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Advances in Mesh Generation for Crystal Plasticity Modeling

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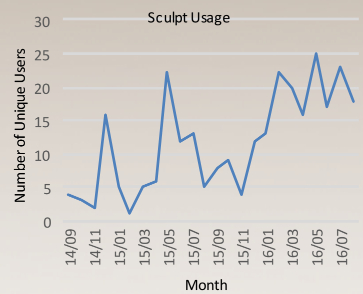
Overview

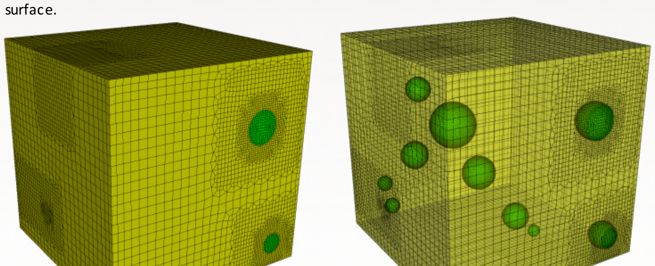
Sandia's Sculpt tool lends itself well to the modeling of microstructures. With initial work begun last year, this capability has advanced to where it is becoming recognized as an indispensable tool for crystal plasticity modeling at the U.S. National Laboratories in the design of materials and composites. This work includes a collection of enhancements implemented during fiscal year 2016 that have been requested by Sculpt users to augment the current capabilities or address deficiencies.



Number of Unique Users of Sculpt (Used Sculpt at least twice during a calendar month)

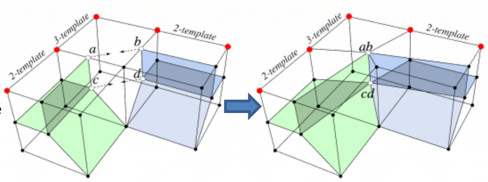
Boundary Pillowing

Sculpt's ability to adaptively refine the Cartesian grid based on geometric criteria has also proven useful in modeling microstructures. The RVE cube that is normally used for microstructures can pose a problem for the standard refinement algorithms. Specifically, the 3-refinement template illustrated below. When adjusting node locations for elements at the RVE boundary, there is a likelihood of generating a hex with two of its faces on the surface.



Geometry adaptive mesh of a microstructures model where sphere's represent air voids in the material

Application of a three-refinement template in Sculpt to refine concave regions

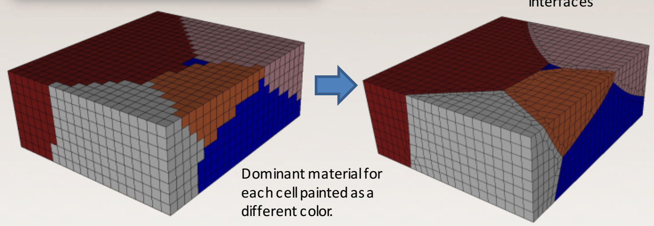


Performance Improvements

```
TITLE = triple line system
VARIABLES = x y z, phi_1, phi_2, phi_3
ZONE i = 2 , j = 2 , k = 2
0.0000      0.0000      0.0000      0.5000      0.5000      0.0000
1.0000      0.0000      0.0000      0.3333      0.3333      0.3334
0.0000      1.0000      0.0000      1.0000      0.0000      0.0000
1.0000      1.0000      0.0000      0.0000      1.0000      0.0000
0.0000      0.0000      1.0000      0.2000      0.4000      0.4000
1.0000      0.0000      1.0000      0.6000      0.1000      0.3000
0.0000      1.0000      1.0000      0.0000      0.0000      1.0000
1.0000      1.0000      1.0000      0.9000      0.0000      0.1000
```

Volume Fraction file format used by Sculpt representing all materials in every cell of the model.

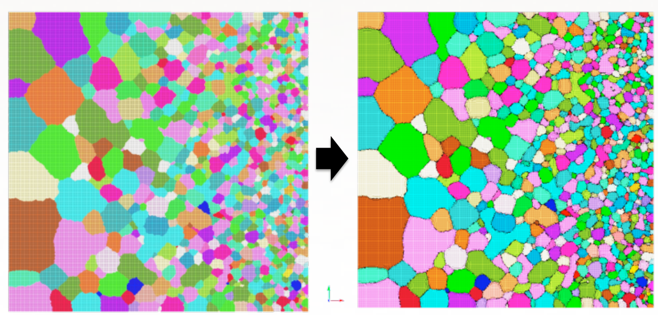
Resulting Sculpt mesh with smooth interfaces



Dominant material for each cell painted as a different color.

Sculpt utilizes volume fraction data on a Cartesian grid to represent material information. To represent the data in Sculpt, each cell would hold a volume fraction floating point value for each unique volume in the model, regardless of whether the volume fraction was zero for a given cell. For models with only a few materials, this was relatively efficient, however, Microstructures RVE models with hundreds or even thousands of grains would quickly become intractable in terms of memory usage and performance.

Significant work was done to revamp Sculpt's data management, including modifications for MPI, to store a minimum amount of data per cell. The result was a major reduction in memory requirements and significant performance improvements for models with large numbers of materials.



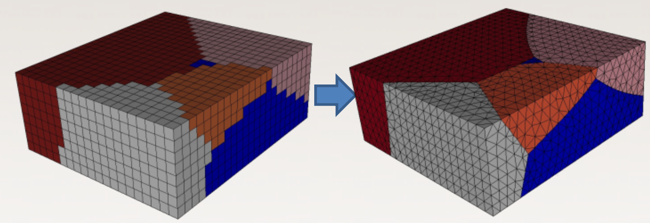
Exodus Block Mesh
75 Material Blocks
500x500x1
250,000 Elements

Sculpt Mesh
75 Material Blocks
307,166
Elements

Discrete Geometry Export

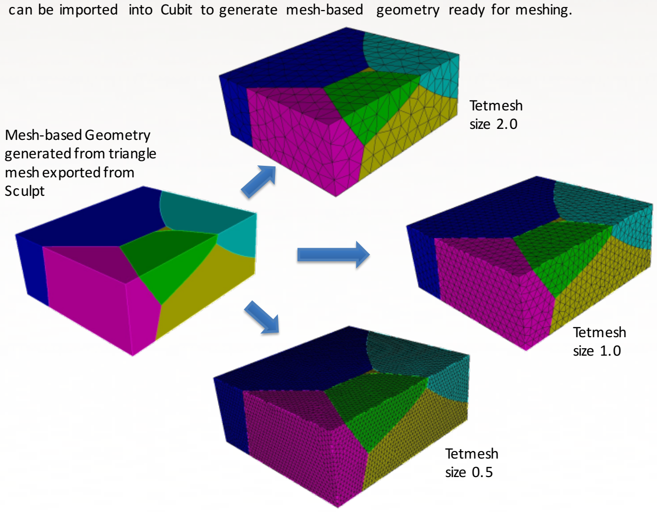
The objective of this on-going work is to build a discrete geometry representation that could be used externally in other applications such as Cubit. The primary motivation was to take advantage of Cubit's built-in adaptive tetrahedral meshing capability for Microstructures while using Sculpt to generate a discrete geometry from Volume Fractions.

Sculpt has the ability to generate a mesh directly from volume fraction data, without the need for a discrete geometry definition. As part of the internal procedure in Sculpt, a temporary geometry representation must be generated in order to perform operations such as smoothing and pillowing. This work uses Sculpt's geometry foundation and exports a triangle mesh that can be used in Cubit for the basis for its discrete geometry.



Using a series of quad splitting and triangle flipping procedures, a triangle mesh with acceptable quality elements is generated and exported as an Exodus file. The Exodus file can be imported into Cubit to generate mesh-based geometry ready for meshing.

Mesh-based Geometry generated from triangle mesh exported from Sculpt



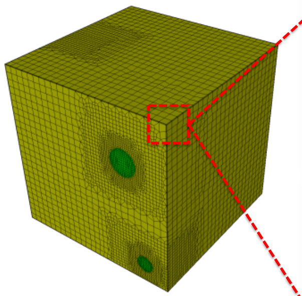
Tetmesh size 2.0

Tetmesh size 1.0

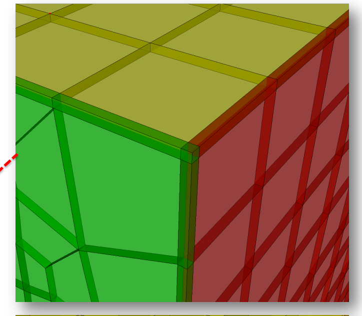
Tetmesh size 0.5

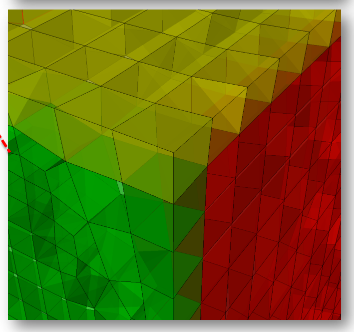
To address this issue a new option to insert pillows or layers of hexes at the faces of the RVE was introduced.

New Pillow Option

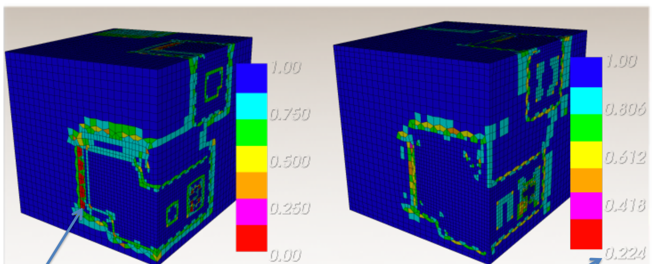


One layer of hexes inserted on each boundary plane





Smoothing performed to improve mesh quality



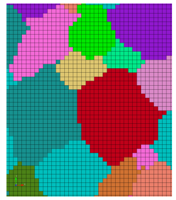
Scaled Jacobian = 0

Minimum SJ acceptable

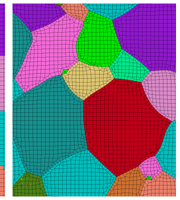
Before

After

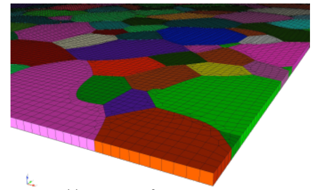
By inserting pillow layers, the adaptive capability is able to produce acceptable quality hexes at the boundaries of the RVE.



Close-up of above data



Resulting Sculpted mesh

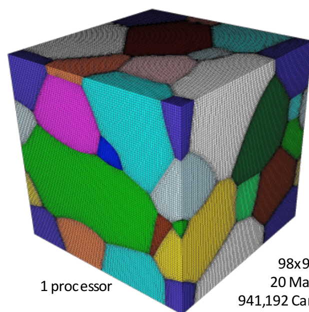


Oblique view of 2D mesh.

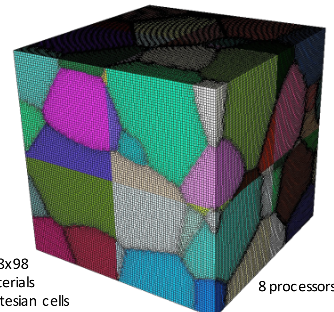
As part of this work, Sculpt was also enhanced to generate 2D meshes from a 2D Cartesian grid of data. The following illustrates results from a 75 material 2D model comparing before and after timings and mesh quality on a single processor.

1 Processor	Time	Num Elems	Min Quality	Num < 0.2	Num < 0.0
Sculpt 15.1	7.25 hrs	307150	-0.998	18	8
Sculpt 15.2	36 sec	307166	0.097	1	0

Comparison of results from 2D Phase Field Data

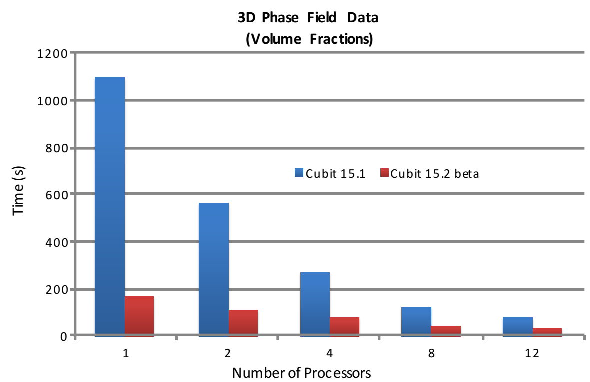


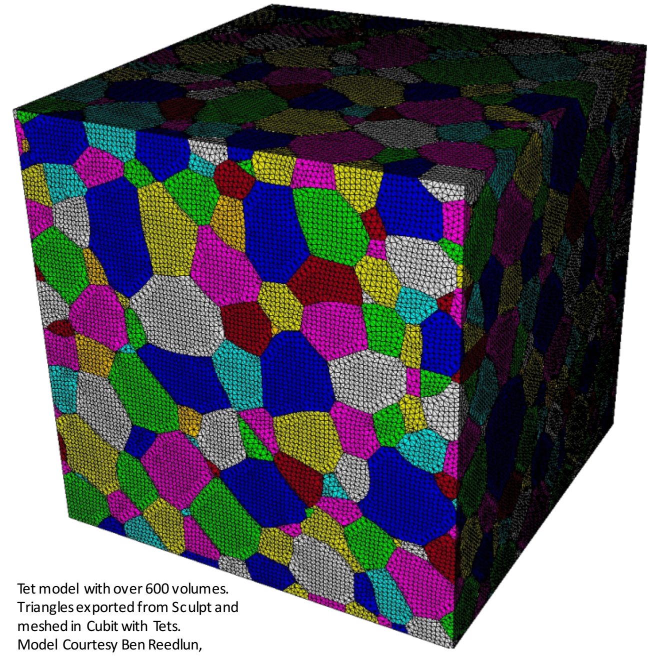
1 processor



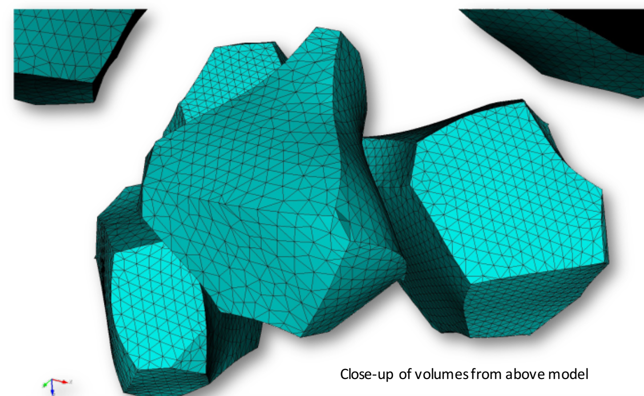
8 processors

98x98x98
20 Materials
941,192 Cartesian cells
1,350,362 elements
Min Quality = 0.1975





Tet model with over 600 volumes.
Triangles exported from Sculpt and meshed in Cubit with Tets.
Model Courtesy Ben Reedlun, Sandia National Laboratories



Close-up of volumes from above model

Paper Reference: Lim, Hojun; Abdeljawad, Fadi; Owen, Steven; Hanks, Byron; Foulk, James; Battaile, Corbett, Incorporating physically-based microstructures in materials modeling: Bridging phase field and crystal plasticity frameworks, Modelling and Simulation in Materials Science and Engineering Volume 24, Number 4, April 25, 2016

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