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

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COMSOL CONFERENCE
2018 BOSTON

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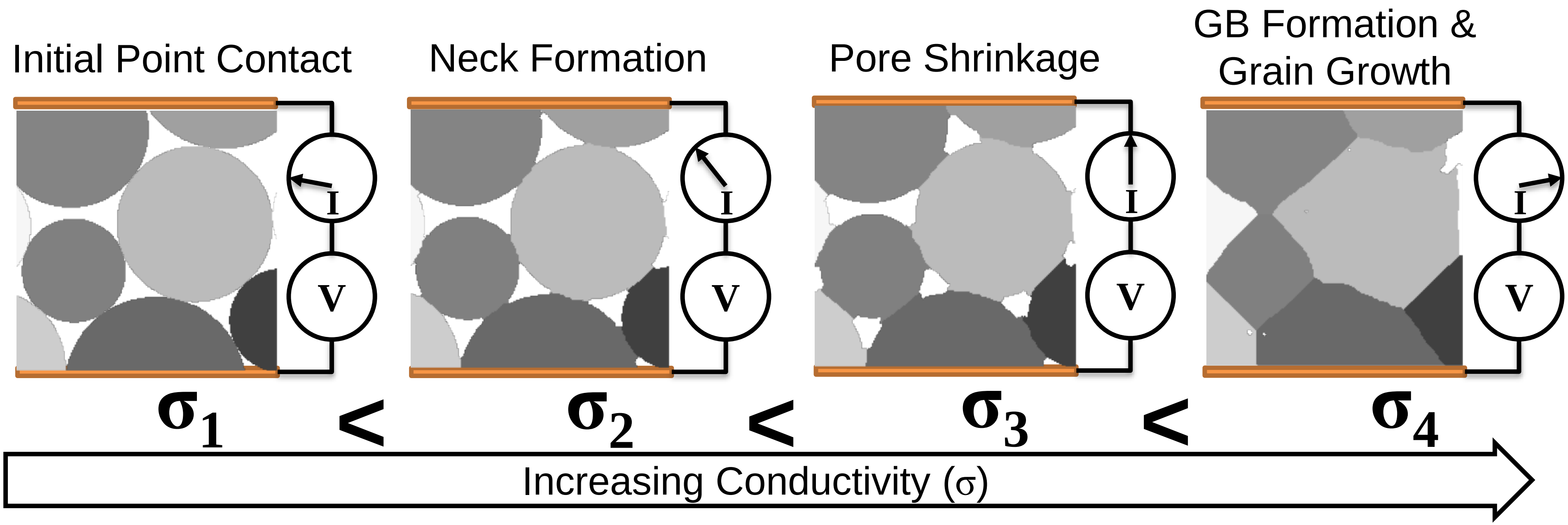
THE DENSIFICATION PROCESS (SINTERING)



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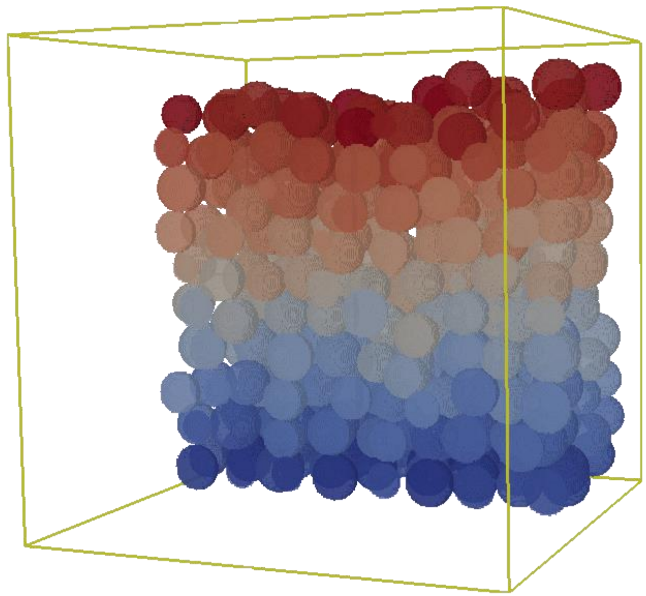
MICROSTRUCTURE DENSIFICATION SIMULATION USING SPPARKS

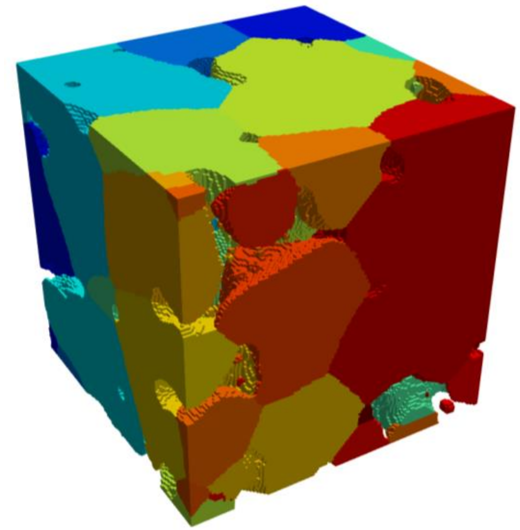
Stochastic **P**arallel **P**article **K**inetic **S**imulator

Sandia National Laboratories

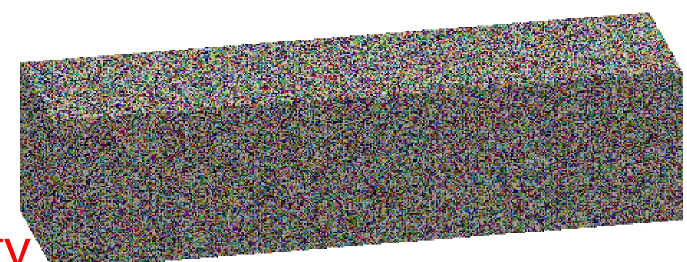
Monte Carlo
Potts Model

*Pore Removal
*Mass Transport
*Grain Coarsening





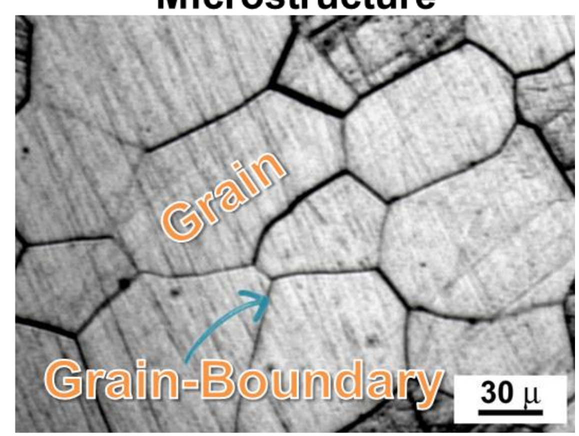
High GB Mobility



Low GB Mobility

Three-Dimensional Simulation of Grain Growth in a Thermal Gradient with Non-Uniform Grain Boundary Mobility, A. L. Garcia, V. Tikare and E. A. Holm, Scripta Materialia 59, 661-664 (2008).

Microstructure



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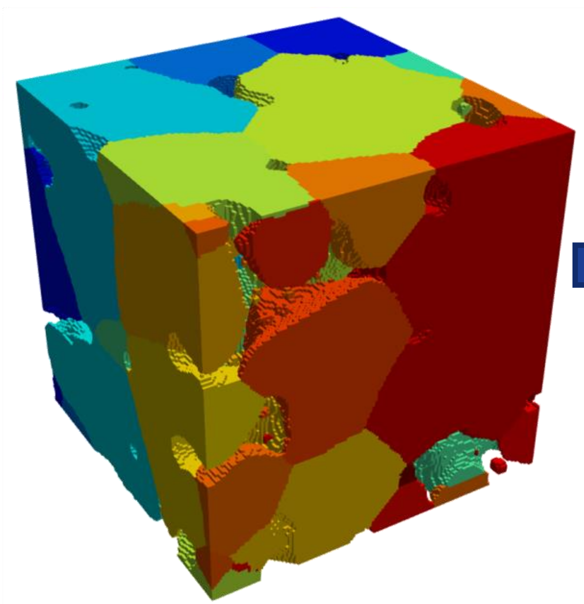
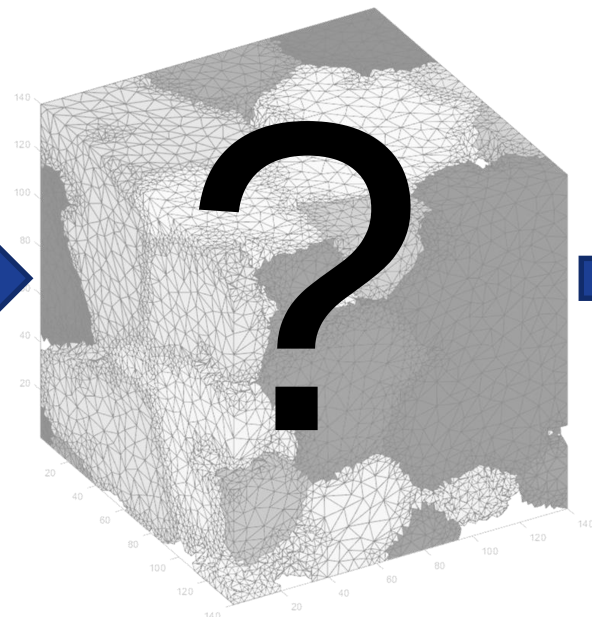
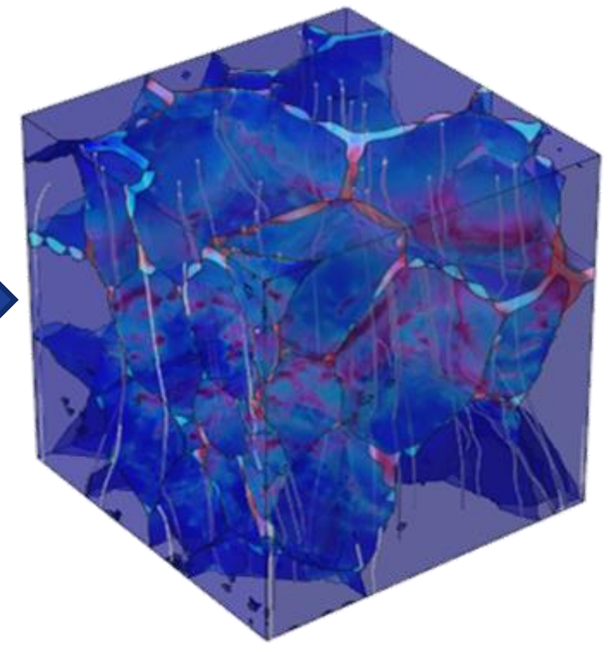
HOW DO YOU GET COMPLEX GEOMETRIES INTO COMSOL?



Grain Growth Simulation



Mesh



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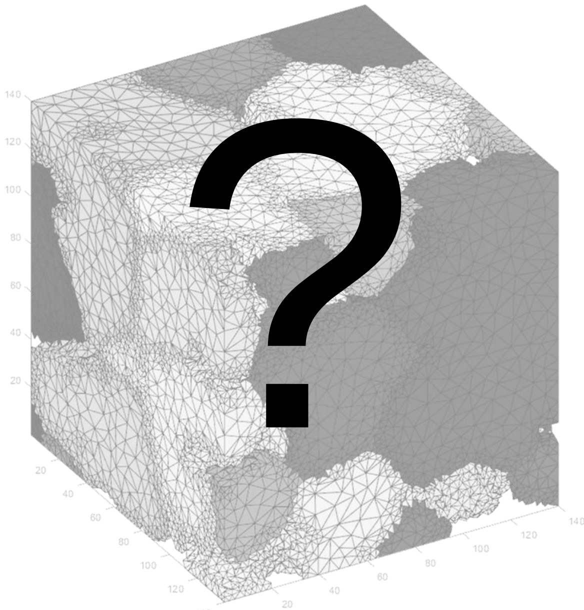
HOW TO MESH MICROSTRUCTURES?

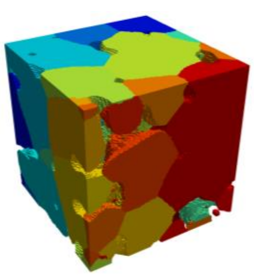


Requirements:

- Automated
- Robust
- Efficient
- Extensible

OUR SOLUTION

SPPARKS



MATLAB

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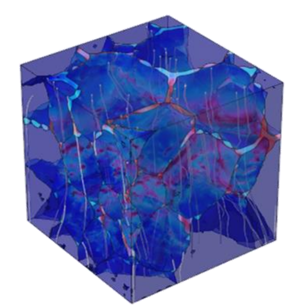
COMSOL MULTIPHYSICS



ISO2MESH

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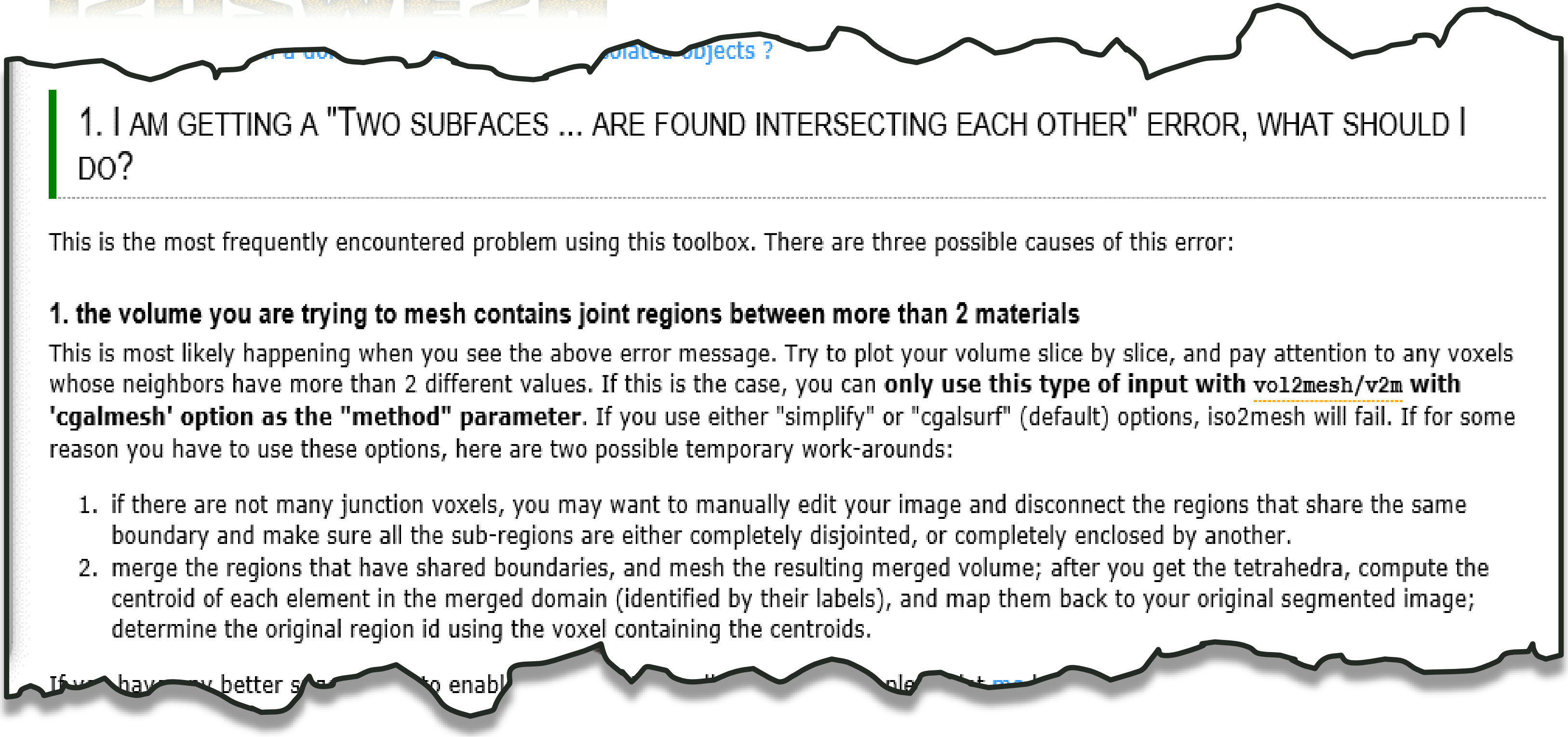
IT'S ALWAYS SOMETHING…

ISO2MESH



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.

COMSOL rejects meshes of these geometries using ISO2MESH high-level functions, but there are useful helper functions to provide a work-around.

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MESHING PROCEDURE

(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 *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.

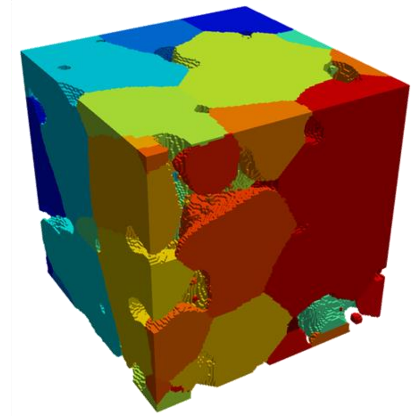
(4) Determine which tetrahedra are at a grain boundary interface (where one or more of the tet's nodes are in a different domain).

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

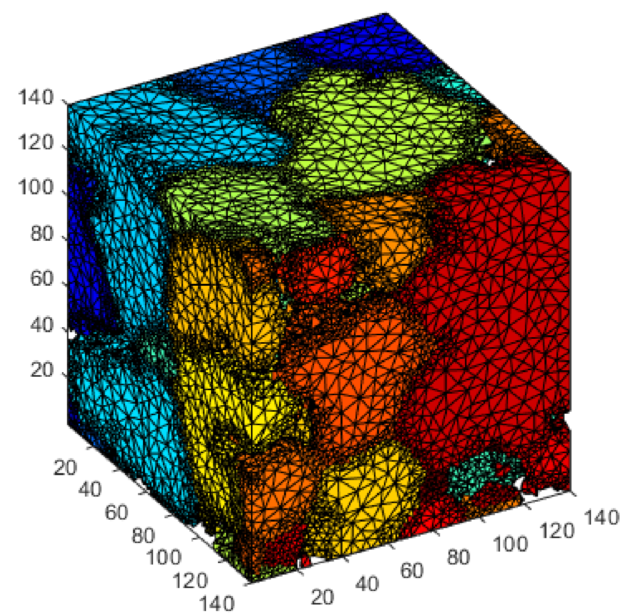
(6) Repeat once steps 3 through 5 with the refined mesh.

(7) Assign each tetrahedral to a domain (grain ID or pore) according to the *xx,yy,zz* position of its centroid (as found via *meshcentroid*) in the microstructure.

OBJECTIVE



RESULT



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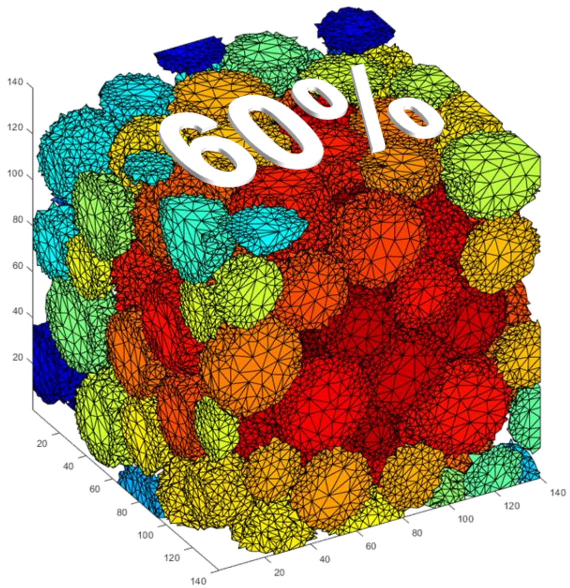
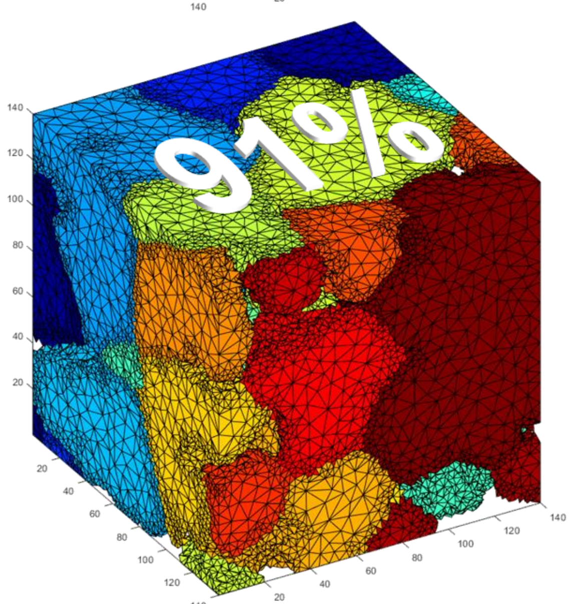
U.S. ARMY RDECOM ARL RESEARCH LABORATORY

CREATE MODEL, IMPORT MESH

INITIAL DENSITY



INTERMEDIATE DENSITY



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```
%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');
```


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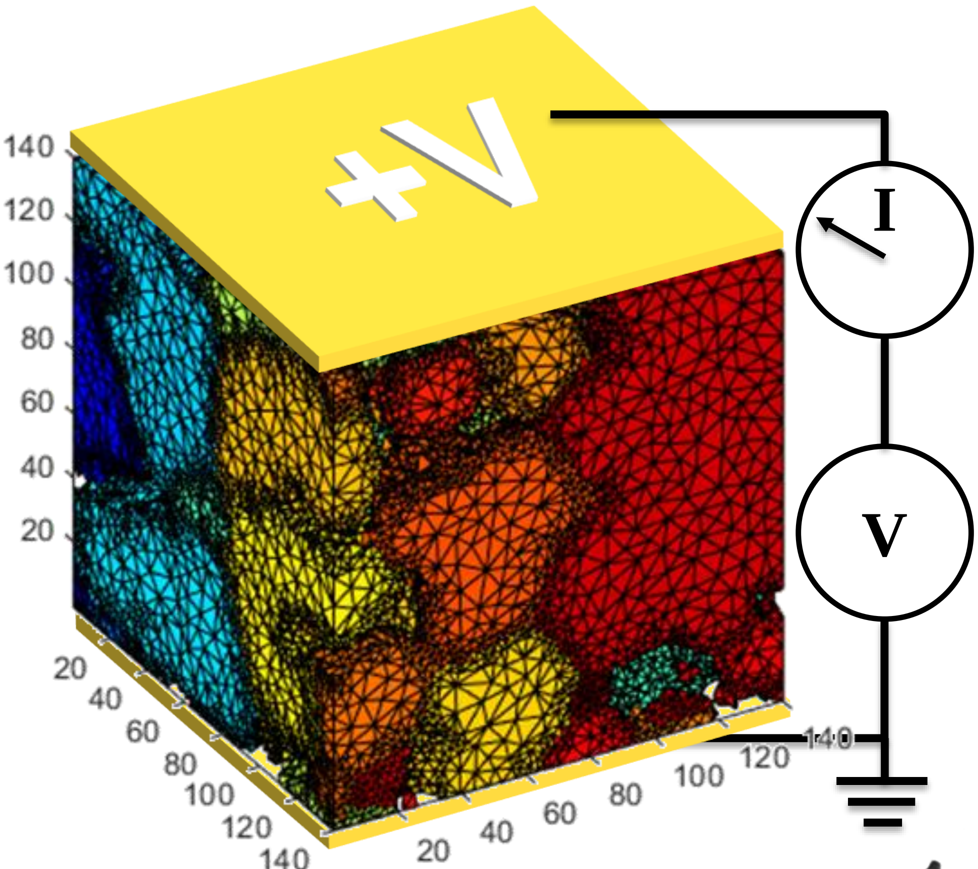
FEA OF MICROSTRUCTURES

Q: What is the conductivity of the microstructures?



Alumina Ceramic @ 1450ºC

Feature	σ (S/m)	ε	thickness
Grain	0.105	9.7	as given
Grain boundary	2	9.7	3 (nm)
Pore	1E-15	1	as given

Material electrical properties assigned to features of the microstructure

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');
```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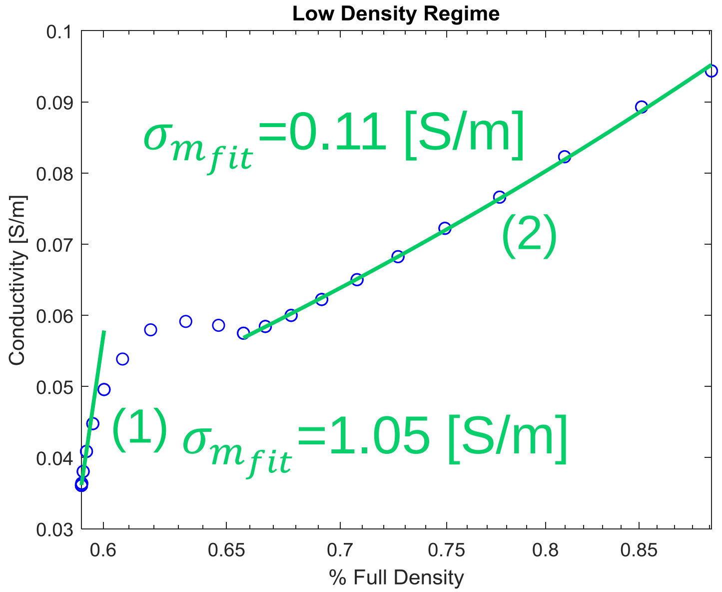
SIMULATION RESULTS (90 STRUCTURES)

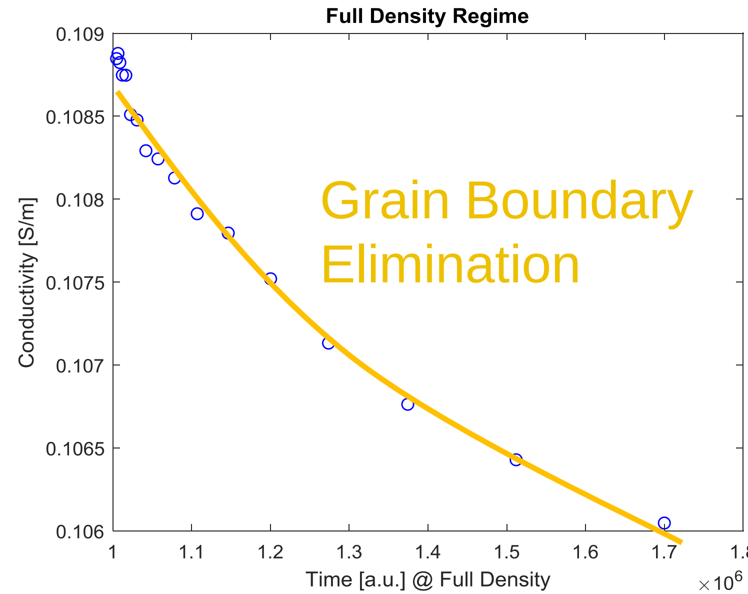


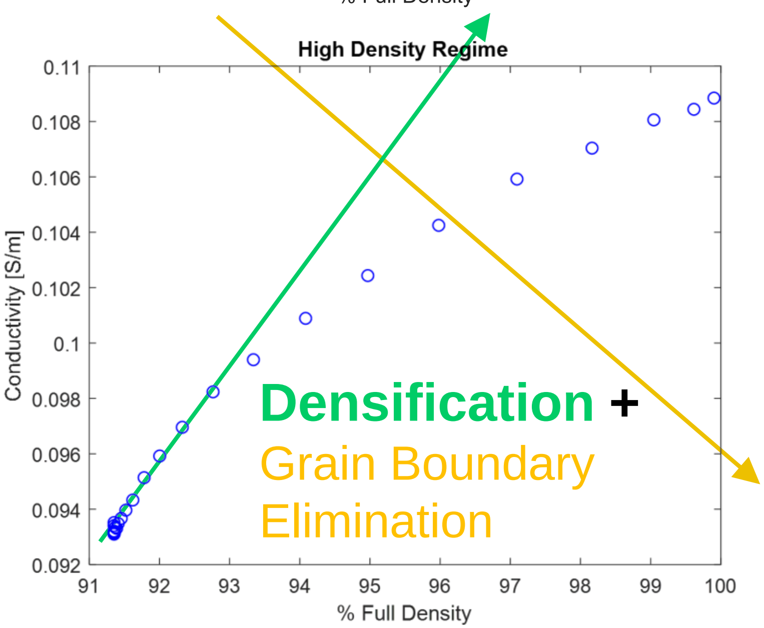
Percolation model

$$\sigma = \sigma_m \left(\frac{\varphi_m - \varphi_c}{1 - \varphi_c} \right)$$

(1) Network Formation

(2) Densification





Feature	σ (S/m)	ε	thickness
Grain	0.105	9.7	as given
Grain boundary	2	9.7	3 (nm)
Pore	1E-15	1	as given

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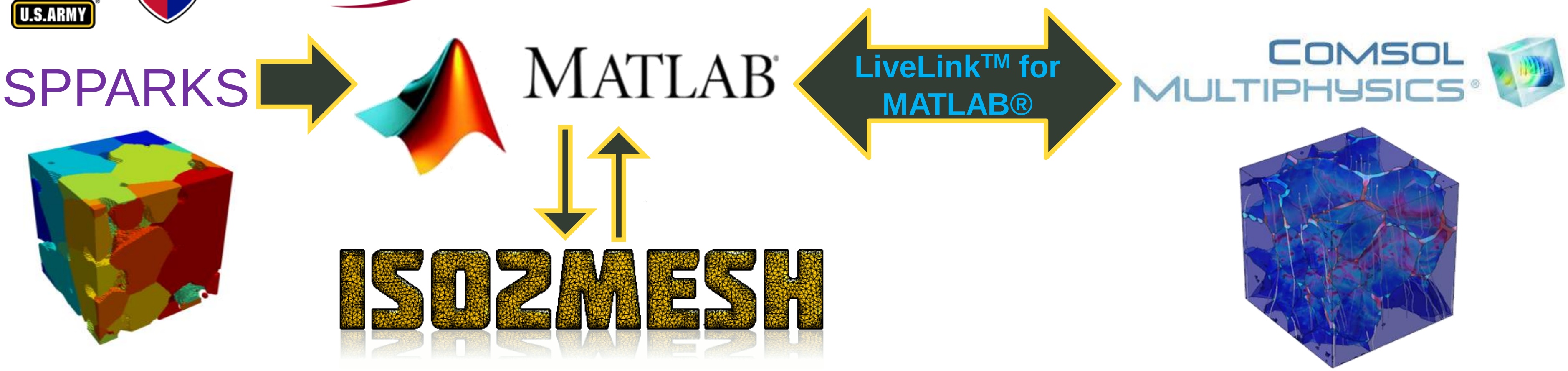
THANK YOU!



THIS PAPER: Golt, M., Hernández-Rivera, E. (2018). An Automated Workflow for Meshing Evolving Microstructures from High-Throughput Grain Growth Simulations. *Proceedings of the 2018 COMSOL Conference in Boston*.

SPPARKS: S. Plimpton, C. Battaile, M. Chandross, L. Holm, A. Thompson, V. Tikare, G. Wagner, E. Webb, X. Zhou, C. Garcia Cardona, A. Slepoy, “Crossing the Mesoscale No-Man's Land via Parallel Kinetic Monte Carlo”, *Sandia Report: SAND2009–6226* (Oct 2009).

SPPARKS: Cristina Garcia Cardona, Veena Tikare, Steven J. Plimpton, “Parallel simulation of 3D sintering”, *Int. Journal of Computational Materials Science and Surface Engineering*, **Vol. 4**, 37-54 (2011)

SPPARKS: Tikare, Veena, et al. "Numerical simulation of microstructural evolution during sintering at the mesoscale in a 3D powder compact." *Computational Materials Science* **48.2** (2010): 317-325.

PARTICLE POURING: Bjørk, Rasmus, et al. "The effect of particle size distributions on the microstructural evolution during sintering." *Journal of the American Ceramic Society* 96.1 (2013): 103-110.

ISO2MESH: Qianqian Fang and David Boas, "Tetrahedral mesh generation from volumetric binary and gray-scale images," *Proc. of IEEE Int. Symposium on Biomedical Imaging 2009*, pp. 1142-1145, 2009

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AC/DC Module Application Library Manual, ©Comsol (2009-2017)

ALUMINA ELECTRICAL: "Electrical Conduction in Single-Crystal and Polycrystalline Al2O3 at High Temperatures." *Journal of the American Ceramic Society* **57.6** (1974): 245-250.

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