible finite element modeling tool with a focus on users from the materials science community, encapsulating sophisticated image processing, mesh construction, material specification and linear algebra capabilities in an interface aimed at the materials science community. It takes as inputs 2D or 3D microstructural images, and exposes powerful tools to allow users to segment these images, construct efficient finite-element meshes with good fidelity to the image but a small number of degrees of freedom, and then run virtual experiments or other structure-property explorations, given suitable boundary conditions.
A good overview is available on-line here: https://mgi.nist.gov/object-oriented-finite-elements-oof.

Identified Data-Science Collaborative Need (approx. 100 words)

The OOF software, developed over the past several years, performs the task for which it was designed very well, i.e. structure-property explorations of small numbers of microstructures. But it is turning out to be difficult to integrate OOF into higher-level workflows. Although the image-processing and meshing tools are quite powerful, there remains a trial-and-error character to the mesh construction process in particular. One of the directions where we would like the project to go is to become a component in higher-level, possibly automated structure-property workflows. This “componentization” is frustrated by the manual character of some of the operations. While it’s possible to write scripts to run a previously-validated sequence of meshing operations on a segmented microstructure, this solution does not generalize robustly across multiple problems. It would be high-value for us to, as far as possible, automate the image-based mesh construction step of the OOF workflow.

Data Origin and Access (*data must be available and sharable with data science teams* – please address: data source/origin, access privileges, sharing privileges)

We do not currently have a specific data set that we need to work, but in the event that this project were selected for the workshop, we could quickly come up with several tens of synthetic microstructures and associated, manually-generated, high-quality meshes. The program itself also has a way of quantifying mesh quality, so given a microstructure and a generated candidate mesh, a score can be automatically generated. We have a small number of 3D micrographs from real experiments that we have been given permission to share.

Project Description (approx. 1.5 pages, plus figures and references; please describe data size, form, dimensionality, uncertainties, number of examples, etc.)

The data transformation we want to try to automate is the step from a segmented 3D microstructure to a finite-element mesh. In the parlance of the OOF code, this is actually called a "skeleton", consisting of nodes and segments, but none of the finite-element mathematical infrastructure, like degrees of freedom and Gauss points and so forth.

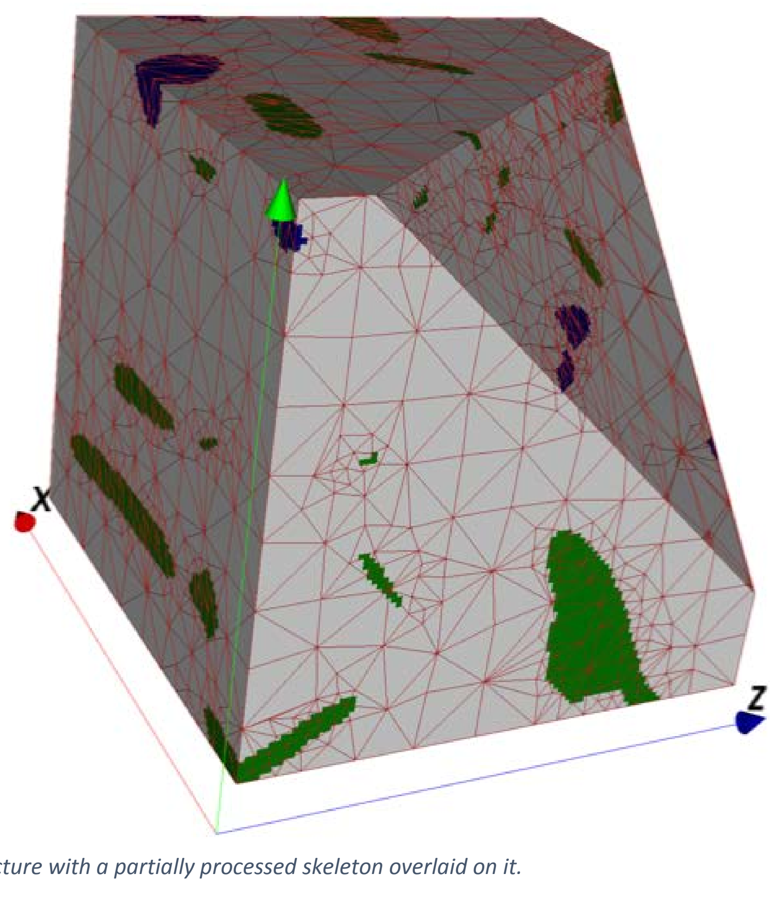
Microstructures consist internally of an array of voxels, with each voxel being assigned a "category". Voxels with different categories have different physical properties. For the skeleton to be a good representation of the microstructure, all boundaries between voxel categories should roughly correspond to faces between elements (but not vice versa). In OOF 3D, a skeleton is a space-filling set of tetrahedra. Skeleton quality can be quantified by two values, homogeneity and regularity, or shape. The homogeneity score is high for a given element if the element only encloses voxels of a single category, and the regularity or shape score is high for a given element if the element is close to being a regular tetrahedron, and low for "needle" or "plate" elements. For each of homogeneity and regularity, the overall score of the skeleton is just the sum over elements. A single scalar score for the entire skeleton is obtained by combining the homogeneity and shape scores with a user-defined weighting factor.

Operationally speaking, the way the skeleton construction process works now is that the software begins with a regular, space-filling skeleton that does not align well with the boundaries in the segmented microstructure. The user can the apply various tools, such as an element-bisection tool, simulated annealing, "snapping" tools which move nodes directly to their nearest microstructure category boundary, or "smoothing" tools, which move nodes close to the average position of their neighbors. The general flow is that a user starts with refinement, focusing on the homogeneity, and then as the homogeneity score goes up, begins pinning nodes that are on boundaries to lock in the homogeneity, and then changes emphasis to node motion tools and element shape modifiers, to regularize the mesh without over-refining.

Assessing skeleton quality, by eye or using the built-in quantitative tools, is reasonably easy, but generating a quality skeleton can be a lengthy trial-and-error process.

This is the step we'd like to try to automate, not only to relieve users of the burden of trial and error, but also because if this step were automatic, the OOF tool could be "componentized" and integrated into high-throughput modeling workflows more effectively.

Below is an example picture of what a typical multi-phase, segmented microstructure looks like, with a skeleton, part-way through the construction process, overlaid on it. The image is clipped, microstructural data occupies the full cube.



A microstructure with a partially processed skeleton overlaid on it.