An Automated Workflow for Meshing Evolving Microstructures from High-Throughput Grain Growth Simulations

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THE DENSIFICATION PROCESS (SINTERING)

- **Initial Point Contact**
- **Neck Formation**
- **Pore Shrinkage**
- **GB Formation & Grain Growth**

Increasing Conductivity ($\sigma$)

$\sigma_1 < \sigma_2 < \sigma_3 < \sigma_4$
MICROSTRUCTURE DENSIFICATION SIMULATION USING SPPARKS

Stochastic Parallel Particle Kinetic Simulator

Monte Carlo Potts Model

* Pore Removal
* Mass Transport
* Grain Coarsening


High GB Mobility

Low GB Mobility

Microstructure
HOW DO YOU GET COMPLEX GEOMETRIES INTO COMSOL?

Grain Growth Simulation  Mesh  COMSOL
HOW TO MESH MICROSTRUCTURES?

Requirements:
- Automated
- Robust
- Efficient
- Extensible

OUR SOLUTION
1. I AM GETTING A "TWO SUBFACES ... ARE FOUND INTERSECTING EACH OTHER" ERROR, WHAT SHOULD I DO?

This is the most frequently encountered problem using this toolbox. There are three possible causes of this error:

1. the volume you are trying to mesh contains joint regions between more than 2 materials
   This is most likely happening when you see the above error message. Try to plot your volume slice by slice, and pay attention to any voxels whose neighbors have more than 2 different values. If this is the case, you can only use this type of input with vol2mesh/v2m with 'cgalmesh' option as the "method" parameter. If you use either "simplify" or "cgalsurf" (default) options, iso2mesh will fail. If for some reason you have to use these options, here are two possible temporary work-arounds:
   1. if there are not many junction voxels, you may want to manually edit your image and disconnect the regions that share the same boundary and make sure all the sub-regions are either completely disjointed, or completely enclosed by another.
   2. merge the regions that have shared boundaries, and mesh the resulting merged volume; after you get the tetrahedra, compute the centroid of each element in the merged domain (identified by their labels), and map them back to your original segmented image; determine the original region id using the voxel containing the centroids.

If you have any better suggestions to enable these options, please contact us via email.

COMSOL rejects meshes of these geometries using ISO2MESH high-level functions, but there are useful helper functions to provide a work-around.
(1) Remove extremely small grains (if <0.04% the total volume) by converting them to pores.

(2) Create a default box with a coarse mesh using \textit{meshabox}, the same size as the microstructure bounds.

(3) For each node of the mesh, determine which domain (grain ID or pore) it would reside in according to its $xx, yy, zz$ position.

(4) Determine which tetrahedra are at a grain boundary interface (where one or more of the tet’s nodes are in a different domain).

(5) Refine the mesh at the grain boundary interface nodes using \textit{meshrefine} with an order-of-magnitude reduced volume.

(6) Repeat once steps 3 through 5 with the refined mesh.

(7) Assign each tetrahedral to a domain (grain ID or pore) according to the $xx, yy, zz$ position of its centroid (as found via \textit{meshcentroid}) in the microstructure.
CREATE MODEL, IMPORT MESH

LiveLink™ for MATLAB®

%Create model in COMSOL v5.3
import com.comsol.model.*
import com.comsol.model.util.*
model = ModelUtil.create('Model');
model.component.create('comp1', true);
model.component('comp1').geom.create('geom1', 3);
model.component('comp1').mesh.create('mesh1');
model.component('comp1').physics.create('ec', 'ConductiveMedia', 'geom1');
model.study.create('std1');
model.study('std1').create('stat', 'Stationary');
model.study('std1').feature('stat').activate('ec', true);
%Upload the mesh
model.mesh('mesh1').data.setElem('tet', elem(:, 1:4)'-1);
model.mesh('mesh1').data.setVertex(node');
model.mesh('mesh1').data.setElemEntity('tet', elem(:,5));
model.mesh('mesh1').data.createMesh;
disp('COMSOL mesh created.')

Determine Pore/Grain Domain IDs:
id=mphselectcoords(model,'geom1',node(porenodes(i, :), :)', 'domain', 'include', 'all');
Q: What is the conductivity of the microstructures?

Material electrical properties assigned to features of the microstructure:

<table>
<thead>
<tr>
<th>Feature</th>
<th>( \sigma ) (S/m)</th>
<th>( \varepsilon )</th>
<th>thickness</th>
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<tbody>
<tr>
<td>Grain</td>
<td>0.105</td>
<td>9.7</td>
<td>as given</td>
</tr>
<tr>
<td>Grain boundary</td>
<td>2</td>
<td>9.7</td>
<td>3 (nm)</td>
</tr>
<tr>
<td>Pore</td>
<td>1E-15</td>
<td>1</td>
<td>as given</td>
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Electric Shielding condition used at the grain boundaries

Determine the boundaries:

top_boundaries = mphselectbox(model,'geom1',[0, sx; 0, sy; sz-1, sz], 'boundary', 'include', 'any');
**SIMULATION RESULTS (90 STRUCTURES)**

\[ \sigma_{mfit} = 0.11 \text{ [S/m]} \]  
(2)

Percolation model
\[ \sigma = \sigma_m \left( \frac{\varphi_m - \varphi_c}{1 - \varphi_c} \right) \]

(1) Network Formation  
(2) Densification

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